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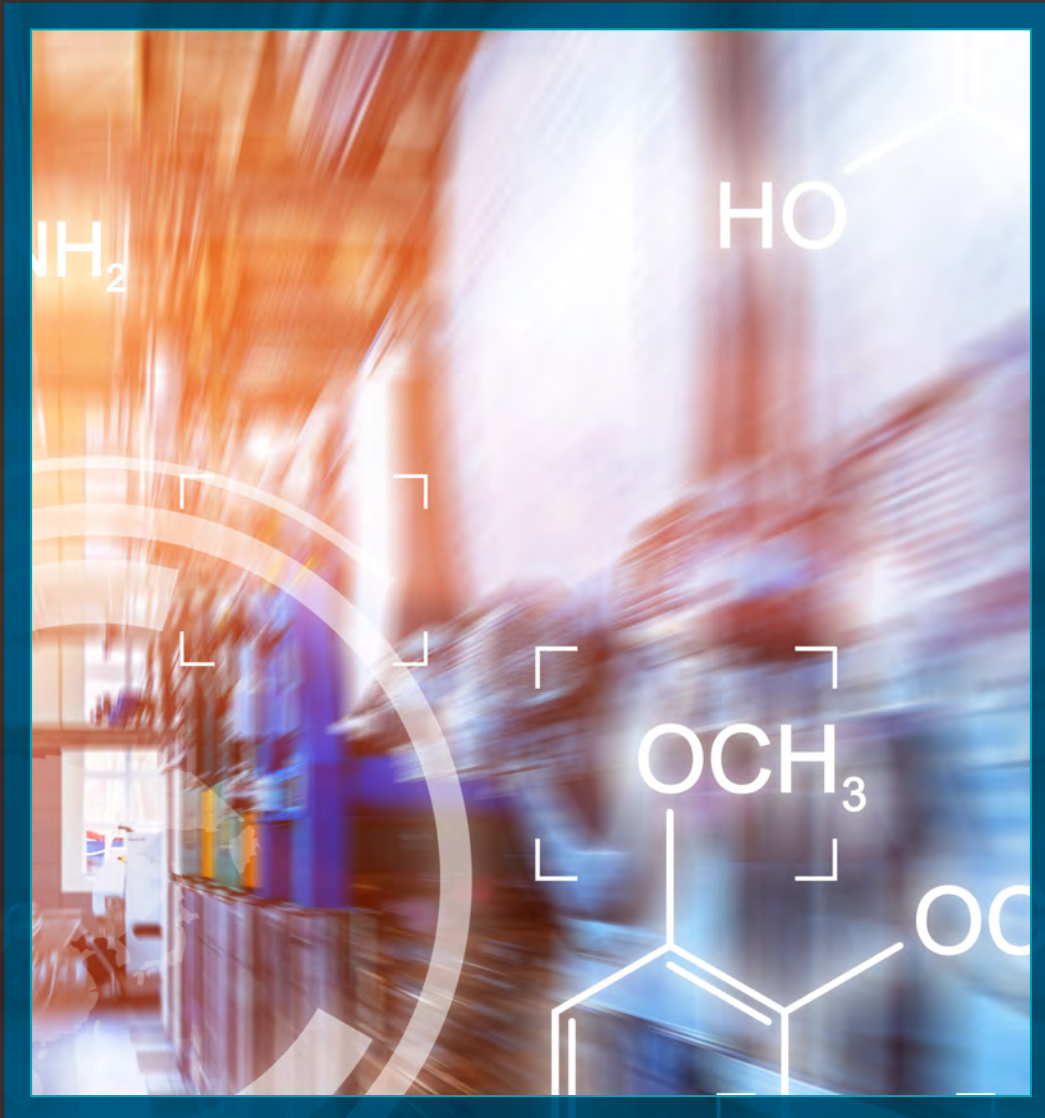
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14. ABSTRACT This report is intended to be a record of key activities describing the research programs of the U.S. Army Research Laboratory - Army Research Office (ARL-ARO) for fiscal year 2018 (FY18; 1 Oct 2017 through 30 Sep 2018). This report provides: (i) an overview of the mission and strategy employed to guide ARO research investments and factors affecting the implementation of that strategy, (ii) a snapshot of end-of-year statistics of basic research funding (i.e., "6.1" funding) and program proposal activity, and (iii) research trends and key annual scientific discoveries and accomplishments of the ARO scientific divisions.					
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ARO IN REVIEW 2018



U.S. ARMY COMBAT CAPABILITIES DEVELOPMENT COMMAND (CCDC)
ARMY RESEARCH LABORATORY (ARL)
ARMY RESEARCH OFFICE (ARO)



Army Research Laboratory (ARL)
Army Research Office (ARO)
P.O. Box 12211
Research Triangle Park, NC 27709-2211

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CHAPTER 1 | ARO MISSION AND INVESTMENT STRATEGY

This report presents an overview of the programs, investment strategies, and accomplishments of the Army Research Office (ARO) for fiscal year 2018 (FY18; 1 Oct 2017 through 30 Sep 2018). This report provides:

- ▶ A brief review of the strategy employed to guide ARO research investments and noteworthy issues affecting the implementation of that strategy
- ▶ Statistics regarding basic research funding (i.e., “6.1” funding) and program proposal activity
- ▶ Selected success stories from each of the ARO scientific divisions and special programs

ARO MISSION

The mission of ARO, as part of the U.S. Army Futures Command (AFC) - U.S. Army Combat Capabilities Development Command (CCDC) - U.S. Army Research Laboratory (ARL), is to execute the Army's extramural basic research program in the following scientific disciplines: chemical sciences, computing sciences, electronics, life sciences, materials science, mathematical sciences, mechanical sciences, network sciences, and physics. The goal of this basic research is to drive scientific discoveries that will provide the Army with significant advances in operational capabilities through high-risk, high pay-off research opportunities, primarily with universities, but also with large and small businesses. ARO ensures that this research supports and drives the realization of future research relevant to all of the Army Functional Concepts, the ARL Core Competencies, and the ARL Essential Research Programs. The results of these efforts are transitioned to the Army research and development community, industry, or academia for the pursuit of long-term technological advances for the Army.

ARO STRATEGY AND FUNCTION

ARO's mission represents the most long-range Army view for changes in its technology, with system applications often 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities. ARO competitively selects and funds basic research proposals from educational institutions, nonprofit organizations, and private industry. ARO executes its mission through conduct of an aggressive basic science research program on behalf of the Army to create cutting-edge scientific discoveries and the general store of scientific knowledge that is required to develop and improve weapons systems for land force dominance. The ARO research portfolio consists principally of extramural academic research efforts consisting of single investigator efforts, university-affiliated research centers, and specially tailored outreach programs. Each program has its own objectives and set of advantages as described further in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES.

ARO's research strategy is organized into the ARL Core Competencies, with current areas of emphasis designated by the Essential Research Programs (ERPs), which aim to address particular technology gaps for the current and future Army. ARO drives fundamental research efforts that will lead to new discoveries and increased understanding of the physical, engineering, and information sciences as they relate to long-term national security needs, in support of all of the ARL Core Competencies and ERPs.

ARO's research strategy is organized into the ARL Core Competencies, with current areas of emphasis designated by the Essential Research Programs (ERPs), which aim to address particular technology gaps for the current and future Army. ARO drives fundamental research efforts that will lead to new discoveries and increased understanding of the physical, engineering, and information sciences as they relate to long-term national security needs, in support of all of the ARL Core Competencies and ERPs.

ARO strategy and programs are formulated in concert with the ARL Technical Implementation Plan, the ARL Research Management and Leadership Strategy, the CCDC Centers, the Army Medical Research and Materiel Command (MRMC), the Army Corps of Engineers, and the Army Research Institute for the Behavioral and Social Sciences. ARO programs and research areas are intimately aligned with, and fully supportive of, the research priorities set within the DoD Quadrennial Defense Review, the Army Modernization Priorities, the Army Functional Concepts, the Assistant Secretary of Defense for Research and Engineering [ASD(R&E)] Science and Technology (S&T) Priorities, the Army S&T Master Plan, the Assistant Secretary of the Army for Acquisition, Logistics, and Technology [ASA(ALT)] Special Focus Areas, and the CCDC Lines of Effort.

ARO serves the following functions in pursuit of its mission:

- ▶ Execute an integrated, balanced extramural basic research program
- ▶ Create and guide the discovery and application of novel scientific phenomena leading to leap-ahead technologies for the Army
- ▶ Drive the application of science to generate new or improved solutions to existing needs
- ▶ Accelerate research results transition to applications in all stages of the research and development cycle
- ▶ Strengthen the research infrastructures of academic, industrial, and nonprofit laboratories that support the Army
- ▶ Focus on research topics that support technologies vital to the Army's future force, combating terrorism and new emerging threats
- ▶ Leverage S&T of other defense and government laboratories, academia and industry, and organizations of our allies
- ▶ Foster training for scientists and engineers in the scientific disciplines critical to Army needs
- ▶ Actively seek creative approaches to enhance the diversity and capabilities of future U.S. research programs by enhancing education and research programs at historically black colleges and universities, and minority-serving institutions

IMPLEMENTING ARO STRATEGY

ARO employs multiple programs, initiatives, and investment strategies to fulfill its mission. A snapshot of the ARO research programs is provided in this section, and each program is described further in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES.

PROGRAM SNAPSHOT

The research programs managed by ARO range from single investigator research to multidisciplinary/multi-investigator centers. A typical basic research grant within a program may provide funding for a few years, while in other programs, such as research centers affiliated with particular universities, a group of investigators may receive funding for many years to pursue novel research concepts. The programs for the Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI) are aimed at providing infrastructure and incentives to improve the diversity of U.S. basic research programs. In addition to supporting the education of graduate students through basic research grants, the National Defense Science and Engineering Graduate (NDSEG) fellowship program is another mechanism through which ARO fosters the training of a highly-educated workforce skilled in DoD and Army-relevant research, which is critical for the future of the nation. ARO also has extensive programs in outreach to pre-graduate education to encourage and enable the next generation of scientists. In addition, ARO guides the transition of basic research discoveries and advances to the appropriate applied-research and advanced-development organizations. ARO is actively engaged in speeding the transition of discovery into systems, in part through involvement in the development of topics and the management of projects in the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs.

COORDINATION FOR PROGRAM DEVELOPMENT AND MONITORING

ARO's extramural research programs are formulated in concert with the ARL-wide strategy, including the:

- ▶ ARL Core Competencies
 - Materials and Manufacturing Sciences
 - Computational Sciences
 - Ballistics Sciences
 - Human Sciences
 - Propulsion Sciences
 - Network and Information Sciences
 - Protection Sciences
 - ▶ ARL Essential Research Programs (ERPs)
 - Discovery
 - Human Agent Teaming
 - Artificial Intelligence and Machine Learning
 - Cyber and Electromagnetic Technologies for Complex Environments
 - Distributed and Cooperative Engagement in Contested Environments
 - Tactical Unit Energy Independence
 - Manipulating Physics of Failure for Robust Performance of Materials
 - Science of Manufacturing at the Point of Need
 - Accelerated Learning for a Ready and Responsive Force
 - ▶ ARL Directorates
 - Computational and Information Sciences Directorate (ARL-CISD)
 - Human Research and Engineering Directorate (ARL-HRED)
 - Sensors and Electron Devices Directorate (ARL-SEDD)
 - Vehicle Technology Directorate (ARL-VTD)
 - Weapons and Materials Research Directorate (ARL-WMRD)
- ARO programs are also formulated through collaborations and consultation with the following DoD and other Federal agencies to ensure complementary investment strategies:
- ▶ The CCDC Centers (formerly known as RDECs)
 - CCDC Armaments Center (CCDC AC)
 - CCDC Aviation and Missile Center (CCDC AvMC)
 - CCDC Army Research Laboratory (CCDC ARL)
 - CCDC Chemical Biological Center (CCDC CBC)
 - CCDC Command, Control, Computers, Communications, Cyber, Intelligence, Surveillance and Reconnaissance Center (CCDC C5ISR)
 - CCDC Data and Analysis Center (CCDC DAC)
 - CCDC Ground Vehicle Systems Center (CCDC GVSC)
 - CCDC Soldier Center (CCDC SC)
 - ▶ Army Medical Research and Materiel Command (MRMC)
 - ▶ Army Corps of Engineers (ACE)
 - ▶ Army Research Institute for the Behavioral and Social Sciences
 - ▶ U.S. Army Special Operations Command (USASOC)
 - ▶ AFC Futures and Concepts Center

- ▶ Office of Naval Research (ONR)
- ▶ Air Force Office of Scientific Research (AFOSR)
- ▶ National Institute of Standards and Technology (NIST)
- ▶ Defense Advanced Research Projects Agency (DARPA)
- ▶ Defense Threat Reduction Agency (DTRA)
- ▶ Office of the Secretary of Defense (OSD)
- ▶ Intelligence Advanced Research Projects Activity (IARPA)
- ▶ National Security Agency (NSA)
- ▶ Federal Bureau of Investigation (FBI)
- ▶ Department of Energy
- ▶ National Institutes of Health (NIH)
- ▶ Environmental Protection Agency
- ▶ National Science Foundation (NSF)

ARO's extramural research program provides foundational discoveries in support of the ARL Core Competencies and ERPs. While the ARL Directorates and the CCDC Centers are the primary users of the results of the ARO research program, ARO also supports research of interest to ACE, MRMCM, other Army Commands, and DoD agencies. The coordination of the ARO extramural program and proposal monitoring by other

ARL Directorates, CCDC Centers, and other Army laboratories ensures a highly productive and cost-effective Army research effort. The University Affiliated Research Centers (UARC) and Multidisciplinary University Research Initiative (MURI) centers benefit from the expertise and guidance provided by the ARL Directorates and other DoD, academic, and industry representatives who serve on evaluation panels for each UARC.

The ARO-managed OSD research programs include the University Research Initiative (URI) programs, and the Research and Educational Program (REP) for HBCU/MSIs. These programs fall under the executive oversight of the Defense Basic Research Advisory Group. This group is led by the ASD(R&E) Director for Research, representatives from the ONR, AFOSR, DARPA, ARO, and the Assistant Secretary of the Army (Acquisition, Logistics and Technology) [ASAALT].

ARO programs are also developed and managed with a focus on supporting future Army needs as identified in the Army Modernization Priorities and the Army Functional Concepts. These priorities were published in FY18, with details available at the Army's website (<https://www.army.mil/e2/c/downloads/500971.pdf>). These priorities emphasize a significant change in how the Army pursues solutions for the current and future warfighter. ARO's strategy is clearly aligned with the needs of the future warfighter and supports all of the Army Modernization Priorities and Army Functional Concepts. As described earlier, ARO's mission represents the most long-range Army view for changes in its technology, with research focused on fundamental discoveries with system applications to

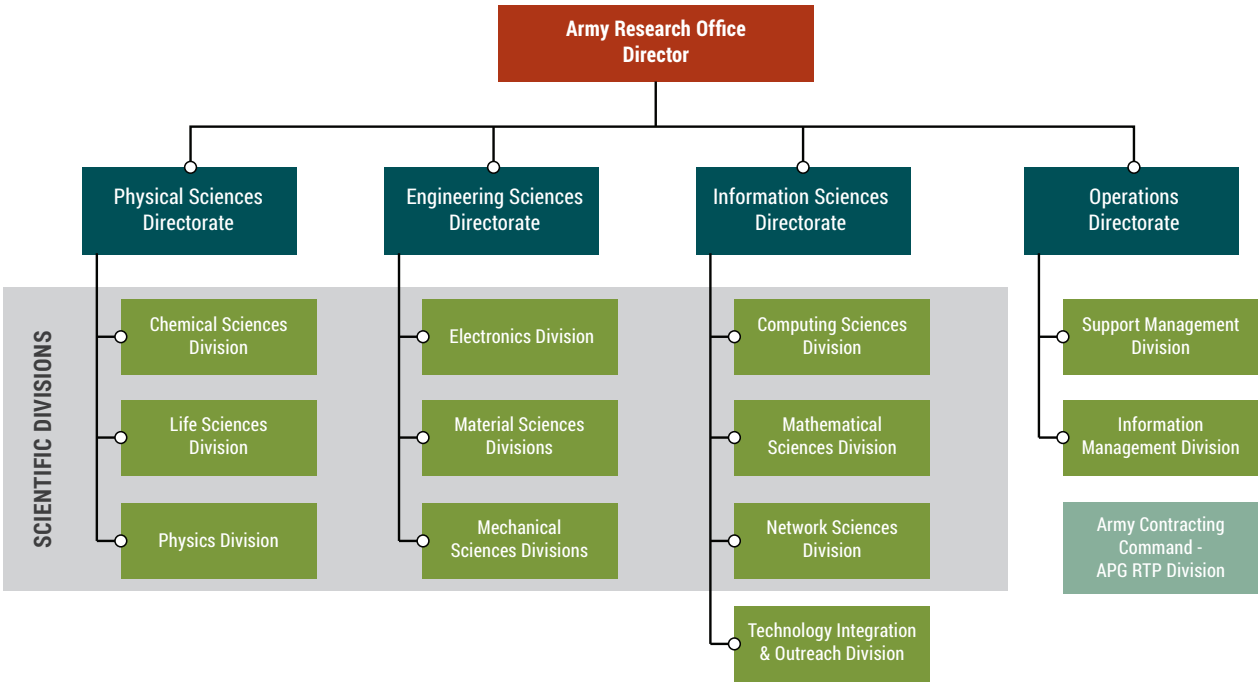


Figure 1. ARO Organizational Structure. ARO's scientific divisions fall under the Physical Sciences, Engineering Sciences, and Information Sciences Directorates. *Army Contracting Command – Army Proving Ground (APG), Research Triangle Park (RTP) Division executes the contracting needs for ARO-funded research; however, as part of the Army Contracting Command (i.e., not ARL), it also performs contracting activities throughout CCDC.

ensure technological superiority 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities.

REVIEW AND EVALUATION

The ARO Directorates, Divisions, and Programs are evaluated by a wide range of internal (Army) and external (academic, other government) reviews, such as the former biennial ARO Division Reviews and the National Research Council's Technical Assessment Board (TAB) Review. For additional information regarding these review processes, the reader is encouraged to refer to the corresponding presentations and reports from each review (not included here).

ARO ORGANIZATIONAL STRUCTURE

The organizational structure of ARO mirrors the departmental structure found in many research universities. ARO's scientific divisions are aligned to a specific scientific discipline (e.g., physics), with outreach activities managed through the Technology Integration and Outreach Division, and supported by the Operations Directorate (see FIGURE 1).

ARO SCIENTIFIC LEADERSHIP AND DIRECTORATE STAFF

ARO DIRECTOR'S OFFICE

Dr. Barton H. Halpern
Director, ARO

Dr. Stephen Lee
Chief Scientist

LTC Thomas "Bull" Holland (retired)
Military Deputy

LTC David Dykema (current)
Military Deputy

Mr. John Stone, Esq.
Legal Counsel

Mr. Richard Freed
Associate Director for Business and Research Administration

Dr. Brian Ashford
Special Assistant to the Director, ARO

Ms. Tish Torgerson
Executive Assistant

PHYSICAL SCIENCES DIRECTORATE (PSD)

Dr. Hugh De Long
Director, PSD

Dr. Peter Reynolds
Senior Scientist

Dr. J. Aura Gimm (moved to AFOSR)
Program Manager, Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies

Dr. Kelby Kizer
Special Assistant to the Director, PSD

Mr. John McConville
Technology Transfer Officer, Institute for Soldier Nanotechnologies

Ms. Ivory Chaney
Administrative Specialist

CHEMICAL SCIENCES DIVISION

Dr. Robert Mantz
Division Chief
Program Manager, Electrochemistry

Dr. Dawanne Poree
Program Manager, Polymer Chemistry
Program Manager (Acting), Reactive Chemical Systems

Dr. James Parker
Program Manager, Molecular Structure and Dynamics
Program Manager (Acting), Environmental Chemistry

Dr. Wesley Henderson
Program Manager (International), Energy Transport and Storage

LIFE SCIENCES DIVISION

Dr. Micheline Strand
Division Chief
Program Manager, Genetics

Dr. Stephanie McElhinny
Program Manager, Biochemistry

Dr. Frederick Gregory
Program Manager, Neurophysiology of Cognition
Program Manager (International), Human Dimension

Dr. Robert Kokoska
Program Manager, Microbiology

Dr. Lisa Troyer

Program Manager, Social and Behavioral Science

Dr. Valerie Martindale

Program Manager (International), Synthetic Biology

PHYSICS DIVISION

Dr. Marc Ulrich

Division Chief

Program Manager, Condensed Matter Physics

Dr. Richard Hammond (retired)

Program Manager, Optical Physics and Fields

Dr. Paul Baker

Program Manager, Atomic and Molecular Physics

Dr. Sara Gamble

Program Manager, Quantum Information Science (QIS)

Dr. T. R. Govindan (NASA)

Program Manager, QIS Quantum Computation and Networking

Dr. Thomas Bahder

Program Manager (International), Quantum Scale Materials

ENGINEERING SCIENCES DIRECTORATE (ESD)

Dr. David Stepp

Director, ESD

Dr. Larry Russell

Program Manager, ARO University Research Initiatives

Ms. Liza Wilder

Administrative Specialist

ELECTRONICS DIVISION

Dr. David Stepp

Division Chief (Acting), Electronics

Dr. Michael Gerhold

Program Manager, Optoelectronics

Program Manager (Acting), Electronic Sensing

Dr. James Harvey

Program Manager (Acting), Biotronics

Dr. Joe Qiu

Program Manager, Solid State and Electromagnetics

MATERIALS SCIENCE DIVISION

Dr. Chakrapani (Pani) Varanasi

Division Chief, Materials Science

Program Manager, Physical Properties of Materials

Program Manager (International, Acting), Innovations in Materials

Dr. Michael Bakas

Program Manager, Synthesis & Processing

Dr. John Prater (retired)

Program Manager, Materials Design

Dr. Evan Runnerstrom (current)

Program Manager, Materials Design

Dr. David Stepp

Program Manager, Mechanical Behavior of Materials

MECHANICAL SCIENCES DIVISION

Dr. Ralph Anthenien

Division Chief, Mechanical Sciences

Program Manager, Propulsion & Energetics

Program Manager (Acting), Solid Mechanics (former)

Dr. Julia Barzyk

Program Manager, Earth Materials & Processes

Dr. Matthew Munson

Program Manager, Fluid Dynamics

Dr. Samuel Stanton

Program Manager, Complex Dynamics & Systems

Dr. Denise Ford

Program Manager, Solid Mechanics (current)

INFORMATION SCIENCES DIRECTORATE (ISD)

Dr. Randy Zachery

Director, ISD

Dr. Bruce West

Senior Scientist

Ms. Debra Brown

Administrative Specialist

Ms. Diana Pescod

Administrative Support Assistant

COMPUTING SCIENCES DIVISION

Dr. Cliff Wang

Division Chief
Program Manager, Information and Software Assurance

Dr. Mike Coyle

Program Manager, Computational Architectures and Visualization

Dr. Liyi Dai (retired)

Program Manager, Information Processing and Fusion

MATHEMATICAL SCIENCES DIVISION

Dr. Joseph Myers

Division Chief
Program Manager, Computational Mathematics
Program Manager (Acting), Modeling of Complex Systems

Dr. Virginia Pasour

Program Manager, Biomathematics

Dr. Michael Lavine

Program Manager, Probability and Statistics

NETWORK SCIENCES DIVISION

Dr. Purush Iyer

Division Chief
Program Manager, Intelligent Information Networks

Dr. Derya Cansever

Program Manager, Multi-Agent Network Control
Program Manager (Acting), Wireless and Hybrid Communication Network

Dr. Edward Palazzolo

Program Manager, Social and Cognitive Networks

Dr. Robert Ulman

Program Manager, Network Science and Intelligent Systems (International Program)

TECHNOLOGY INTEGRATION AND OUTREACH DIVISION

Mr. Michael Caccuitto

Division Chief

Mr. Tylar Temple

Program Manager, OSD Science, Mathematics and Research for Transformation Program

Mr. Michael J. Smith

Program Manager, Department of the Army STTR Program

Ms. Nicole Fox

Program Specialist, ARO SBIR and STTR Programs

Ms. Patricia Huff

Program Specialist, HBCU/MSI Programs

Ms. Jennifer Ardouin

Program Specialist, STEM Education Outreach



CHAPTER 2 | PROGRAM DESCRIPTIONS AND FUNDING SOURCES

As described in the previous chapter, ARO pursues a variety of investment strategies to meet its mission as the Army's lead extramural basic research agency in chemical sciences, computing sciences, electronics, life sciences, materials science, mathematical sciences, mechanical sciences, network sciences, and physics. In this role, ARO, as part of CCDC-ARL, is an essential component of ARL's Discovery ERP and a critical provider of fundamental discoveries in support of all ARL ERPs and Core Technical Competencies. ARO implements its investment strategies through research programs and initiatives that have unique objectives, eligibility requirements, and receive funding from a variety of DoD sources. The visions, objectives, and funding sources of these programs are presented in this chapter.

The selection of research topics, proposal evaluation, and project monitoring are organized within ARO Divisions according to scientific discipline (refer to CHAPTER 1 - Figure 1). ARO's Divisions and Programs are aligned with these disciplines, each with its own vision and research objectives. Each Division identifies topics that are included in the ARO Core Broad Agency Announcement (BAA). The ARO Core BAA is provided for reference in CHAPTER 5. Researchers are encouraged to submit white papers and proposals in areas that support the Division's objectives. The ARO Divisions are not confined to only funding research in the academic departments that align with the Division names; they have the flexibility to find and fund the most promising research to advance their mission regardless of the academic department pursuing a particular research idea.

OVERVIEW OF PROGRAM FUNDING SOURCES

ARO oversees and participates in the topic generation, proposal solicitation, evaluation, and grant-monitoring activities of programs funded through a variety of DoD agencies, as listed in the following subsections.

ARMY FUNDING

The Army funds the majority of the extramural basic research programs managed by ARO, as listed below.

- ▶ The Core (BH57) Research Program, funded through basic research “BH57” funds.
- ▶ The University Research Initiative (URI), which includes these component programs:
 - Multidisciplinary University Research Initiative (MURI) program
 - Presidential Early Career Awards for Scientists and Engineers (PECASE)
 - Defense University Research Instrumentation Program (DURIP)
- ▶ Three University Affiliated Research Centers (UARCs)

ARO coordinates with the Office of the Secretary of Defense (OSD) in managing the URI programs and also manages the Army’s Small Business Technology Transfer (STTR) program.

OFFICE OF THE SECRETARY OF DEFENSE (OSD) FUNDING

The funds for a variety of programs managed or supported by ARO are provided by OSD. These include:

- ▶ Research and Educational Program (REP) for Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI)
- ▶ National Defense Science and Engineering Graduate (NDSEG) Fellowships
- ▶ Educational Outreach Activities

These activities are mandated by DoD’s Chief Technology Office, the Office of the Assistant Secretary of Defense for Research and Engineering [OASD(R&E)]. Each of these OSD-funded programs has a unique focus and/or a unique target audience. ARO has been designated by OASD(R&E) as the lead agency for the implementation of REP for HBCU/MSI activities on behalf

of the three Services. OSD oversees ARO management of the Army-funded URI and its component programs (MURI, PECASE, and DURIP).

OTHER FUNDING SOURCES

In addition to the Army- and OSD-funded programs described earlier in this section, ARO leverages funds from other DoD sources (e.g., DARPA) to support a variety of external programs with specific research focuses. These joint programs have objectives consistent with the strategies of the corresponding ARO Program. Due to the unique nature of these cooperative efforts, each externally-funded effort is discussed within the chapter of the aligned scientific Division.

ARO CORE (BH57) RESEARCH PROGRAM

ARO’s Core Research Program is funded with Army basic research “BH57” funds and represents the primary basic research funding provided to ARO by the Army. Within this program and its ongoing BAA, research proposals are sought from educational institutions, nonprofit organizations, and commercial organizations for basic research in electronics, physics, and the chemical, computing, life, materials, mathematical, mechanical, and network sciences. The goal of this program is to utilize world-class and worldwide academic expertise to discover and exploit novel scientific discoveries, primarily at universities, to provide the current and future force with critical new or enhanced capabilities.

ARO Core Research Program activities fall under five categories, discussed in the following subsections: (a) Single Investigator awards; (b) Short Term Innovative Research efforts; (c) Young Investigator Program; (d) support for conferences, workshops, and symposia; (e) international programs; and (f) special programs. ARO’s Core (BH57) Research Program represents the principal mission of ARO and is where the majority of the Army funds are used. A summary of the Core (BH57) Research Program budget is presented in Table 5 on page 23.

SINGLE INVESTIGATOR (SI) PROGRAM

The goal of the SI program is to pursue the most innovative, high-risk, and high-payoff ideas in basic research. Research proposals within the SI Program are received throughout the year in a continuously-open, worldwide BAA solicitation. This program focuses on basic research efforts by one or two faculty members along with supporting graduate students and/or postdoctoral researchers and is typically a three-year grant. This program, as for all program elements that fall under the overarching ARO Core Program, enables the Army to invest

and drive national academic research toward areas of interest to the future Army. As the grants are on a three-year cycle, approximately one third of the extramural portfolio can be reinvested into new or advancing areas each year. This program provides the Army with a dynamic method for rapidly investing or divesting in research to ensure the realization of foundational discoveries that will enable future Army capabilities.

SHORT TERM INNOVATIVE RESEARCH (STIR) PROGRAM

The objective of the STIR Program is to explore high-risk initial proof-of-concept ideas within a nine-month timeframe. Research proposals are sought from educational institutions, nonprofit organizations, or private industry. If a STIR effort's results are promising, the investigator may be encouraged to submit a proposal to be evaluated for potential longer-term funding options, such as an SI award.

YOUNG INVESTIGATOR PROGRAM (YIP)

The objective of the YIP is to attract outstanding young university faculty to Army-relevant research questions, to support their research, and to encourage their teaching and research careers. Outstanding YIP projects may be considered for the prestigious PECASE award.

CONFERENCES, WORKSHOPS, AND SYMPOSIA SUPPORT PROGRAM

The ARO Core Program also provides funding for organizing and facilitating scientific and technical conferences, workshops, and symposia. This program provides a method for conducting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army and help define research needs, thrusts, opportunities, and innovation. In particular, workshops are a key mechanism ARO uses to identify new research areas with the greatest opportunities for scientific breakthroughs that will revolutionize future Army capabilities.

INTERNATIONAL PROGRAMS

Beginning in FY16, ARO initiated international programs with the goal of identifying academic investigators who are the forerunners in particular fields of research of which U.S. scientists do not currently hold the lead. Based on a detailed data analytics study that assessed 39 countries and their research publication output from 2009-2014, ARO identified seven scientific areas critical to the future Army, components of which are led by researchers outside of the U.S. These areas were grouped into three key geographic locations: the Atlantic, Pacific, and Americas regions.

These international programs are part of ARL and ARO's comprehensive approach to ensure that Army basic research funds are used efficiently to find the scientists best suited to drive high-risk, high-payoff Army crucial research, regardless of whether these researchers are in the U.S. or abroad. The seven ARO International Program Managers (PMs) are each aligned to an ARO Division and focus on key research areas to identify international investigators with skills and ideas in areas not led by researchers within the U.S., as well as to engage and partner those researchers with existing Army and DoD programs. These international research areas, the corresponding aligned Division, and the locations where the International PMs are stationed are listed below:

- ▶ Energy Transport and Storage (Chemical Sciences Division) - Tokyo, Japan
- ▶ Advanced Computing (Computing Sciences Division) - São Paulo, Brazil (currently vacant)
- ▶ Synthetic Biology (Life Sciences Division) - Tokyo, Japan
- ▶ Human Dimension (Life Sciences Division) - London, United Kingdom
- ▶ Innovation in Materials (Materials Science Division) - London, United Kingdom (currently vacant)
- ▶ Network Science and Intelligent Systems (Network Sciences Division) - London, United Kingdom
- ▶ Quantum Scale Materials (Physics Division) - Tokyo, Japan

SPECIAL PROGRAMS

Although the programs listed earlier in this section constitute the primary use of BH57 funds, the ARO Core Research Program also supports a variety of special programs. The Research Instrumentation (RI) Program is designed to improve the capabilities of U.S. institutions of higher education to conduct research and educate scientists and engineers in areas important to national defense, and funds may be provided to purchase instrumentation in support of this research or in the development of new research capabilities. However, the majority of instrumentation support awarded through ARO is provided through the Defense University Research Instrumentation Program (DURIP). The ARO Core Research Program also co-funds awards selected through the Army's High School Apprenticeship Program (HSAP) and Undergraduate Research Apprenticeship Program (URAP), which is managed through ARO's Educational Outreach Activities.

MULTIDISCIPLINARY UNIVERSITY RESEARCH INITIATIVE (MURI)

The MURI Program is part of the University Research Initiative (URI) and supports research teams whose research efforts intersect more than one traditional discipline. A multidisciplinary effort can accelerate research progress in areas particularly suited to this approach by cross-fertilization of ideas, can hasten the transition of basic research findings to practical applications, and can help to train students in science and/or engineering in areas of importance to DoD. In contrast with ARO Core program SI research projects, MURI projects support centers whose efforts require a large and highly collaborative multidisciplinary research effort. These are typically funded at \$1.25 million per year for three years with an option for two additional years. The efforts are expected to enable more rapid research and development breakthroughs and to promote eventual transition to Army applications.

Oversight of the MURI program comes from the Basic Research Office of OASD(R&E) to the Service Research Offices (OXRs), where OXR PMs manage the MURI projects. The OXRs include ARO, the Air Force Office of Scientific Research (AFOSR), and the Office of Naval Research (ONR). OXR PMs have significant flexibility and discretion in how the individual projects are monitored and managed, while OASD(R&E) defends the program to higher levels in OSD and has responsibility for overall direction and oversight. Selection of Army research topics and the eventual awards are reviewed and approved by OASD(R&E) under a formal acquisition process.

The full list of all ARO-managed MURI projects that were active in FY18 are described in CHAPTER 4.

Eight MURI projects were selected for funding and began in FY18. These projects are based on proposals submitted to the FY18 MURI FOA, which was released in late FY17. Each new-start project, lead investigator, and lead performing organization are listed here, immediately below the corresponding MURI topic, topic authors/PMs, and the ARO Division responsible for monitoring the project.

The following eight proposals were selected to be the FY18 new starts for the MURI Program.

- ▶ **Topic:** Novel solid- state materials and color centers for quantum science and engineering
PMs: Dr. Pani Varanasi (Materials Science), Dr. T.R. Govindan (Physics), & Dr. Paul Baker (Physics)
Project Selected: Ab-Initio Solid-State Quantum Materials: Design, Production, and Characterization at the Atomic Scale
Lead PI: Professor Dirk Englund, Massachusetts Institute of Technology
- ▶ **Topic:** Controlling Protein Function Using Dynamic Chemical Switches to Modulate Structure
PMs: Dr. Stephanie McElhinny (Life Sciences) and Dr. Dawanne Poree (Chemical Sciences)
Project Selected: Stimuli-Responsive Control of Protein-Based Molecular Structure
Lead PI: Professor Milan Mrksich, Northwestern University
- ▶ **Topic:** Consolidation of Novel Materials and Macrostructures from a Dusty Plasma
PMs: Dr. Michael Bakas (Materials Science), Dr. Richard Hammond (Physics), and Dr. James Parker (Chemical Sciences)
Project Selected: New Materials from Dusty Plasmas
Lead PI: Professor Uwe Kortshagen, University of Minnesota
- ▶ **Topic:** Embodied Learning and Control
PM: Dr. Samuel Stanton (Mechanical Sciences)
Project Selected: Science of Embodied Innovation, Learning and Control
Lead PI: Professor Daniel Koditschek, University of Pennsylvania
- ▶ **Topic:** Coevolution of Neural, Cognitive, & Social Networks: Mind-Body-Community Connections
PMs: Dr. Edward T. Palazzolo (Network Science) and Dr. Frederick Gregory (Life Sciences)
Project Selected: Multiscale integration of neural, social, and network theory to understand and predict transitions from illness to wellness
Lead PI: Professor Emily Falk, University of Pennsylvania
- ▶ **Topic:** Network Games
PMs: Dr. Purush Iyer (Network Science) and Dr. Edward Palazzolo (Network Science)
Project Selected: MultiScale Network Games of Collusion and Competition
Lead PI: Professor Mingyan Liu, University of Michigan
- ▶ **Topic:** Modeling Interdependence among Natural Systems and Human Population Dynamics
PMs: Dr. Lisa Troyer (Life Sciences) and Dr. Derya Cansever (Network Science)
Project Selected: Towards a Multi-Scale Theory on Coupled Human Mobility and Environmental Change
Lead PI: Professor Rachata Muneeppeerakul, University of Florida Gainesville

The following eight topics were published in FY18 and constitute the ARO portion of the FY19 MURI BAA.

- ▶ *Clearing Your Head: The Glymphatic System and Restorative Effects of Sleep*
PMs: Dr. Matthew Munson (Mechanical Sciences) and Dr. Frederick Gregory (Life Sciences)
- ▶ *Foundations of Emergent Computation and Self-Organized Adaptation*
PMs: Dr. Samuel Stanton (Mechanical Sciences) and Dr. Paul Baker (Physics)
- ▶ *Multi-layer Network Modeling of Plant and Pollen Distribution across Space and Time*
PMs: Dr. Micheline Strand (Life Sciences) and Dr. Lisa Troyer (Life Sciences)
- ▶ *Near Field Radiative Heat Energy Transfer between Nanostructured Materials*
PMs: Dr. Pani Varanasi (Materials Science) and Dr. Marc Ulrich (Physics)
- ▶ *Networked Interactions Governing Community Dynamics*
PMs: Dr. Robert Kokoska (Life Sciences) and Dr. Derya Cansever (Network Science)
- ▶ *Prediction and Control in Particulate Systems*
PMs: Dr. Joseph Myers (Mathematical Sciences) and Dr. Julia Barzyk (Engineering Sciences)
- ▶ *Reactive and non-Reactive Scattering from Targeted Molecular Quantum States*
PMs: Dr. James Parker (Chemical Sciences) and Dr. Paul Baker (Physics)
- ▶ *Unified Decision Theory: From Bounded to Unbounded Rationality*
PMs: Dr. Purush Iyer (Network Science) and Dr. Edward Palazzolo (Network Science)

PRESIDENTIAL EARLY CAREER AWARD FOR SCIENTISTS AND ENGINEERS (PECASE)

The PECASE program, also part of the URI program, attracts outstanding young university faculty members, supporting their research, and encouraging their teaching and research careers. PECASE awards are the highest honor bestowed by the Army to extramural scientists and engineers beginning their independent research careers. Each award averages \$200K/year for five years. PECASE awards are based in part on two important criteria: (i) innovative research at the frontiers of science and technology that is relevant to the mission of the sponsoring

agency, and (ii) community service demonstrated through scientific leadership, education, and outreach.

The PECASE winners for each calendar year's competition are typically announced by the White House. In order to ensure the PECASE program continues with regard to funding FY15+ PECASE nominees, ARO created the ECASE-Army to begin funding FY15-FY18 PECASE nominees as ECASE-Army awards while Presidential selection and approval of candidates is pending. These awards will begin as new-start projects in FY19, to be reported in ARO in Review 2019.

DEFENSE UNIVERSITY RESEARCH INSTRUMENTATION PROGRAM (DURIP)

DURIP, also part of the URI program, supports the purchase of state-of-the-art equipment that augments current university capabilities or develops new capabilities to perform cutting-edge defense research. DURIP meets a critical need by enabling university researchers to purchase equipment costing \$50K or more to conduct DoD-relevant research. In FY18, the Army awarded 47 grants at \$10.2M total, with an average award of \$324K.

UNIVERSITY AFFILIATED RESEARCH CENTERS (UARCs)

The Army's University Affiliated Research Centers (UARCs) are strategic DoD-established research organizations at universities. The UARCs were formally established in May 1996 by OASD(R&E) to advance DoD long-term goals by pursuing leading-edge basic research and to maintain core competencies in specific domains unique to each UARC, for the benefit of DoD. One DoD Agency is formally designated by OASD(R&E) to be the primary sponsor for each UARC. The primary sponsor ensures DoD UARC management policies and procedures are properly implemented. Collaborations among UARCs and the educational and research resources available at the associated universities can enhance each UARC's ability to meet the long-term goals of DoD. ARO is the primary sponsor for two UARCs, with involvement in a third.

- ▶ The Army's Institute for Soldier Nanotechnologies (AISN), located at the Massachusetts Institute of Technology (MIT).
- ▶ The Army's Institute for Collaborative Biotechnologies (AICB), located at the University of California - Santa Barbara, with academic partners at MIT and the California Institute of Technology.

- ▶ The Army's Institute for Creative Technologies (AICT), located at the University of Southern California. In contrast to the AISN and AICB, the AICT is co-managed within ARL by both ARO and the Human Research and Engineering Directorate (HRED). Funding for the AICT is managed through ARO while HRED provides technical guidance with ARO support.

MINERVA RESEARCH INITIATIVE (MRI)

The Minerva Research Initiative (MRI) is a DoD-sponsored, university-based social science basic research program initiated by the Secretary of Defense and focuses on areas of strategic importance to U.S. national security policy. It seeks to increase the intellectual capital in the social and behavioral sciences and improve DoD's ability to address future challenges and build bridges between DoD and the social and behavioral sciences community, with a focus on the National Defense Strategy and basic research missions of the tri-service branches (U.S. Army, U.S. Air Force, U.S. Navy). Minerva brings together universities, research institutions, and individual scholars and supports multidisciplinary and cross-institutional projects addressing specific topic areas determined by DoD.

Minerva projects are funded up to a five-year base period, with awards ranging from small, single investigator grants for two to three years to large multidisciplinary projects for \$1-2 million per year for five years. The program is overseen by the U.S. Air Force and U.S. Navy and OSD; with currently managing projects (2-5 year duration) dealing with models of multi-state burden-sharing to mitigate conflict and establish sociopolitical stability in fragile states, assessment of post-conflict crises and factors impacting of social order; and development of new models to predict causes and consequences of sociopolitical stability and rise of violent extremist organizations. ARO also provides scientific, technical, and managerial support to OSD in managing projects in these areas.

The titles of ARO-managed FY18 new-start Minerva projects are listed below, followed by the name of the lead PI, the performing organization, and the award duration.

- ▶ *All Intervention is Local*, PI: Professor Pierre Englebort, Pomona College, FY18-FY21
- ▶ *Refugee Psychology and Its Potential for Refugee Radicalization*, Professor Arie Kruglanski, University of Maryland – College Park, FY18-FY21
- ▶ *The Political, Economic, and Social Effects of the United States Overseas Military Presence*, Professor Michael Allen, Boise State University, FY18-FY21

- ▶ *Displace, Return, and Reconstruct: Population Movement and Resilience to Instability*, Professor James Walsh, University of North Carolina – Charlotte, FY18-FY21
- ▶ *Integrating Structural Theories of Revolution with Evolutionary Models to Predict Societal Resilience*, Professor Sergey Gavrillets, University of Tennessee – Knoxville, FY18-FY21
- ▶ *Informal Economies, Societal Stability, and Regime Resilience in China and Russia*, Professor Marina Zaloznaya, University of Iowa, FY18-FY21

SMALL BUSINESS INNOVATION RESEARCH (SBIR) AND SMALL BUSINESS TECHNOLOGY TRANSFER (STTR) PROGRAMS

Congress established the SBIR and STTR programs in 1982 and 1992, respectively, to provide small businesses and research institutions with opportunities to participate in government-sponsored R&D. The DoD SBIR and STTR programs are overseen by the Office of the Under Secretary of Defense for Research and Engineering. The Army-wide SBIR Program is managed at Headquarters, CCDC, while the Army-wide STTR Program is managed by CCDC-ARL at ARO. In contrast to the basic research programs managed by ARO, the SBIR and STTR programs focus primarily on feasibility studies leading to prototype demonstration of technology for specific applications.

PURPOSE AND MISSION

The purpose of the SBIR and STTR programs is to: (i) stimulate technological innovation; (ii) use small business to meet Federal R&D needs; (iii) foster and encourage participation by socially and economically disadvantaged small business concerns (SBCs), in technological innovation; and (iv) increase private sector commercialization of innovations derived from Federal R&D, thereby increasing competition, productivity, and economic growth. The STTR program has the additional requirement that small companies must partner with universities, federally funded research and development centers, or other non-profit research institutions to work collaboratively to develop and transition ideas from the laboratory to the marketplace.

THREE-PHASE PROCESS

The SBIR and STTR programs use a three-phase process, reflecting the high degree of technical risk involved in funding research, and developing and commercializing cutting edge technologies. The basic parameters of this three-phase process for both programs within the Army are shown in TABLE 1.

Phase I. Phase I of the SBIR and STTR programs involves a feasibility study that determines the scientific, technical, and commercial merit and feasibility of a concept. Each SBIR and STTR BAA contains topics seeking specific solutions to stated government needs. Phase I proposals must respond to a specific topic in the BAA, and proposals are competitively judged on the basis of scientific, technical, and commercial merit. The Phase I evaluation and award process marks the entry point to the program and cannot be bypassed.

Phase II. Phase II represents a major research and development effort, culminating in a well-defined deliverable prototype (i.e., a technology, product, or service). The Phase II selection process is also competitive. Phase I contractors can submit Phase II proposals during one of the respective program’s submissions cycles, as there are no separate Phase II BAAs. Typically 50% of Phase II proposals are selected for award. SBIR Phase II awardees may be selected to receive additional funds as an invited Subsequent Phase II, Phase II Enhancement, or via the Commercialization Readiness Program (CRP). STTR Phase II awards may also be selected to receive additional funds as an invited Sequential Phase II.

Phase III. In Phase III, the small business or research institute is expected to obtain funding from the private sector and/or non-SBIR/STTR government sources to develop products, production, services, R&D, or any combination thereof into a

viable product or service for sale in military or private sector markets. Commercialization is the ultimate goal of the SBIR and STTR programs.

ARMY FY18 STTR PROGRAM

ARO manages the Army-wide STTR program and has since the program’s inception in 1992. ARO coordinates participation of nine (9) Army components and commands. In FY18, the budget was \$35 million, up 25% from FY17 when it was \$28 million. Participating components include: CCDC-Aviation and Missile Center, CCDC-Armaments Center, CCDC-ARL/ARO, CCDC-C5ISR, CCDC-Chem Bio Center, CCDC-Soldier Center, CCDC-Ground Vehicle Systems Center, Corp of Engineers (CoE)-ERDC, and MRDC.

The Army STTR program conducted an aggressive outreach program as it was showcased on the Small Business Administration (SBA) “Eastern SBIR/STTR Road Tour” stopover at the North Carolina Biotechnology Center in Durham, NC, where attendees were provided detailed insight to participate in future Army STTR research projects. Additional outreach events were conducted in support of the following: “Taking the Pentagon to the People” at Fayetteville State University, DASA(R&T)-sponsored “xTechSearch” pitch events at the USC-Playa Vista CA campus and at ARL’s Open Campus Northeast site in Burlington, MA, the NC Defense Business Association (NCDBA), and the Spring National SBIR/STTR Summit in Anaheim, CA, where hundreds of small businesses and research institutes were provided more insight to participate in future Army S&T opportunities.

An Army STTR small business/university team (Simulation Technologies and the University of Alabama-Huntsville) developed a high-fidelity, missile sensor simulation model to create realistic scenes of flight scenarios in lieu of expensive flight tests. In FY18, they were awarded a five-year, \$20 million IDIQ contract to become part of the DoD-level simulations used to evaluate missile system designs and performance.

TABLE 1

Three-phase process of the SBIR and STTR programs. Phase I is an assessment of technical merit and feasibility, Phase II is a larger R&D effort often resulting in a deliverable prototype, and Phase III is a project derived from, extending, or logically concluding prior SBIR/STTR work, generally to develop a viable product or service for military or commercial markets.

	SBIR Contract Limits	STTR Contract Limits
Phase I	<ul style="list-style-type: none"> 6 months, \$100K max 3-month option (at Government’s discretion), \$50K max, to fund interim Phase II efforts 	<ul style="list-style-type: none"> 6 months, \$150K max No options
Phase II	<ul style="list-style-type: none"> 2 years, \$1 million max 	<ul style="list-style-type: none"> 2 years, \$1 million max
Subsequent Phase II	<ul style="list-style-type: none"> 2 years, \$1 million max 	<ul style="list-style-type: none"> 2 years, \$1 million max
Phase II Enhancement	<ul style="list-style-type: none"> 2 years, \$500K matching funds max 	<ul style="list-style-type: none"> n/a
Phase III	<ul style="list-style-type: none"> No time or size limit No SBIR/STTR set-aside funds 	<ul style="list-style-type: none"> No time or size limit No SBIR/STTR set-aside funds

ARO FY18 SBIR AND STTR TOPICS

The following SBIR topics were published in an FY18 SBIR BAA. The lead topic author (who serves as the topic PM) and corresponding Division are listed with each topic.

- ▶ *Biologically-Derived Targeted Antifungals for Textiles*; Dr. Michael Coyle, Computing Sciences Division
- ▶ *CMOS Compatible Deposition of Multi-Ferroic Films for Tunable Microwave Applications*; Dr. James Harvey, Electronics

The following STTR topics were published in an FY18 STTR BAA. The lead topic author and corresponding Division are listed following each topic title.

- ▶ *Additive Manufacturing Feedstock Designed for Uniform Printing of Metallic Builds*; Dr. Michael Bakas, Material Sciences
- ▶ *Carbon Nanotube Based Monolithic Millimeter-wave Integrated Circuits*; Dr. Joe Qiu, Electronics
- ▶ *Diffusiophoresis for Water Purification*; Dr. Matthew Munson, Mechanical Sciences
- ▶ *Deep Ultraviolet Light Sources for Water Purification and Surface Sterilization*; Dr. Michael Gerhold, Electronics
- ▶ *Resource Sharing Platforms for Improved Operational Logistics*; Dr. Purush Iyer, Network Sciences
- ▶ *Effective Human Teaming Supported by Social Sensing*; Dr. Edward Palazzolo, Network Sciences
- ▶ *Wavelet-Based Adaptive Antenna Systems*; Dr. Joseph Myers, Mathematical Sciences
- ▶ *Mitigation of Ransomware*; Dr. Cliff Wang, Computing Sciences
- ▶ *Software Tools for Scalable Quantum Validation and Verification*; Dr. TR Govindan, Physics
- ▶ *Hybrid Nano-Bio-Electronic Odor Detector*; Dr. Fredrick Gregory, Life Sciences
- ▶ *Disabling of Vehicles and/or Remote Weapon Stations in an Urban Environment*; Dr. Stephen Lee, Chemical Sciences
- ▶ *Robust High-Performance Laser Sources for Scalable Quantum Technology*; Dr. T R Govindan, Physics
- ▶ *Microporous Flexible Electrodes for Lithium Metal Secondary Batteries*; Dr. Robert Mantz, Chemical Sciences
- ▶ *Cell-Free Screening System for Genetically-Derived Small Molecule Biosensors*; Dr. Stephanie McElhinny, Life Sciences
- ▶ *Freeze Dried Plasma for Canines*; Dr. Robert Mantz, Chemical Sciences
- ▶ *Lithium Ion Battery Electrodes Manufacturing to Improve Power and Energy Performance*; Dr. Robert Mantz, Chemical Sciences
- ▶ *Lead Acid Battery Monitoring, Diagnostics, and Prognostics*; Dr. Robert Mantz, Chemical Sciences
- ▶ *Electromagnetically Catalyzed Decontamination (EMCAT) Development*; Dr. Stephen Lee, Chemical Sciences

The following STTR and CBD STTR topics were selected for Phase II contracts in FY18. The lead topic author/PM and corresponding Division are listed following each topic title.

- ▶ *High Dynamic Range Heterodyne Terahertz Imager*; Dr. Joe Qiu, Electronics
- ▶ *3D Tomographic Scanning Microwave Microscopy with Nanometer Resolution*; Dr. Joe Qiu, Electronics
- ▶ *Scalable Manufacturing of Graphite Yarn via Wet Spinning Process*; Rob Mantz, Chemical Sciences
- ▶ *Engineered Strain for Bioconversion of Food Waste to Fuels*; Dr. Bob Kokoska, Life Sciences
- ▶ *Monolithic photonic platform for high-power InGaAs/AlInAs quantum cascade laser beam combining and steering*; Dr. Michael Gerhold, Electronics
- ▶ *In Theater Additive Manufacturing of Ceramic Armor for Dismounted Soldiers and Structures*; Dr. Stephen Lee, Chemical Sciences
- ▶ *Multiscale Fast and Distributed Data and Statistics Summarization*; Dr. Joseph Myers, Mathematical Sciences
- ▶ *Low-Loss Commercial Deposition Technology for Thick Ferrites and Ferrite/Insulator Films on Printed Circuit Boards*; Dr. James Harvey, Electronics
- ▶ *Monolithic Slow Light Enhanced Chip-Integrated Absorption Spectrometer from 3-15 microns*; Dr. Michael Gerhold, Electronics
- ▶ *Scalable Manufacturing of Functional Yarns for Textile-based Energy Storage*; Dr. Robert Mantz, Network Sciences
- ▶ *Multiple Hit Performance of Small Arms Protective Armor*; Dr. David Stepp, Engineering Sciences
- ▶ *Method for Locally Measuring Strength of a Polymer-Inorganic Interface During Cure and Aging*; Dr. Dawanne Poree, Chemical Sciences

ARO FY18 SBIR AND STTR PHASE II CONTRACT AWARDS

The following SBIR and Chemical Biological Defense (CBD) SBIR topics were selected for Phase II contracts in FY18. The lead topic author/PM and corresponding Division are listed following each topic title.

- ▶ *Biologically-Derived Targeted Antifungals for Textile Applications*; Dr. Stephanie McElhinny, Life Sciences
- ▶ *CMOS Compatible Deposition of Multi-Ferroic Films for Tunable Microwave Applications*; Dr. James Harvey, Electronics
- ▶ *High-Speed Free-Space Optical Link for Cryogenic Focal Plane Array Read-Out*; Dr. Michael Gerhold, Electronics

ARO FY18 SBIR AND CBD SBIR SUBSEQUENT PHASE II CONTRACT AWARDS

The following CBD SBIR topic was selected for a Subsequent Phase II contract in FY18. The lead topic author/PM and corresponding Division are listed following the topic title.

- ▶ *Electromagnetically Catalyzed Decontamination (EMCAT) Development*; Dr. Stephen Lee, Chemical Sciences

ARO FY18 STTR AND CBD STTR SUBSEQUENT PHASE II CONTRACT AWARDS

The following STTR topics were selected for Subsequent Phase II contracts in FY18. The lead topic author/PM and corresponding Division are listed following each topic title.

- ▶ *On Demand Energy Activated Liquid Decontaminants and Cleaning Solutions*; Dr. Dawanne Poree, Chemical Sciences
- ▶ *Biologically-Derived Targeted Antimicrobials for Textile Applications*; Dr. Stephanie McElhinny, Life Sciences
- ▶ *ADA Conformable Wearable Battery-Hybrid Electrical Energy Storage System: A Rechargeable, Safe and High Performance Energy Storage Solution*; Dr. Robert Mantz, Chemical Sciences
- ▶ *EMS Monitor & Broadcast Training Capacity Enhancement*; Dr. Robert Ulman, Network Sciences

ARO FY18 SBIR AND CBD SBIR PHASE III CONTRACT AWARDS

The following SBIR and CBD SBIR topics were awarded a Phase III contract in FY18. The lead topic author/PM and corresponding Division are listed following each topic title. Phase III revenues can be obtained from Government or private customers but cannot be SBIR/STTR funds.

- ▶ *Research and Development Supporting New EW Capabilities*; Dr. Joe Qiu, Electronics
- ▶ *Advancement of Capabilities, Products, and Sensors in Chem/Bio Detection, Quantification, and Mitigation IDIQ*; Dr. Stephen Lee, Chemical Sciences

ARO FY18 STTR PHASE III CONTRACT AWARDS

The following STTR topics were awarded a Phase III contract in FY18. The lead topic author/PM and corresponding Division are listed following each topic title. Phase III revenues can be obtained from Government or private customers but cannot be SBIR/STTR funds.

- ▶ *Hybrid System for Beyond Lithium Rechargeable Batteries*; Dr. Robert Mantz, Chemical Sciences
- ▶ *Nondestructive Concrete Characterization System*; Dr. Dawanne Poree, Chemical Sciences

CONTRACT EVALUATION AND FUNDING

The Army receives Phase I and Phase II proposals in response to SBIR, STTR, CBD-SBIR/STTR, and OSD-SBIR/STTR topics that are published during solicitation periods throughout each fiscal year. Proposals are evaluated against published evaluation criteria and selected for contract award. Contract awards are made pending completion of successful negotiations with the small businesses and availability of funds.

HISTORICALLY BLACK COLLEGES AND UNIVERSITIES AND MINORITY-SERVING INSTITUTIONS (HBCU/MSI) PROGRAMS

The programs for HBCU/MSIs are a significant part of the ARO portfolio. These programs are discussed in the following subsections.

ARO (CORE) HBCU/MSI PROGRAM

Academic institutions classified as HBCU/MSIs may submit proposals to the ARO Core BAA, as for any other institution, and are evaluated and selected according to the same evaluation criteria and process established for all proposal submissions to the Core BAA. In FY18, ARO supported 127 agreements with HBCU/MSIs receiving over \$9.4 million in FY18 funding, including 24 new starts listed here.

The new-start HBCU/MSI research grants are listed below, with the project title followed by the PI, performing organization, ARO PM, and corresponding scientific division.

- ▶ *Acoustic Simulation in Real World Scenes*, Professor Dinesh Manocha, University of Maryland – College Park; Dr. J. Michael Coyle, Computing Sciences Division
- ▶ *Mission Critical Survivable and Recoverable Cyber Systems*, Professor Swastik Brahma, Tennessee State University; Dr. Cliff Wang, Computing Sciences Division
- ▶ *Dynamics of Stratified Particulate Flows with Erosion and Deposition*, Professor Eckart Meiburg, University of California – Santa Barbara; Dr. Julia Barzyk, Materials Science Division

- ▶ *Intracellular pathway explorations enabled by liquid based scanning microwave microscopy*, Professor Peter Burke, University of California - Irvine; Dr. James Harvey, Electronics Division
 - ▶ *Excitons and exciton-polaritons in novel organic-inorganic hybrids with sub-nano II-VI or III-V layers*, Professor Yong Zhang, University of North Carolina - Charlotte; Dr. Chakrapani Varanasi, Materials Science Division
 - ▶ *Anyonic Quantum Matter in Atomic Optical Lattices*, Professor Victor Galitskiy, University of Maryland – College Park; Dr. Paul Baker, Physics Division
 - ▶ *Conference and Symposia Grants: Microscale Ocean Biophysics*, Professor Shilpa Khatri, University of California - Merced; Dr. Virginia Pasour, Mathematical Sciences Division
 - ▶ *Biomimetic Artificial Cells with Multiple Internal Compartments: Novel Microstructures with Bioinspired Properties and Functions*, Professor Srinivasa Raghavan, University of Maryland – College Park; Dr. Stephanie McElhinny, Chemical Sciences Division
 - ▶ *Towards understanding the urban surface energy budget*, Professor Prathap Ramamurthy, CUNY – City College of New York; Dr. Julia Barzyk, Materials Science Division
 - ▶ *Investigations of Proximity-Induced Topological Superconductors as a Path to Non-Abelian Anyons in the Solid State*, Professor James Williams, University of Maryland – College Park; Dr. Marc Ulrich, Physics Division
 - ▶ *2018 Controversies Colloquium: Stability of Nanostructures*, Professor Timothy Rupert, University of California – Irvine; Dr. Michael Bakas, Materials Science Division
 - ▶ *Czech Republic - U.S. Workshop on Artificial Intelligence*, Professor William Regli, University of Maryland – College Park; Dr. Purush Iyer, Network Sciences Division
 - ▶ *A workshop on creation of an artificially intelligent organic chemist: applied machine learning for multiphase chemistry*, Professor Ann Marie Carlton, University of California - Irvine; Dr. Robert Mantz, Chemical Sciences Division
 - ▶ *26th Current Trends in Computational Chemistry*, Professor Jerzy Leszczynski, Jackson State University; Dr. Robert Mantz, Chemical Sciences Division
 - ▶ *Understanding the instability of particle-laden liquids over soft porous media*, Professor Parisa Mirbod, University of Illinois – Chicago; Dr. Matthew Munson, Mechanical Sciences Division
 - ▶ *Large scale dynamics and geometry in stochastic systems*, Professor Sunder Sethuraman, University of Arizona; Dr. Michael Lavine, Mathematical Sciences Division
 - ▶ *Exotic Transport Properties and Unique Applications of Intercalated van der Waals Materials*, Professor Kaustav Banerjee; University of California – Santa Barbara; Dr. Joe Qiu, Electronics Division
 - ▶ *Fundamental studies on the evolution of stress and other defects during additive manufacturing*, Professor Enrique Lavernia, University of California - Irvine; Dr. Michael Bakas, Materials Science Division
 - ▶ *Mathematical modeling of limbic system dynamics, pathophysiology, and response to stress*, Professor Maria-Rita D’Orsogna, California State University - Northridge; Dr. Virginia Pasour, Mathematical Sciences Division
 - ▶ *Multi-Agent Network Control - A Brain Emotional Learning-Inspired Approach*, Professor Luis Carrillo, Texas A&M University – Corpus Christi; Dr. Derya Cansever, Network Sciences Division
 - ▶ *Understanding Quantum Effects in 2D polymeric Systems*, Professor Sefaattin Tongay, Arizona State University; Dr. Chakrapani Varanasi, Materials Science Division
 - ▶ *Scalable Universal Quantum Computing and Networking Using Continuous-Variable Entangled Photonic Graphs*, Professor Saikat Guha, University of Arizona; Dr. Derya Cansever, Network Sciences Division
 - ▶ *Acquisition of a controlled environment fabrication system for two-dimensional materials*, Professor Brian LeRoy, University of Arizona; Dr. Joe Qiu, Electronics Division
 - ▶ *Enabling Gigantic Antiferromagnetic Spin Caloritronic Effects through Spin Heat Accumulation*, Professor Richard Wilson, University of California - Riverside; Dr. Chakrapani Varanasi, Materials Science Division
- As for all institutions funded through the ARO Core Program, HBCU/MIs selected for funding were afforded the opportunity to submit add-on proposals to fund high school and/or undergraduate student research apprenticeships through HSAP/URAP. A total of 19 HBCU/MIs were funded under HSAP/URAP in FY18, totaling approximately \$192K (~50/50 mix of PM and Army Education Outreach Program (AEOP) funding). Additional information regarding HSAP/URAP can be found in Section XI: Educational Outreach Activities.

PARTNERED RESEARCH INITIATIVE (PRI)

The PRI Program was established as the next phase of what was previously known as the Partnership in Research Transition (PIRT) Program, which ended in FY16. The focus of the PRI Program is to advance innovative basic research leading to potential technology development in areas of strategic

importance to the Army by bringing competitively selected HBCU/MSI research teams into existing ARL Collaborative Research Alliances (CRAs) and Collaborative Technology Alliances (CTAs). The CTAs and CRAs are large collaborative centers focused on developing and transitioning research in Army critical areas.

In FY18, ARL's PRI Program for HBCUs/MIs continued funding four projects totaling \$1.36 million through the CTA/CRA consortia: The New Mexico Institute of Mining and Technology as part of the Multiscale Modeling of Electronic Materials CRA; City College of New York as part of the Cognition and Neuroergonomics CTA; University of Texas at El Paso as part of the Cyber Security CRA; and North Carolina Agricultural and Technical State University as part of the Materials in Extreme Dynamic Environments (MEDE) CRA. The projects listed below may be funded for up to four years (through FY20) and are performed in collaboration with ARL and CTA/CRA member institutions to maximize the impact of the research and enhance HBCU/MSI research capabilities.

- ▶ **PRI Title:** *Defeating the Dark Triad in Cyber-security Using Game Theory*
Integrated into Cyber Security CRA
CTA/CRA Collaborating Institution: University of Texas at El Paso
PI: Professor Christopher Kiekintveld
Cooperative Agreement Manager (CAM): Dr. Michael Frame
- ▶ **PRI Title:** *Material Design Under Uncertainty*
Integrated into Multiscale Modeling of Electronic Materials CRA
CTA/CRA Collaborating Institution: New Mexico Institute of Mining and Technology (NMT)
PI: Dr. Yanyan He
CAM: Dr. Meredith Reed
- ▶ **PRI Title:** *Tailoring Mg-alloy Systems through Composition / Microstructure/Severe Plastic Deformation for Army Extreme Dynamic Environment Applications*
Integrated into Materials in Extreme Dynamic Environments (MEDE) CRA
CTA/CRA Collaborating Institution: North Carolina A&T State University
PI: Dr. Jagannathan Sankar
CAM: Dr. John Beatty
- ▶ **PRI Title:** *Reliability of Neural Activity as an Assay of Cognitive State*
Integrated into Cognition and Neuroergonomics CTA
CTA/CRA Collaborating Institution: City College of New York (CCNY)
PI: Dr. Jacek Dmochowski
CAM: Dr. Jon Touryan

DOD RESEARCH AND EDUCATIONAL PROGRAM (REP) FOR HBCU/MSIS

ARO has administered programs on behalf of OASD(R&E) since 1992. REP aims to enhance research capabilities of HBCUs and MSIs and to strengthen their education programs in science, technology, engineering, and mathematics (STEM) disciplines that are relevant to the defense mission.

Under this program, qualifying institutions were able to submit proposals to compete for basic research grants. In FY18, Funding Opportunity Announcement (FOA) W911NF-17-S-0010 was issued for the DoD REP for HBCUs/MSIs, with 139 proposals identified as eligible under the solicitation. In FY18, 45 grants totaling \$25.7 million were made to 22 unique HBCUs and 17 to unique MSIs under the DoD REP solicitation.

OTHER HBCU/MSI ACTIVITIES

On 19 June 2018, ARO in partnership with the Office of the Under Secretary of Defense for Research and Engineering (OUSD (R&E)) hosted a workshop to provide technical assistance on DoD research proposal writing for the HBCUs/MIs. This event was attended by over 210 registered participants from across the country, representing 25 HBCUs, 10 MSIs, 7 federal agencies, and 15 private sector businesses. Participants received assistance in developing competitive proposals in response to DoD funding opportunities. The knowledge gained by their attendance, the breakout sessions dialogues, and their interactions with the DoD program managers are expected to increase the number of opportunities available to the HBCUs, MIs, and their students. ARO will continue the dialogue initiated with the HBCU/MI representatives at the event to further develop areas of shared scientific interests to bolster HBCU/MI participation in DoD funding and research opportunities.

Also, in FY18, ARL's ARO announced its first-ever HBCU/MI Undergraduate Student Design Competition. The goals of the competition are to:

- ▶ Introduce HBCU/MI students to Army research and technical challenges and increase student interest in Army science and engineering;
- ▶ Engage HBCU/MI students with the Army's technical and operational communities;
- ▶ Implement ARL's HBCU/MI engagement strategy; and,
- ▶ Stimulate innovation and entrepreneurship.

Science and engineering talent and capability lie at the heart of the Army's ability to field the world's most advanced and capable ground fighting forces. To maintain this combat edge, it is vital that the Army attracts students from a wide variety of academic

and personal backgrounds to ensure it stays on the forefront of discovery and innovation. The inaugural year of the competition focuses on unmanned aerial vehicle (UAV) technology gaps in two topic areas. The first challenges students to eliminate wire bundles in an innovative way in small UAVs. The second topic seeks a way to replace UAV parts with biologically-based materials.

NATIONAL DEFENSE SCIENCE AND ENGINEERING GRADUATE (NDSEG) FELLOWSHIP PROGRAM

The NDSEG Fellowship Program is a tri-service program administered by the Air Force Office of Scientific Research (AFOSR), designed to increase the number of U.S. citizens trained in disciplines of science and engineering important to defense goals. ARO supports the NDSEG Fellowship Program along with the Office of Naval Research (ONR) and AFOSR. NDSEG is a highly competitive fellowship awarded to U.S. citizens who have demonstrated a special aptitude for advanced training in science and engineering, and who intend to pursue a doctoral degree in one of fifteen scientific disciplines of interest to the military. NDSEG Fellowships are for years of sponsorship. Fellows are provided full tuition and fees at any accredited university of choice, a monthly stipend very competitive with other top-tier fellowships (\$3,200/month), up to \$1,200/year in medical insurance, and \$5,000 to support travel during the duration of the fellowship.

With the funds made available to the Army to support candidates in FY18, ARO selected 23 NDSEG Fellows from 13 categories relevant to Army fundamental research priorities. These awardees began their fellowships in the fall of 2018. Each of ARO's divisions reviewed the applications assigned to NDSEG topic categories within their particular areas of expertise, and selected Fellows whose doctoral research topics most closely align with the Army's missions and research needs. Historically, the number of Fellows chosen from each discipline was based roughly on the percentage of applicants who submitted topics in that category. However, in FY18, far fewer fellowships could be funded. Selections were therefore almost evenly drawn from all relevant disciplines, with only candidates showing the greatest potential and alignment with Army research interests getting selected. The number of Fellows chosen from each scientific discipline for the FY18 NDSEG program is shown in TABLE 2.

TABLE 2

FY18 NDSEG fellows by discipline. The table displays the number of NDSEG Fellows chosen in FY18, according to topic categories relevant to the designated Army research priorities.

Scientific Discipline	NDSEG Fellows Selected in FY18
Aeronautical and Astronautical Engineering	1
Biosciences	2
Chemical Engineering	2
Chemistry	2
Civil Engineering	1
Cognitive, Neural, and Behavioral Sciences	2
Computer and Computational Sciences	2
Electrical Engineering	2
Geosciences	3
Materials Science and Engineering	1
Mathematics	1
Mechanical Engineering	2
Physics	2
TOTAL 23	

EDUCATIONAL OUTREACH ACTIVITIES

All the programs managed by the Army Educational Outreach Program (AEOP) STEM Outreach Office at CDCD Headquarters share one principal purpose: to increase the number of future adults with careers in science, technology, engineering, and mathematics. These programs accomplish this through a variety of mechanisms, including: providing a work/study laboratory experience, sponsoring hands-on science workshops during the summer, showcasing talented young high school scientists at symposia, and supporting student science fairs nationwide. Of these many programs, ARO continued to administer the High School and Undergraduate Research Apprenticeship Programs in FY18.

During the summer of FY18, 114 students served as apprentices and worked in university laboratories with mentors through the High School Apprenticeship Program (HSAP) and the Undergraduate Research Apprentice Program (URAP). This was about the same number of participants as in FY17. These programs are described further in the following subsections.

UNDERGRADUATE RESEARCH APPRENTICESHIP PROGRAM (URAP)

URAP funds the STEM apprenticeship of promising undergraduates to work in university-structured research environments under the direction of ARO-sponsored PIs or their senior research staff serving as mentors. In FY18, URAP awards provided 66 students with research experiences at 26 different universities in 20 different states. Fifteen of the universities were HBCU/MIs. ARO invested approximately \$182K of the \$364K total in the FY18 URAP effort, a mix of ARO core funding and AEOP matching funds.

HIGH SCHOOL APPRENTICESHIP PROGRAM (HSAP)

HSAP funds the STEM apprenticeship of promising high school juniors and seniors to work in university-structured research environments under the direction of ARO-sponsored PIs or their senior research staff serving as mentors. In FY18, HSAP awards provided 48 students with research experiences at 20 different universities in 22 different states. Fifteen of the universities were HBCU/MIs. ARO invested approximately \$85K of the \$169K total in the FY18 HSAP effort, which includes ARO core funding and AEOP matching funds.

LOCAL OUTREACH

ARO participated in the following local outreach efforts in FY18:

- ▶ North Carolina Science and Engineering Fair: ARO PMs volunteered to judge posters for a special category that presents awards to high school juniors and seniors based upon the overall quality and Army relevance of their projects.
- ▶ Regional JSHS: ARO attended and judged high school student posters for the regional competition. Top winners advance to the national JSHS competition.
- ▶ JSHS National Symposium: scientists from ARO and sponsored PIs attended and judged student posters as well as oral presentations of students that have previously won regional competitions. Winners are awarded various scholarships ranging from \$4,000 to \$12,000. Sponsored PIs also conducted tours of their labs for JSHS participants.

- ▶ Site visits to local and out of state universities that host HSAP/URAP participants: the HSAP/URAP Program Coordinator visited ten (10) host sites in North Carolina, Texas, and New York to measure program efficacy.
- ▶ STEM Expo/Fests: ARO joined the RTP STEM in the Park, a nonprofit organization that facilitates Science, Technology, Engineering and Mathematics outreach and mentoring opportunities for underrepresented minorities, during their two 2018 Expos/Fairs. Program Managers from ARO in the fields of chemistry, physics, mathematics, environmental, social and life sciences volunteered as speed mentors to an estimated 550 students ranging from grades 5 to 12 at the Frontier building in Research Triangle Park, North Carolina. The Youth Sciences Program Coordinator also staffed displays promoting Army research/technology and the AEOP at the event, including HSAP and URAP.

SCIENTIFIC SERVICES PROGRAM (SSP)

ARO established the SSP in 1957. This program provides a rapid means for the Army, DoD, OSD, and other federal government agencies to acquire the scientific and technical analysis services of scientists, engineers, and analysts from small and large businesses, colleges and universities, academics working outside their institutions, and self-employed persons not affiliated with a business or university. Annual assistance is provided through the procurement of short-term, engineering and scientific technical services in response to user-agency requests and funding. Through the SSP, these individuals provide government sponsors with scientific and technical results and solutions to problems related to R&D by conducting well-defined studies, analyses, evaluations, interpretations, and assessments in any S&T area of interest to the government.

SSP services are administered and managed for ARO through the Battelle Eastern Science and Technology (BEST) Center located in Aberdeen, Maryland, on behalf of Battelle Memorial Institute (BMI), headquartered in Columbus, Ohio. Battelle's responsibilities include the selection of qualified individuals, universities, businesses, and/or faculty to perform all tasks requested by ARO, and for the financial, contractual, security, administration, and technical performance of all work conducted under the program.

SSP awards tasks in a wide variety of technical areas, including mechanical engineering, computer sciences, life sciences, chemistry, material sciences, and military personnel recruitment/retention. In FY18, 12 new SSP tasks were awarded with 32 modifications to the scope and/or funding of ongoing tasks. A summary of the agencies served under this program and the corresponding number of FY18 new SSP tasks is provided in TABLE 3.

TABLE 3

FY18 new SSP tasks and sponsoring agencies. In FY18, 12 new SSP tasks were awarded in addition to 32 modifications of the scope and/or funding of ongoing tasks in SSP contracts.

Sponsoring Organization	SSP Tasks
CCDC (formerly RDECOM)	
Army Research Laboratory (ARL)	1
C5ISR Center (formerly CERDEC)	1
Ground Vehicle Systems Center (GVSC; formerly TARDEC)	3
TOTAL: CCDC	5
Other U.S. Army	
Headquarters Department of Army (HQDA)	2
Training & Doctrine Command (TRADOC)	1
Intelligence and Security Command (INSCOM)	1
TOTAL: Other U.S. Army	4
Other DoD	
U.S. Navy	3
TOTAL: Other DoD	3
TOTAL FY18 New SSP Tasks	12

SUMMARY OF PROGRAM FUNDING AND ACTIONS

FY18 RESEARCH PROPOSAL ACTIONS

ARO PMs receive white papers throughout the year and discuss these topic ideas with the potential investigator to identify any ways the proposed research could better align with program vision and Army needs. PMs then encourage a subset of the white papers to be submitted as full proposals; however, any eligible investigator can submit a full proposal, regardless of PM recommendations. It is rare for a potential investigator to submit a full proposal without first submitting a white paper. Approximately one-third of the white papers received by ARO PMs from academic institutions are ultimately submitted as formal, full proposals. The actions for FY18 extramural basic research white papers and full proposal submissions are summarized in TABLE 4.

TABLE 4

FY18 ARO Research Proposal Actions. The status of white papers and research proposals received by ARO within FY18 (i.e., 1 Oct 2017 through 30 Sep 2018) is listed for each scientific division, based on proposal actions reported through 8 July 2019. The table reports actions for extramural proposals in the basic research categories: SI, STIR, YIP, HBCU/MSI, MRI, MURI, and DURIP. White papers are defined as potential research concepts submitted to an ARO Program Manager for discussion and potential submission as a full proposal, in line with the process outlined in the ARO BAA.

	White Papers	Full Proposals				
	Received	Received	Accepted	Declined	Pending	Withdrawn
Chemical Sciences	375	120	46	30	44	0
Computing Sciences	128	53	29	6	18	0
Electronics	138	52	34	1	16	1
Life Sciences	367	78	42	14	21	1
Materials Science	324	96	36	40	20	0
Mathematical Sciences	215	43	8	5	30	0
Mechanical Sciences	170	81	25	31	24	1
Network Sciences	89	60	40	17	2	1
Physics	265	66	30	16	20	0
Educational Outreach	n/a ¹	190	60	127	3	0
TOTAL	2,071	839	350	287	198	4

¹White papers for projects awarded through Educational Outreach Activities were submitted through OASD(R&E) and/or the ARO division most closely aligned to each proposal's scientific discipline

SUMMARY OF ARO CORE PROGRAM BUDGET

The ARO FY18 Core (BH57) Research Program budget is shown in TABLE 5, below.

TABLE 5

ARO Core (BH57) Program funding. The ARO Core Program FY18 Budget is listed according to each scientific discipline (Division) or special program. The FY18 Allotment totals shown here are the funds ARO had received and allotted within FY18, regardless of the year of appropriation, based on the 31 Jan 2019 transactions report from the General Fund Enterprise Business System (GFEBS) and the corresponding ARO Status of Funds Report.

ARO Core (BH57) Program Type	Division or Program Title	FY18 Allotment
Scientific Disciplines	Chemical Sciences	\$9,560,857
	Computing Sciences	\$6,087,049
	Electronics	\$7,518,933
	Life Sciences	\$8,956,572
	Materials Science	\$10,179,999
	Mathematical Sciences	\$6,656,978
	Mechanical Sciences	\$8,596,961
	Network Sciences	\$7,750,872
	Physics	\$8,495,860
	SUBTOTAL: Core Program Funding by Scientific Discipline	
Special Programs	Senior Scientist Research Programs	\$486,300
	International Offices ¹	\$2,326,977
	Technology Integration and Outreach	\$869,549
	ARL General and Administrative Support	\$3,712,240
	In-House Operations	\$11,579,075
SUBTOTAL: Core Program Funding by Scientific Discipline		\$73,804,081
TOTAL ARO Core (BH57) Program		\$92,778,222

¹Includes funds for research grants monitored through ARO International PMs (refer to Section II-E)

SUMMARY OF OTHER PROGRAMS MANAGED OR CO-MANAGED BY ARO

The FY18 allotments and funding sources for other ARO managed or co-managed programs (i.e., not part of the ARO Core Program) are shown in TABLES 6-8.

TABLE 6

FY18 allotments for other Army-funded programs. These programs, combined with the ARO Core (BH57) Program elements shown in TABLE 5, represent all of the Army funds managed through ARO. The FY18 allotments include funds ARO received and allotted within FY18, regardless of the year of appropriation. Data source: ARO 31 Jan 2019 GFEBS Status of Funds Report (for FY18 funds received in FY18) and 30 Sep 2018 Status of Funds Report (for FY17 funds received in or reallocated for FY18).

Other Army-funded Program	FY18 Allotment
Multidisciplinary University Research Initiative	\$43,506,689
Presidential Early Career Award for Scientists and Engineers	\$2,399,999
Defense University Research Instrumentation Program	\$11,036,768
University Research Initiative Support	\$4,712,544
Minerva Program (Project V72) ¹	\$793,000
HBCU/MSI – PIRT Centers (Project H04)	\$1,475,000
Army Institute for Collaborative Biotechnologies (AICB; Project H05)	\$5,759,000
Army Institute for Soldier Nanotechnologies (AISN; Project J12) ²	\$6,182,091
Army Institute for Creative Technologies (AICT; Project J08)	\$6,057,000
Board of Army Science and Technology (BAST; Project C18)	\$865,646
Small Business Innovation Research (SBIR; Project M40) ^{1,3}	\$7,006,842
Small Business Technology Transfer (STTR; Project 861) ^{1,4}	\$14,002,826
SBIR/STTR Services / Contract Support (Project 720) ⁵	\$679,852
URI Congressional (D58)	\$10,000,000
TOTAL: Other Army-funded Programs	\$114,477,257

¹Does not show additional funds provided by OSD (see TABLE 8)

²Includes \$423,091 of FY17 funds received in or reallocated for FY18

³Includes \$3,044,421 of FY17 funds received in or reallocated for FY18

⁴Includes \$3,471,955 of FY17 funds received in or reallocated for FY18

⁵Includes \$35,943 of FY17 funds received in or reallocated for FY18

TABLE 7

FY18 allotment for externally-funded programs. FY18 funds received from sources other than Army or OSD are indicated below. The Other Agencies category includes funds from a range of sources, such as the Defense Threat Reduction Agency (DTRA). Data source: GFEB Status of Funds Reports from 30 Sep 2018 (for FY17 funds received in or reallocated for FY18) and 31 Jan 2019.

External Program	FY18 Allotment
Scientific Services Program (SSP) ¹	\$3,267,278
Defense Advanced Research Projects Agency (DARPA) ²	\$117,549,623
Other Agencies (e.g., DTRA) ³	\$130,149,832
TOTAL: External Programs	\$250,966,733

¹Includes \$117,989 of FY17 funds received in or reallocated for FY18

²Includes \$8,974,619 of FY17 funds received in or reallocated for FY18

³Includes \$41,859,647 of FY17 funds received in or reallocated for FY18

TABLE 8

OSD direct-funded programs. These funds were allocated directly from OSD to the indicated program. Data source: 31 Jan 2019 GFEB Status of Funds Report.

OSD Direct-funded Programs	FY18 Allotment
SBIR/STTR (Project BP0) ^{1,2}	\$427,029
Minerva ²	\$7,117,798
HBCU/MSI Research and Educational Program (REP) ³	\$27,665,000
TOTAL: OSD Direct Funding	\$35,209,827

¹Does not include additional Army funds provided for SBIR/STTR (see TABLE 6).

²This allotment was FY17 funds received in or reallocated for FY18

³This amount does not include the additional Army Core Program funds provided for the HBCU/MSI Program (see TABLE 5).

GRAND TOTAL FY18 ALLOTMENT FOR ARO MANAGED OR CO-MANAGED PROGRAMS

TABLE 9

Summary of FY18 allotment for all ARO managed or co-managed programs. This table lists the subtotals from TABLES 6-9 and the grand total FY18 allotment for all ARO managed or co-managed programs. The FY18 allotments include funds ARO received and allotted within that FY, regardless of the year of appropriation (e.g., FY18 allotment includes any FY17 funds received during or allocated for FY18). Refer to TABLES 6-9 for data source information.

Program Category	FY18 Allotment
Core (BH57) Programs	\$92,778,222
Other Army-funded Programs	\$114,477,257
External Program Funds	\$250,966,733
OSD Direct-funded Programs	\$35,209,827
GRAND TOTAL: (all sources)	\$493,432,039





CHAPTER 3 | ARO FY18 SUCCESS STORIES

This chapter provides a brief summary of the ARO Success Stories in FY18, organized by ARO Directorate, Division, and the associated program manager (PM) or other ARO staff. Each success story represents fundamental studies that will also impact one or more ARL Core Competencies, as indicated in the following table.

INDEX OF ARO FY18 SUCCESS STORIES WITH LINKS TO ARL CORE TECHNICAL COMPETENCIES

ARL CORE TECHNICAL COMPETENCIES (CTCs)

A brief description of each Core Technical Competency is provided after the table.

The CTCs are abbreviated as follows.

- ▶ Materials and Manufacturing Sciences (**M**)
- ▶ Computational Sciences (**C**)
- ▶ Ballistics Sciences (**B**)
- ▶ Human Sciences (**H**)
- ▶ Propulsion Sciences (**P1**)
- ▶ Network and Information Sciences (**N**)
- ▶ Protection Sciences (**P2**)

Success Story	Associated ARO PM/staff	Pg #	M	C	B	H	P1	N	P2
PHYSICAL SCIENCES DIRECTORATE									
CHEMICAL SCIENCES DIVISION									
Cascade Catalysis	Mantz, Stepp	34	●				●		
Electron-mediated chemistry without wires	Mantz	36	●				●		
The First Melt-Castable Energetic Co-crystal	Parker, Varanasi	38	●		●				
Development of Attosecond Pulsed Lasers	Parker, Hammond	40	●		●				
Mechanochemistry in Materials	Poree, Stepp	44	●						●
Towards Laser-Based 3D printing of Thermally Cured Polymeric Materials	Poree	46	●						
Supersoap: Development of a Non-Reactive Decontaminant	Poree, Becker, Lee	48		●					●
Nanocatalyst Communication	Poree, Becker	50	●						●
LIFE SCIENCES DIVISION									
Accelerating Learning by Defining the Neural Basis of Expert Performance	Gregory, Pasour	52				●	●		
ARO-Funded Investigator For 20 Years Awarded The 2018 Nobel Prize In Chemistry	Kokoska	55	●	●	●				●
Study of the Human Microbiome – Army Leadership within the Tr-Service Research Community	Kokoska	57	●			●			●
Artificial Cells for Novel Synthetic Biology Chassis	McElhinny	61	●						●

Success Story	Associated ARO PM/staff	Pg #	M	C	B	H	P1	N	P2
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LIFE SCIENCES DIVISION (CONTINUED)

Biologically-derived Targeted Antimicrobials for Improved Warfighter Health	McElhinny	63	●			●			●
Elemental Reducing Agents to Modulate Mitochondrial Activity and Reduce Warfighter Mortality	Strand	66							●
Pouchies, Social Biology and the Detection of Unexploded Ordnance	Strand	68							●
Path-Breaking Research in Collective Biometric Dynamics Generates New Capabilities to Identify and Track Adversarial Groups	Troyer	71		●		●		●	

PHYSICS DIVISION

Superradiance	Baker	76		●				●	
Time Crystals	Baker	78	●	●				●	
Hidden Within Quantum Devices	Gamble, Qui	82	●					●	
The Chemical Potential of Light & Synthetic Quantum Matter	Gamble	86	●					●	
A New Form of Matter and Energy, Optical / Plasma Filaments	Ulrich, Harvey	89	●	●			●		
Development and Application of Attosecond Pulsed Lasers	Hammond, Parker	93	●	●					
Impacts of A Decade Of Discoveries In Topological Physics	Ulrich, Qiu	96	●	●					
Impacts of Forty Years of Strategic Discoveries on Ferromagnetic Insulators	Ulrich	101	●	●					

ENGINEERING SCIENCES DIRECTORATE**ELECTRONICS DIVISION**

Pioneering Advances in Low Energy Information Processing	Gerhold	104		●				●	
Mitigating Atmospheric Turbulence with Modal Beam Control	Gerhold	106			●			●	
Digital Alloys Based Upon Binary Semiconductors Produce Unexpected Noise Reductions	Gerhold	107	●					●	
Pb-Salt based Detectors for Superior Uncooled Operation	Gerhold	109	●					●	
A New Form Of Matter and Energy, Optical / Plasma Filaments, Provide New Opportunities For Directed Energy Applications	Harvey, Hammond	111	●		●			●	

Success Story	Associated ARO PM/staff	Pg #	M	C	B	H	P1	N	P2
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ELECTRONICS DIVISION (CONTINUED)

New Focus Area on the Potential for Electronics to Provide New Insight into Biological Cell Internal Functionality	Harvey	115				●			●
Signature of Majorana Fermion in Topological Insulator-Superconductor Heterostructures	Qiu, Ulrich	118	●	●					
ARO-funded Scientists Expose Security Vulnerabilities in Terahertz Data Links	Qiu	120		●				●	

MATERIALS SCIENCES DIVISION

Ultrasonic Manipulation for Creation of Arrayed Reinforcement In Polymer Composites	Bakas, Stepp	123	●	●					
Fifteen Years of Nanocrystalline Alloys Research Creates High Impact Field of Structural Materials Science	Bakas	125	●	●					
Reconfigurable Materials	Prater	128	●	●					
Magnetic Resonance Force Microscopy	Prater	130	●	●					
Mechanochemistry in Materials	Stepp, Poree	133	●	●					
Tunable Shear Jamming at the Forefront	Stepp	135	●	●					
Near-Field Transport of Energy using Nanostructured Materials	Varanasi	137	●						●
Two Dimensional Materials Beyond Graphene	Varanasi	139	●	●				●	

MECHANICAL SCIENCES DIVISION

Fundamental Mechanisms of Impact Initiation of Reactive Materials	Anthenien	142			●		●		
High Pressure Auto-ignition of Hydrocarbon Fuels	Anthenien	144					●		
Building Extramural Research Partnerships to Advance Army Rotorcraft	Munson	145					●		
Leading the Field of Aerospace	Munson	147			●		●		
Operator-Theoretic Approaches to High Dimensional Dynamical Systems	Stanton	149		●			●	●	
New Science of Terradynamics	Stanton	151	●				●		●

EARTH SCIENCES DIVISION

New Foundational Science for Urban Operations	Barzyk	154		●					
Advancing Ground Mobility	Barzyk	155		●			●		

Success Story	Associated ARO PM/staff	Pg #	M	C	B	H	P1	N	P2
INFORMATION SCIENCES DIRECTORATE									

COMPUTING SCIENCES DIVISION

Interactive Computational Algorithms for Acoustic Simulation in Complex Environment and Real-World Scenes	Coyle	158	●	●					
Scalable Techniques for Modeling and Analyzing Big Spatial Data	Coyle	160		●				●	
Compressive Sensing MRI	Dai	161		●				●	
A Novel Machine Learning Algorithm for Unknown Domains	Dai	163		●				●	
Machine Learning Algorithm Discovers New Android Malware	Wang	164		●				●	●
DeepRadio: Deep Learning for Wireless Communications and Security	Wang	165		●				●	●

MATHEMATICAL SCIENCES DIVISION

Reliable Simulation of the Complex Physics of Internal Multiphase Processes	Myers	167	●	●					
Multiscale Mathematical Modeling for Design of 2D Functional Materials	Myers	168	●						
Inferring Social and Psychological Meaning in Social Media	Myers	171				●		●	
Network-based Hard-Soft Fusion	Myers	172						●	
Modeling Rare Events: Multivariate Heavy Tail Phenomena	Lavine	174		●				●	
Deterministic Approach to Solving Stochastic Partial Differential Equations	Lavine	176		●				●	
Circadian Rhythm Monitoring and Regulation	Pasour	177		●		●			●
Computational Cortical Network Model	Pasour	179		●		●			●

NETWORK SCIENCES DIVISION

Interference Alignment	Cansever	181		●				●	
Age of Information	Cansever	183		●				●	
Distributed Systems Optimization and Control	Cansever	185		●				●	
Co-evolutionary Complex Networks	Cansever	186		●				●	
Algorithmic Game Theory – Theory and Applications	Iyer	188		●		●		●	

Success Story	Associated ARO PM/staff	Pg #	M	C	B	H	P1	N	P2
NETWORK SCIENCES DIVISION (CONTINUED)									
Inferring Hidden Network Structure	Iyer	191		●				●	
Toward Predictive Modeling of Deviant Cyber Flash Mobs	Palazzolo	193		●		●		●	
Network Science of Teams	Palazzolo	195		●		●		●	
TECHNOLOGY INTEGRATION AND OUTREACH DIVISION									
The Army's Education Outreach Program STEM Initiatives	Ardouin	198				●			
Pathogen Specific Antimicrobial Coatings for Fabrics	Fox	201	●						●
DeepRadio: Deep Learning for Wireless Communications and Security	Wang	202		●				●	●
ARO Hosts DoD Workshop for HBCU/MSIs	Huff	204	●	●	●	●	●	●	●
Partnership Research Initiative (PRI) Program	Huff	205	●	●	●	●	●	●	●
Army STTR Program Partnership with USASOC	Smith	207	●						●
ARO SPECIAL PROGRAMS									
Support to Ground Vehicle Operating System (Scientific Services Program)	Ashford	208	●	●					

ARL CORE TECHNICAL COMPETENCIES (CTCs)

The ARL technical strategy provides a comprehensive vision of the future technical landscape and is a critical component of its Research Management and Leadership Strategy. Key aspects of ARL's technical strategy are the seven Core Technical Competencies (CTCs) that guide the laboratory in identifying the scientific, technical, and analytical areas of vital importance to the Army of the future. These Core Technical Competencies guide the laboratory in identifying and answering critical research questions in support of the Army's strategy for Multi-domain Operations and the required Army Functional Concepts. A brief summary of each CTC is provided in this section.

ARO's programs support each of the CTCs; however, as noted in CHAPTER 1, ARO's mission represents the most long-range Army view for changes in its technology, with system applications often 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities.



MATERIALS AND MANUFACTURING SCIENCES

Research in this CTC drives the discovery and creation of superior materials and devices needed to enable lasting strategic land power dominance. The future Army will require materials with unprecedented properties rapidly manufactured, grown, synthesized, and produced cost-effectively to enable highly mobile, information reliant, lethal, and protected Army platforms. This technology enables the Army to execute real-time, point-of-need design and fabrication thereby increasing agility and logistical efficiency from the microscale to the infrastructure scale.



COMPUTATIONAL SCIENCES

This CTC focuses on advancing the fundamentals of predictive simulation sciences, data intensive sciences, computing sciences, and emerging computing architectures to transform the future of complex Army applications. Foundational research in artificial intelligence and machine learning will enable autonomous cross-domain maneuver warfighting concepts with intelligent agents that rapidly learn, adapt, and reason faster than the adversary to fight and win in contested, austere, and congested environments.



BALLISTICS SCIENCES

This CTC focuses on gaining a greater understanding and discovery of mechanisms and on generating concepts and emerging technologies that support kinetic lethality. Knowledge and concepts gained will lead to unprecedented enhancements in weapons range, precision, and lethality for the mounted and dismounted Soldier against a spectrum of manned and unmanned ground and aerial combat systems.



HUMAN SCIENCES

This CTC focuses on identifying, creating, and transitioning scientific discoveries and technological innovations underlying Human Behavior; Human Capabilities Enhancement; and Human-System Integration that are critical to the U.S. Army's future operational superiority. Foundational research in human agent teaming provides human agent teams with the capability to perform as well as Soldier teams but with greater team resilience, faster, more informed team decision making, and reduced numbers and risk to Soldiers.



PROPULSION SCIENCES

This CTC focuses on gaining a greater fundamental understanding of advanced mobility and maneuver technologies that enable innovative vehicle configurations and subsystems architectures – critical to the future Army's movement, sustainment, and maneuverability. Foundational research in tactical unit energy independence enables energy-intelligent autonomous squad support systems that lighten the Soldier load, providing a more maneuverable, sustainable, and lethal force and intelligently monitor and distribute power on the move, reducing dismounted Soldiers' cognitive and physical load.



NETWORK AND INFORMATION SCIENCES

This CTC focuses on gaining a greater understanding of emerging technology opportunities that support intelligent information systems that perform acquisition, analysis, reasoning, decision-making, collaborative communication, and assurance of information and knowledge. Understanding gained through these research efforts will lead to technological developments that make it possible to manage, utilize, and maintain trust in information flows and geospatial situational awareness within the battlespace.



PROTECTION SCIENCES

This CTC focuses on gaining a greater understanding and discovery of mechanisms and generating concepts and emerging technologies that support protection systems that adapt to evolving threats, and the mechanisms of injury affecting the Warfighter. Foundational research in understanding and manipulating the physics of failure will lead to technologies that enable a broad array of resilient kinetic and non-kinetic protection systems and focuses on precise and accurate knowledge of materials/system failure for protection overmatch.

CHEMICAL SCIENCES DIVISION: FY18 SUCCESS STORIES

ELECTROCHEMISTRY PROGRAM



Dr. Robert Mantz

Program Manager, Electrochemistry
Chief, Chemical Sciences Division
ARO Physical Sciences Directorate

Dr. Mantz completed his undergraduate studies at the United States Air Force Academy, receiving his B.S. in Chemistry in 1989. He received his M.S. in Chemistry from California State University, Northridge in 1994, and his Ph.D. in Chemistry from North Carolina State University in 1997.

He came to ARO in 2006 as the Program Manager for Electrochemistry and was promoted to the additional role of Chief, Chemical Sciences Division, in 2017.



Dr. David Stepp

Program Manager, Mechanical Behavior of Materials
Director of Engineering Sciences
ARO Engineering Sciences Directorate

Dr. Stepp completed his undergraduate studies at Harvey Mudd College, receiving his B.S. in Engineering in 1993. He trained as a materials scientist at Duke University, receiving his Ph.D. in Mechanical Engineering and Materials Science in 1998.

He came to ARO in 1999 as the Program Manager for Mechanical Behavior of Materials and was promoted to the Chief, Materials Science Division, in 2004 and to the Director, Engineering Sciences, in 2016.

Cascade Catalysis

Drs. Mantz and Stepp recognized the efficiency of biological systems and their ability to cascade enzyme systems. The Krebs cycle is an exquisite example of a regulated enzyme cascade which biological systems use to precisely control charge and reactant transport to convert energy for the cell. Conversely, man-made systems typically involve a series of conversions with intermediate purification steps to achieve a desired product, with yield losses that compound with each step. The current approach to achieve multi-step reactions in a single reactor is an arbitrary combination of multiple catalysts that is likely to lead to poor yield with unreacted intermediates or byproducts of reactants that have reacted with the incorrect catalysts. Recent breakthroughs in materials synthesis, such as self-assembly and lock-and-key type architectures, offer control of surface arrangement and topology that enable a much more effective approach to achieving multi-step reactions through control of spatial and temporal transport of reactants, electrons, intermediates, and products.

Action

Drs. Mantz and Stepp formulated a MURI topic to drive multidisciplinary research to enable multi-step/cascade chemical and electrochemical reactions through the rational design of material architectures that control the spatial and temporal pathways of precursors, intermediates, and products.

This success supports
these ARL Core Technical
Competencies



Human Sciences



Propulsion Sciences

This resulted in an ARO MURI call focused on using biology as an inspiration for designing catalytic cascades. The overall goal of our Catalytic Cascades ARO MURI grant with Utah Science Technology and Research initiative's (USTAR) Prof. Shelley Minteer at the University of Utah is to develop integrated catalytic cascades created from different catalytic modalities such that novel scaffolding and architectures are employed to optimize selectivity, electron transfer, diffusion, and overall pathway flux. This fundamental effort has laid a framework for the production and integration of advanced catalytic systems with optimized performance.

Although the literature over the last 20 years was all focused on the need for specific materials structures (i.e., putting catalysts in close proximity or developing support structures that physical constrain the intermediate between the two catalyst active sites) to induce substrate channeling of intermediates between active sites, this MURI made a breakthrough in determining that the nano- and microscale chemical environment of a catalyst or multicatalyst structure is the PRIMARY factor for both catalytic activity and substrate channeling. The MURI demonstrated that biomolecular scaffolds with binding properties to the reactant of interest can enhance enzyme catalysis by increasing the local concentration of reactant. This current work shows that upward of 10-fold enhancement in reactant binding, and consequently reaction rate at low bulk reactant concentrations, can be obtained when enzymes are modified with designed DNA scaffolds, as shown in Figure 1. This is impressive, because directed evolution of enzyme activity can rarely get a 10-fold increase and materials design of better catalysts or catalyst cascades is usually confined to doubling turnover rate.

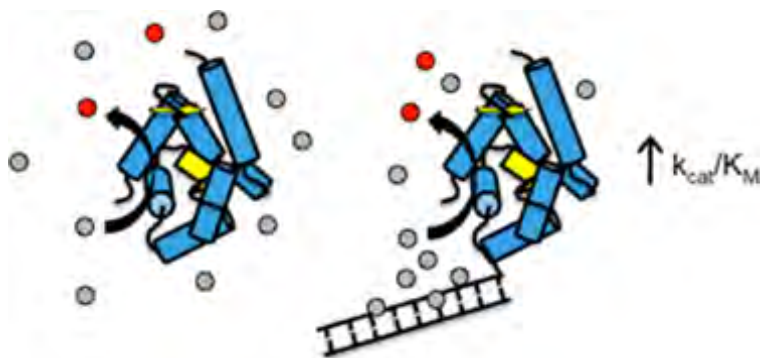


Figure 1. When a DNA scaffold is added to an enzyme (right side), it changes the chemical microenvironment around the active site of the enzyme to increase reactant binding and therefore catalytic rate.

The ARO program managers saw this new breakthrough as a game changer in the field of catalysis, so they have helped this MURI team move this theme into a variety catalytic cascades to improve performance. For instance, the ARO program managers Robert Mantz and David Stepp provided add-on funding to the team to combine this catalytic strategy with covalent attachment of intermediates. This “swing arm” engineering research demonstrated a second mechanism to control local substrate pools and enhance catalytic rates. The MURI team has also demonstrated that intermediate channeling can be engineered and enhanced by controlling the local electrostatic charge separating two catalysts of a cascade. This MURI has shown that catalytic rates can be dramatically enhanced by more than an order of magnitude simply by altering the nano- and/or microscale chemical environment of a catalyst without actually altering the catalyst itself, which was a previously unknown engineering tool for catalysis. These studies provide a set of design rules for scientists and engineers developing catalysts for all Army applications ranging from synthesis to fuel oxidation to decontamination.

SUCCESS

Ability to design and control multi-step/cascade chemical and electrochemical reactions through the rational design of material architectures that control the spatial and temporal pathways of precursors, intermediates, and products.

RESULTS

- ▶ 19 peer-reviewed publications
 - ▶ ARL funded PhD now employed at PNNL
 - ▶ New collaborations with Redstone Arsenal and CCDC Chemical Biological Center
 - ▶ Transitioned nitrogenase technology to Fulcrum – currently funded DOE STTR Phase II after successful DOE STTR Phase I last year
 - ▶ Transitioning technology to Abbvie which is evaluating TEMPO immobilization strategies
-

This success supports these ARL Core Technical Competencies



Human Sciences



Propulsion Sciences

SUCCESS

New understanding of the influence of external photon, electron and plasma fluxes on catalytic processes, as well as underlying physical phenomena that occur at catalytic interfaces.

Result

The MURI team developed a series of biological, organic, and inorganic catalysts that operate in concert under mild conditions. These catalysts were designed to be synergistic, including oxalate decarboxylase, nitroxyl radicals, and precious metal electrocatalytic materials (i.e., Pd nanoclusters, graphene based atomically-dispersed transition metal electrocatalysts, and organometallic reductive catalysts). The MURI team has developed and published a series of design principles to fabricate materials that enable efficient substrate channeling in a variety of catalytic cascades. These include DNA, proteins, polymers, and nanostructured composite scaffolds. Such scaffolds can improve catalytic microenvironments, induce bounded diffusion, sequester cofactors, and ensure compartmentalization to increase the efficiency of catalytic cascades. These design rules can be broadly applied to a range type of complex chemical transformations (biological, inorganic, electrocatalysis, and photocatalysis) that are of interest to DoD.

Way Ahead

Dr. Minter and her team is focusing their future efforts on developing the capability to engineer enzyme microenvironments as another tool to increase enzyme activity. They have also developed collaborations with Fulcrum Bioscience base on their nitrogenase technology and Abbvie which is interested in TEMPO immobilization strategies.

Electron-mediated chemistry without wires

The Army relies on compact power sources to support many different weapons systems, communications, and other devices. This program is focused on fundamental research that may provide the foundation for developing advanced power generation and storage technology. Specifically, electrochemical power generation and storage processes often involve catalytic chemical conversion processes at metal electrodes. Inherent limitations exist in these technologies, specifically with the operation of such devices with sufficient power fluxes at ambient temperatures. The development of approaches to promote electrochemical processes at ambient temperatures is of critical importance for promoting efficiency.

Action

Dr. Mantz recognized recent advances in the use of photons (from LEDs or solar energy flux) to promote catalytic processes and nanostructured metal surfaces and sponsored a workshop on the topic at Rice University in 2014. During this meeting, Assistant Prof. Phillip Christopher gave a lecture the selective activation of Pt-CO bonds using visible photon excitation. Based on this lecture, Dr. Robert Mantz discussed with Prof. Christopher the ideas that would ultimately be funded through an ARO YIP grant to understanding photon driven chemistry at nanostructured metal surfaces and has grown to compare various non-thermal approaches for promoting catalytic processes via laser, electron beam, and non-thermal plasma excitation.

The work by Prof. Christopher in this area has played a role in the development of a new direction in the ARO Electrochemistry Program focused on “electrode-less electrochemistry.” Through this work collaborations have been sparked to visualize the transformation of nanostructured metal catalysts under reaction conditions and explore the use of semiconductors for promoting photon-mediated chemistry at nanostructured metal surfaces. Further, Prof. Christopher has had many informal discussions with ARL scientists on how photons could be used to promote alcohol electro oxidation rates. Prof. Christopher was recently awarded the Presidential Early Career Award for Scientists and Engineers (PECASE) to continue efforts described above.

Result

The overall objective of this research is to develop a holistic understanding of catalysis by photoexcitation of adsorbate-metal bonds on metal nanoparticle surfaces and the know how to exploit this phenomenon to manipulate reaction selectivity in a rational manner (Figure 1). Prof. Christopher's Group identified that unique photon mediated mechanisms for controlling catalytic processes exist on small metal nanoparticle surfaces. Specifically, the adsorption of molecules to metal nanoparticle surfaces creates hybridized metal-molecule orbitals that can be directly photo excited to induce chemical conversions. These electronic transitions are unique to each molecule and can be exploited to selectively deposit the energy of a photon flux into a targeted reaction pathway. This was demonstrated for the case of targeted activation of Pt-CO bonds instead of Pt-O bonds and to control selectivity in the preferential CO oxidation. These results are interesting in the context of various reactions, including low temperature electro-oxidation of alcohol fuels where in-situ produced CO poisons catalytic surfaces and minimizes power production rates. The use of nanostructured metal catalysts and direct photo-excitation of metal-CO bonds may enable enhancements in low temperature power production efficiency.

These initial findings were expanded on to more complicated reactions such as benzyl alcohol dehydrogenation, benzyl amine oxidative coupling, and heck coupling demonstrating the use of this approach to control a range of chemistries over small metal nanoparticles. This work provided strong evidence that photons could be used to control the outcome of catalytic processes at nanostructured metal surfaces via energy deposition into targeted reaction pathways.

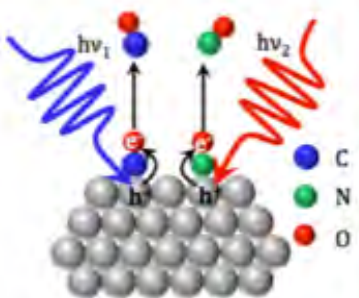


Figure 1. Direct photoexcitation of metal-adsorbate bonds at nanostructured metal surfaces. The schematic highlights how photons provide a bond specific mechanism of promoting catalytic processes.

Overall, Prof. Christopher's research focus has resulted in the development new understanding of the influence of external photon, electron and plasma fluxes on catalytic processes, as well as underlying physical phenomena that occur at catalytic interfaces. These findings have the potential for promoting electrochemical conversion processes that are key to Army missions.

Way Ahead

Prof. Chrostopher is expanding his work to include other chemical systems such as nitrogen oxide, carbon monoxide, methane, and methanol under non-thermal excitation conditions using photon or electron excitation. Prof. Chrostopher is also having discussions with Jonathan Boltersdorf (ARL) on the use of plasmon excitations to promote electrochemical alcohol oxidation.

ELECTROCHEMISTRY PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Synthesize and characterize new electrolyte species to enable advanced power storage and generation devices.
- ▶ Understand transport in heterogeneous charged environments to allow selective control of transport of species enabling advanced sensors, protective gear, fuel cells, etc.
- ▶ Understand how material and morphology affect electron transfer and electrocatalysis to enable synthesis, oxidation, and reduction of Army relevant materials and energy systems.
- ▶ Explore new methods of controlling electrochemistry to enable creation of novel materials.

RESULTS

- ▶ Demonstrated that near fields at metal surfaces can be influenced by adsorbates and can drive catalysis
- ▶ New methodology to efficiently and selectively drive chemical conversion processes at metal nanoparticle surfaces through non-thermal excitation mechanisms
- ▶ New collaborations with ARO
- ▶ Ongoing collaborations with Naomi Rice and Peter Nordlander (Rice), Stephen Cronin (USC), and Tony Murphy (CSIRO)

MOLECULAR STRUCTURE AND DYNAMICS PROGRAM



Dr. James Parker

Program Manager, Molecular and Structure Dynamics
Chemical Sciences Division
ARO Physical Sciences Directorate

Dr. Parker completed his undergraduate studies at Marquette University, receiving his B.S. in chemistry in 1993. He trained as a physical chemist at the University of Mississippi, receiving his Ph.D. in physical chemistry in 1999.

He came to ARO in 2009 as the Manager for what was then called the Physical and Theoretical Chemistry Program.



Dr. Chakrapani Varanasi

Program Manager, Physical Properties of Materials
Division Chief, Materials Science
ARO Engineering Sciences Directorate

Dr. Varanasi completed his M.S. in Materials Science and Engineering at the Indian Institute of Technology, Kanpur, India in 1990. He trained as a Materials Scientist at the University of Notre Dame, IN, receiving his Ph.D. in Materials Science & Engineering in 1994.

He came to ARO in 2009 as the Manager for the Physical Properties of Program and was promoted to Chief, Materials Science Division in 2017.

The First Melt-Castable Energetic Co-crystal

Scientific Challenge

Liquid stability is important for explosives as it enables manufacturers to easily and safely cast the explosive into the desired shape (aka melt-castable). Despite being first synthesized over 150 years ago, TNT remains the most commonly used melt-castable explosive because most other energetic compounds, although more powerful, are not stable in liquid form.

Action

In the year 2011, a MURI topic on molecular co-crystals was conceived of while speaking with Dr. Suithi Peiris (then at the Defense Threat Reduction Agency; DTRA) about the potential of the idea. Encouraged by the discussion I set out to develop the topic with a focus on energetic materials. I then approached Chakrapani Varanasi of the Material Sciences division for his feedback. He made critical suggestions about including ferroelectric and non-linear optical materials as focus areas, since opportunities for progress in these areas existed by exploiting molecular co-crystals. The topic went forward with Varanasi as co-PM and was awarded in 2013 to the University of Michigan with Professor Adam Matzger as the Principal Investigator.

It was thought that physical and chemical properties such as density, sensitivity, explosive velocity, ferroelectricity, and propensity for frequency doubling could be tuned by formation of co-crystals with suitable molecular partners. In contrast to traditional crystallization, research in co-crystallization explores if and how two different compounds can be combined to form a crystal that incorporates both compounds with improved properties versus either component alone.

This success supports these ARL Core Technical Competencies



Materials and Manufacturing Sciences



Ballistics Sciences

SUCCESS

This ARO initiative resulted in the discovery of co-crystals that change the properties of an unstable explosive, enabling it to be safely melted and poured for potential Army applications

Result

This story recounts a particular success that was not envisioned by us: the formation of a melt-castable energetic co-crystal. This story demonstrates that the future cannot be accurately predicted, but it also sometimes comes with fortunate surprises.

Professor Matzger, along with co-investigators Jonathan Bennion (graduate student) and Zohaib Siddiqi (graduate student), prepared an energetic co-crystal between two energetic precursors: 3,4-diaminofurazan (DAF, melting point 177°C) and 4-amino-3,5-dinitropyrazole (ADNP, decomposition at 173°C; see Figure 1). The material is remarkable because interaction between the components leads to melting behavior and melt-state stabilization (absent in ADNP), that allows a melt-castable formulation with explosive performance superior to DAF alone (see Figure 2). This is important because industrially, there are two methods for loading of energetic materials into a munition: (1) hydraulic pressing and subsequent milling of a pure or formulated energetic to required dimensions, and (2) melting and casting (pouring) of a pure or formulated energetic directly into a munition. In addition to the advantage of reducing void space in the munition resulting in density approaching the theoretical limit, the process of melt casting has many added benefits over hydraulic pressing, including greater processing efficiency and allowing for more complex arrangements to be configured within the munition. An ideal melt-castable material should possess a low melting point (70 - 120°C), large range between the melting point and the start of decomposition, and high loading density. It is also very interesting to note that melt phase stabilization allows casting of a thermally unstable molecule (ADNP), revealing yet another advantage of the co-crystal approach to high performance explosives which had not been anticipated. In its pure form, ADNP undergoes decomposition at its melting point of 173°C.

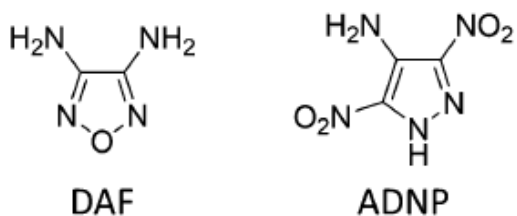


Figure 1. Molecular structures of 3,4-diaminofurazan (DAF) and 4-amino-3,5-dinitropyrazole (ADNP).

This discovery of the co-crystal was recently featured on the cover of the journal *Chemical Communications* [DOI: 10.1039/c7cc02636f]. The scientific article details how the thermally labile explosive ADNP, which was previously limited due to thermal decomposition, could be co-crystallized with another energetic compound resulting in a new explosive material which is stable in liquid form in the temperature range of 162 – 212°C.

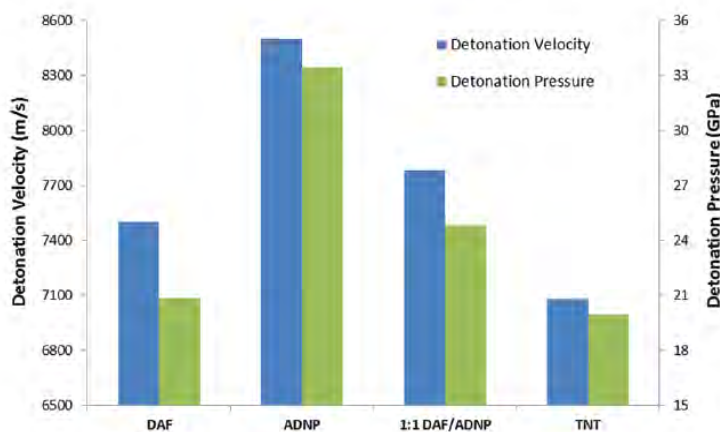


Figure 2. Detonation parameters (velocity and pressure) of DAF, ADNP, 1:1 DAF:ADNP, and TNT were predicted with Cheetah 7.0 using the room-temperature (295 K) crystallographic densities of each material.

RESULTS

- ▶ Co-publication between Army and academic researchers
- ▶ Academic researcher hired by ARL to provide the Army with in-house expertise in this area
- ▶ Co-crystals transitioned to CCDC Armaments Center for characterization and to explore potential new manufacturing methods
- ▶ Discovery of a new class of ferroelectric compounds that are now part of a new ARO initiative into tunable electronic materials

This success supports these ARL Core Technical Competencies



Materials and Manufacturing Sciences



Ballistics Sciences

Way Ahead

ARDEC has received samples of this new co-crystallized compound for detailed characterization of its explosive properties and the potential development of new manufacturing methods for explosives and propellants. A researcher from the EBRC academic laboratory was also hired at ARL-WMRD as a postdoctoral fellow, thereby bringing this expertise to Army in-house laboratories.

The potential Army impact of this research is the use of this new co-crystallization method to harness the latest classes of explosives that may have been dismissed for certain applications due to their instability.

This research also led to the discovery of a new family of tunable organic crystalline ferroelectric materials whereby non-ferroelectric compounds are co-crystallized, resulting in properties not possible with either compound alone. Dr. Varanasi has expanded his program's portfolio to advance this new discovery that in the long term could be integrated with organic electronics through a novel approach of solid-solutions of co-crystals. If successful, this work could develop basic understanding of ferroelectric co-crystal design principles and may also discover new organic ferroelectric materials with unique tunability that can be easily integrated into lightweight organic electronic devices that could replace heavier, more expensive, more power intensive conventional inorganic materials. Although commercial applications based on organic electronic materials are being developed, organic ferroelectrics are still yet to be discovered to replace the currently used inorganic ferroelectrics.

Development and Application of Attosecond Pulsed Lasers



Dr. James Parker

Program Manager, Molecular and Structure Dynamics
Chemical Sciences Division
ARO Physical Sciences Directorate

Dr. Parker completed his undergraduate studies at Marquette University, receiving his B.S. in chemistry in 1993. He trained as a physical chemist at the University of Mississippi, receiving his Ph.D. in physical chemistry in 1999.

He came to ARO in 2009 as the Manager for what was then called the Physical and Theoretical Chemistry Program.



Dr. Richard Hammond (Retired)

Program Manager, Optics
Physics Division
ARO Physical Sciences Directorate

Dr. Hammond completed his undergraduate studies at New Jersey Institute of Technology, receiving his B.S. physics in 1973. He trained as a physicist at Rensselaer Polytechnic Institute, receiving his M.S. and Ph.D. degrees in optics in 1979.

He came to ARO in 2002 as the Program Manager for Optics, and retired from ARO in June 2019.

Scientific Challenge

To develop and apply transient absorption spectroscopy in the attosecond time range for understanding the earliest time processes in electronic excitation in molecules and materials.

Action

In 2005, Richard Hammond, a Program Manager in Physics, submitted a MURI topic on the development of attosecond lasers (10-18 s). Professors Margaret Murnane (U. of Colorado), Henry Kapetyan (U. of Colorado), and Paul Corkum (National Research Council of Canada), had each contributed to the understanding of high harmonic generation, a process in which focused infrared radiation impinging on a noble gas sample causes the atoms to emit high-energy attosecond bursts of radiation. This discovery eventually brought laser pulse times from the femtosecond regime, where they had stalled since about the year 1980, into the attosecond regime (see Figure 1). At the time, Hammond's MURI topic was thought to be too ambitious, but Hammond argued aggressively for the topic and was able to get it approved. The award went to a relatively unknown physicist, Zenghu Chang at Kansas State University, and within the time frame of the MURI Chang had the world's record shortest pulse at 72 attoseconds.

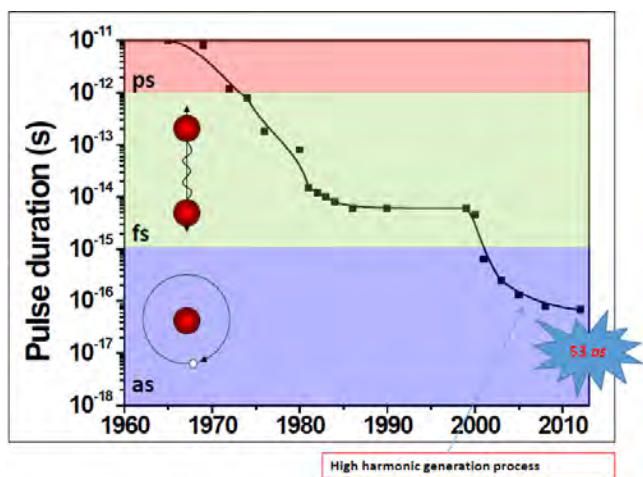


Figure 1. Shortest available laser pulse duration as a function of year.

Hammond was not satisfied yet, and he wanted to develop a whole new world of spectroscopy that would be allowed by these ultrashort laser pulses. Bringing together world's experts, Hammond held a workshop to determine the next steps. The conclusion was that the attosecond pulses needed more photon flux, and should be applied to the study of effects in solid materials. To achieve these goals Hammond funded a single investigator award to the University of Central Florida, where Chang was a faculty member by then, to produce high-flux, isolated attosecond pulses. Within a few years they set the world's record on making the shortest laser pulse, 53 attoseconds. By now, Chang was an international leader in ultrashort laser physics. With the success of this program, everything was in place to use the high-energy, ultrashort pulse to open a new door in the study of molecules and materials.

At this time James Parker, a Program Manager in Chemistry, was looking for a way to study ultrashort electronic phenomena in molecules and recognized the need for attosecond lasers. Parker and Hammond jointly developed a MURI topic on Attosecond Electron Dynamics whose objective was to increase the power of attosecond pulses and to apply them to the study of molecular electronic processes. At the same time, Enrique Parra of the Air Force Office of Scientific Research independently proposed a MURI topic on studying the effects of attosecond pulses on materials. The two MURIs were awarded in 2014. The Army MURI went to the University of California, Berkeley with Professor Stephen Leone as the Principal Investigator and with Chang among

Attosecond beamline at Berkeley

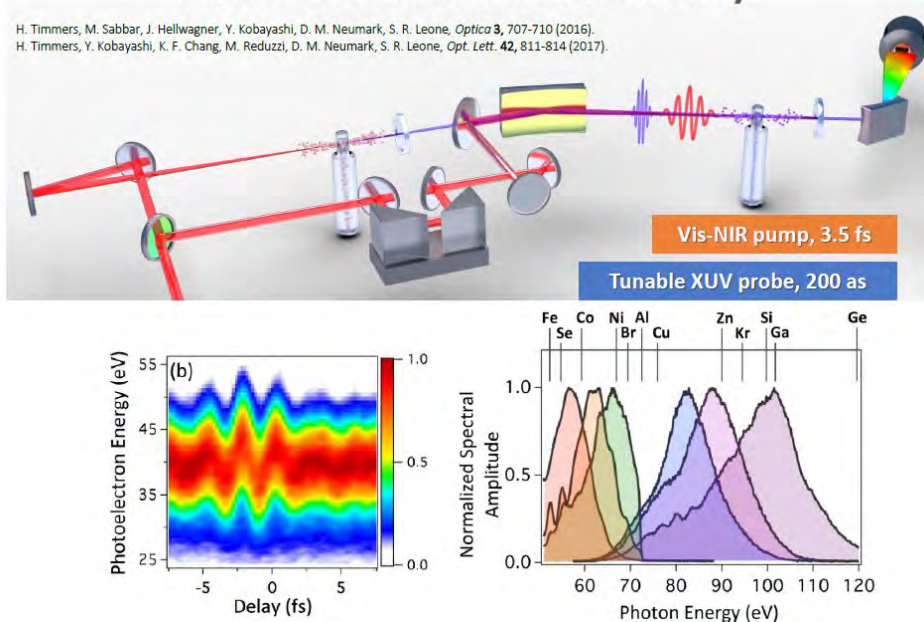


Figure 2. Schematic of the attosecond transient absorption spectroscopy technique showing the range of photon energies available, coinciding with numerous L, M, and N-edge electron binding energies of chemically relevant elements.

SUCCESS

This ARO initiative resulted in the development of attosecond science for probing the electron dynamics in molecules on the natural timescale of the electron, approximately 50 attoseconds.

RESULTS

- ▶ URI team holds the world's shortest laser pulse of 53 as
- ▶ The role of conical intersections for non-adiabatic transitions and resulting reactions impacts understanding of the chemistry of energetic materials
- ▶ Understanding charge migration on the attosecond timescale in nanoparticles aids in the development of more efficient devices for solar energy conversion

the co-PIs on the team. The AFOSR MURI went to the University of Central Florida with Professor Zenghu Chang as the Principal Investigator and with Leone among the co-PIs on the team. A major accomplishment of the Army MURI was the development of the attosecond transient absorption spectroscopy technique (see Figure 2), which has been applied to study a variety of physical processes: probing dark states in oxygen, discovering signatures of light-induced conical intersections, observing electronic coherences in atomic ions, resolving surface crossing dynamics in ethylene, observing strong field-induced dynamics in methyl bromide, understanding how conical intersections can lead to branching in chemical reactions, studying Auger phenomena in real time, and understanding intramolecular charge migration at the moment a molecule absorbs a photon.

Result

The Army MURI topic on the development of attosecond sources and their applications to the study of molecules and materials have yielded a plethora of physical information about the electron dynamics in atoms and molecules at this timescale. Areas where significant progress has been made include development of attosecond transient absorption spectroscopy (ATAS) to probe valence reaction dynamics in atoms, molecules, and solids on timescales approaching the electronic domain, understanding charge migration in nanoparticles, development of velocity map imaging for studying electronic structure changes when a molecules absorbs a XUV pulse, driving laser development, new polarization gating techniques for attosecond pulses, extending theory for charge migration in molecules, and development of new theory for light-induced conical intersections.

As an example of a scientific result from ATAS, let us consider non-adiabatic molecular dynamics initiated by strong field excitation. The investigators have been studying the fragmentation of methyl bromide (CH_3Br) as the molecule relaxes through multiple conical intersections. In the experiment, a few-cycle NIR pulse is used for strong-field

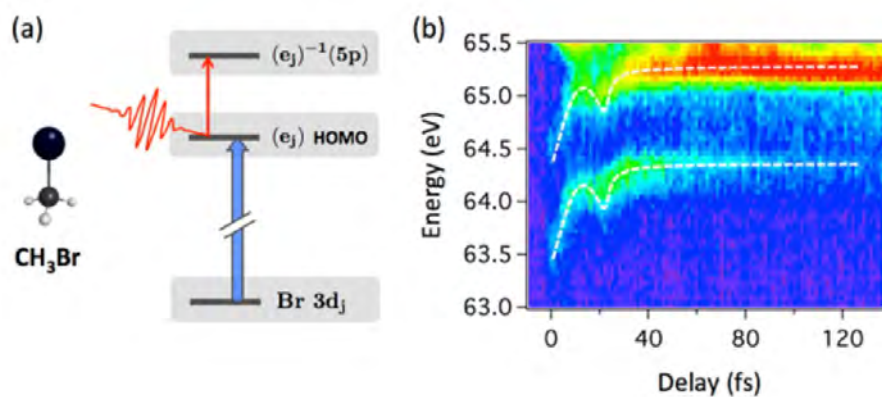


Figure 3: (a) Experimental probing scheme for probing non-adiabatic dynamics in methyl bromide. (b) Experimental ATAS trace in methyl bromide depicting non-stationary motion of Rydberg absorption lines.

excitation of the molecule to the 5p Rydberg state (Figure 3a). As the Rydberg state relaxes and breaks apart through a series of conical intersections, the quantum state of the system is probed by resonantly exciting the Br 3d inner-shell electron with a time delayed attosecond pulse to fill the HOMO hole in the excited molecule. The resulting ATAS trace is depicted in Figure 3b. The non-stationary, energetic motion of the absorption features is representative of the non-adiabatic motion of the excited state wavepacket as it passes through multiple conical intersections. The superb temporal and energy resolution of ATAS is paramount for probing such a transient molecular reaction.

The information obtained from this MURI has proven extremely valuable for understanding ultrashort time scale phenomena which occur on the timescale of the motion of bound electrons and will continue to be of high value for future studies.

Way Ahead

It is possible that scientists at ARL/SEDD will adopt the attosecond techniques described here to study Army relevant problems in photovoltaics, energy storage, and detonation chemistry. These attosecond techniques require specialized training for their implementation, and it is likely therefore that ARL could hire graduate students or post-docs who graduate from this MURI.

MOLECULAR STRUCTURE AND DYNAMICS PROGRAM –CURRENT SCIENTIFIC OBJECTIVES

- ▶ Achieve control for state-to-state chemical reactions, quantum state preparation, and intermolecular interactions that if successful, will enable future technologies in keyed detonation of explosives, sensitive and selective chemical threat detection at range, synthetic routes to new energetic materials, and support applications in quantum computing, solar
- ▶ Develop attosecond spectroscopic methods and utilize them to understand electron dynamics and associated phenomena in atoms, molecules, and materials that if successful, will enable future technologies in plasmonics, solar voltaics, energetic materials, and catalysis.
- ▶ Model and explain novel dynamics phenomena, including reaction mechanisms and electron-transfer rates that if successful, will enable a deep understanding of chemical kinetics, thermochemistry, and catalysis. This information will help to close the gap between how chemical structure and physical properties relate.

POLYMER CHEMISTRY PROGRAM



Dr. Dawanne Poree

Program Manager, Polymer Chemistry
Program Manager (Acting), Reactive Chemical Systems
Chemical Sciences Division
ARO Physical Sciences Directorate

Dr. Poree completed her undergraduate studies at Nicholls State University, receiving her B.S. in Chemistry in 2004. She trained as a polymer chemist at Tulane University, receiving her Ph.D. in Chemistry in 2010.

She came to ARO in 2011 as a SETA Contractor to support the Polymer Chemistry Program and was hired as the Program Manager in 2014. In addition, Dr. Poree has served as the Program Manager (A) for Reactive Chemical Systems since 2014.



Dr. David Stepp

Program Manager, Mechanical Behavior of Materials
Director of Engineering Sciences
ARO Engineering Sciences Directorate

Dr. Stepp completed his undergraduate studies at Harvey Mudd College, receiving his B.S. in Engineering in 1993. He trained as a materials scientist at Duke University, receiving his Ph.D. in Mechanical Engineering and Materials Science in 1998.

He came to ARO in 1999 as the Program Manager for Mechanical Behavior of Materials and was promoted to the Chief, Materials Science Division, in 2004 and to the Director, Engineering Sciences, in 2016.

Mechanochemistry in Materials

Challenge

Structural materials are inherently susceptible to damage, and this damage is usually in the form of cracks that can occur deep within the structure where detection is difficult and repair is almost impossible.

The concept of a material that could repair or heal itself when subjected to force or damage has long captivated the chemistry and materials science research communities. Self-healing materials research blossomed under the National Nanotechnology Initiative and into the early 2000's. However, this work was based on classical composite designs and traditional manufacturing strategies, and was therefore limited to additive approaches that required a "payload" to drive self-healing. What disruptive opportunities might the frontiers of materials science or chemistry provide? Could a molecular-scale mechanism be discovered?

The Army Research Office began an initiative in 2006 that strategically pursued answers to these questions.

Action

Sensing an opportunity for a disruptive breakthrough, ARO Mechanical Behavior of Materials program manager David Stepp and Polymer Chemistry program manager Doug Kiserow organized a unique workshop in January 2006 to bring internationally renowned researchers in the areas of self-healing and self-repairing polymers and materials together with DoD scientists and engineers to establish emerging research

This success supports
these ARL Core Technical
Competencies



Materials and
Manufacturing Sciences



Protection Sciences

opportunities. The workshop was organized for academic researchers to give tutorial presentations to highlight recent findings and approaches in their respective areas, Army and DoD attendees to describe potential applications in DoD for self-healing materials, and ARO program managers to actively moderate in-depth discussion by all attendees. This workshop identified a particular opportunity in the area of productive mechanochemistry where forces induced by mechanical stress could be harnessed and used to drive pre-defined, beneficial chemical reactions. More specifically, this opportunity was manifested in such research targets as: new compositions of matter; mechano-chemical transduction; molecular reconfiguration before failure; and advances in reversible chemistry.

Drs. Stepp and Kiserow devised the first ever multidisciplinary research opportunity at the forefront of materials and mechanochemistry, calling for “molecular dynamic and thermodynamic theory to be extended to describe mechanochemical transduction, to develop predictive computational methodologies, and to guide the rapid design and synthesis of novel mechanophores.” This opportunity not only defines the etymology of “mechanophore” (a force-activated molecular unit), but captured the imagination and attention of researchers internationally who envisioned the ability to embed these force-activated molecules into polymeric materials to realize a range of new materials with Army-relevant functional capabilities such as early-warning indicators for failure and the ability to remodel and strengthen in response to mechanical stress. ARO funded research soon produced the first-ever demonstration of mechano-responsive behavior in a solid-state material, when the spiropyran mechanophore was demonstrated to undergo a stress-induced conversion to merocyanin, resulting in an inherent and reversible color change in the region of damage (Figure 1). In recognition of this breakthrough, ARL-ARO was invited to organize and chair a Mechanochemical Transduction Convergence Workshop. This workshop served as a model study for scientific research forecasting, building upon the concept of research convergences in the advancement of science, and was published by the Center for Technology and National Security Policy at National Defense University.

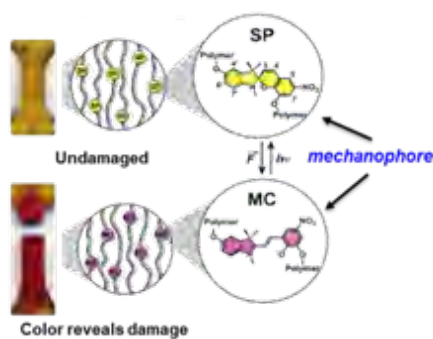


Figure 1. First demonstration of mechano-responsiveness in solid-state materials

Continued Army leadership and investment in this field by ARO program managers Dawanne Poree and David Stepp, integrating Polymer Chemistry and Mechanical Behavior of Materials respectively, has positioned the Army at the forefront of this research community. Symposia at major professional societies have begun to emerge (including Mechanochemistry in Materials Science at the Materials Research Society in Fall 2009 and Fundamental Studies of Mechanochemical and Tribochemical Processes at Interfaces at the American Chemical Society National Meeting in

2017). Furthermore, mechanochemistry has emerged as a powerful methodology in the search for sustainable alternatives to conventional solvent-based synthetic routes that has received broad support from federal and international funding agencies.

Result

More recently, ARO extramural research investments have led to the development of new mechanophores with novel functional outputs including the ability to undergo a complete change in material properties by incorporating multiple mechanophore units in a single polymer chain. In particular, researchers at Stanford University have developed a unique polymechanophore system, termed polyladderane, which undergoes

SUCCESS

Initiating the first ever research effort to exploit mechanochemistry in materials led to new polymers that self-report damage and can be transformed from insulating to conducting with the application of force, and are expected to enable new classes responsive polymers for self-healing structural materials, adaptive fabrics, and self-repairing electronics.

RESULTS

- ▶ Defined the new term “mechanophore” (a force-activated molecular unit) that captured the imagination and attention of researchers internationally.
- ▶ First-ever demonstration of a stress-induced molecular conversion that resulted in an inherent and reversible color change in the region of damage.
- ▶ First-ever demonstration of transforming a polymer from insulating to conducting with the application of force.
- ▶ Positioned the Army at the forefront of this research community.

a force-induced rearrangement to polyacetylene. This effort received extraordinary acclaim when it successfully demonstrated transforming a polymer from insulating to conducting with the application of force. In 2018, this research team further showed that these responsive poly ladderanes could be copolymerized with other commodity polymers which would impart stress-responsive capabilities to a diversity of materials that are not mechano-responsive on their own (Figure 2). The ability to extend this unique mechano-responsive behavior to more practically used polymers now enables new classes responsive polymers for use in a wide-range of applications, such as self-healing structural materials for Army vehicles or aircraft, breathable fabrics for uniforms that detect chemical agents and automatically close pores to protect the Soldier, and electronic components that self-repair or are programmed to deactivate if captured.

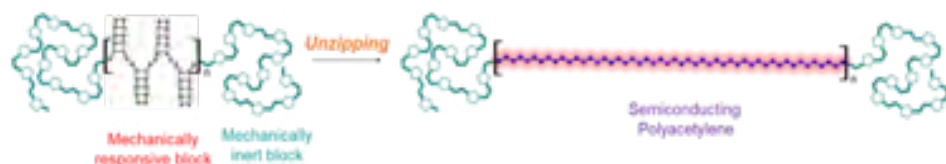


Figure 2. Mechanoactivation of poly ladderane-containing copolymer

Way Ahead

The next objective in this effort is to target scale-up and integration of mechanochemistry into bulk materials more broadly. Collaborations with ARL-WMRD, CCDC Soldier Center, and DARPA are exploring new paradigms for detecting damage in composite structures and to revolutionize additive manufacturing and 3D printing with mechanochemistry and mechanophores. Additional collaborations with ONR are exploring opportunities to amplify the effects and sensitivity of force activation in bulk materials.

Towards Laser-Based 3D printing of Thermally Cured Polymeric Materials

Challenge

There is currently much interest in 3D printing of materials as 'on demand' means of manufacturing useful devices promises to revolutionize fields such as machining, medicine, and consumer goods, to name a few. 3D printing may be particularly enabling for DoD applications where manufacturing at the point of use may provide unique capabilities and ease supply chain and logistics issues. Though significant advances in 3D printing have been made, there remain several classes of materials for which additive manufacturing has yet to be realized.

Action

In 2015, recognizing the ubiquitous nature of polymeric materials and lack of additive manufacturing techniques amenable to their use, ARL-ARO Polymer Chemistry program manager Dr. Dawanne Poree began focusing programmatic resources on novel approaches for integrating functional polymeric materials with additive manufacturing processes.

Of particular interest were thermally cured thermoset polymers. These polymers are widely used, and include materials such as epoxy resins, polyurethane, and polydimethylsiloxane (PDMS) that possess a myriad of industrial and military-relevant applications. The difficulty in 3D printing these materials largely stems from a need for extremely rapid (sub microsecond) heating/cooling cycles that span large (thousands

This success supports these ARL Core Technical Competencies



Materials and Manufacturing Sciences

SUCCESS

Developed a laser-based photothermal curing methodology that can be harnessed to additively manufacture thermally cured thermoset polymers, a class of widely used materials with a myriad of industrial and military-relevant applications.

of degrees) temperature changes – a requirement that cannot be easily met using conventional heating. To address this challenge, Dr. Poree strategically supported researchers at Pennsylvania State University to develop a unique methodology that utilizes the photothermal effect of nanoparticles to provide the rapid heating and cooling cycles required for precise control over polymerization in time and space (Figure 1a).

Results

The laser-based photothermal curing method enabled heating of the monomers by over 1,000 degrees in less than one second, resulting in an enhanced rate of polymerization by a factor of one billion versus a traditional thermal curing process, providing an underlying technology that could be harnessed to 3D print thermally cured thermoset polymers (Figure 1b). In FY18, the research team was awarded instrumentation funding to construct a printer that will leverage the photothermal curing process to enable a practical demonstration of additively manufactured objects of thermally cured thermoset materials with micron resolution which may ultimately lead to more rapid and economical manufacturing creation of protective coatings, structural elements, wound-dressings, and textiles.

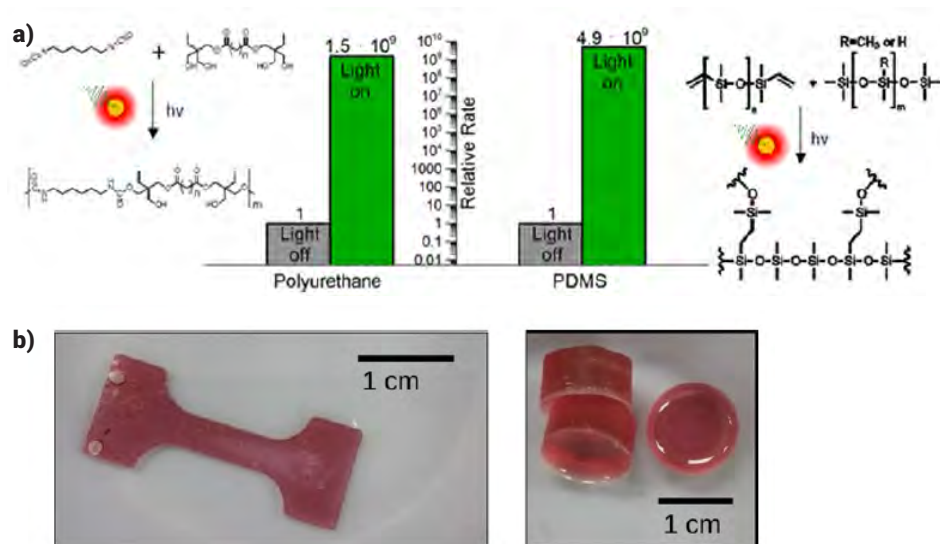


Figure 1. a) Photothermal effect of nanoparticles provides billion-fold enhancement to the rate of curing for both poly(urethane)s and poly(dimethylsiloxane)s; **b)** Images of bulk-scale objects made of PDMS cured using high power pulsed YAG systems and the team's photothermal approach.

Way Ahead

The investigators recently launched the company Actinic to transition this method to industry to determine how this method could be scaled for use in additive manufacturing methods. Collaborative efforts among ARL-ARO, ARL-WMRD, and CCDC-SC will be sought and leveraged to transition key knowledge products towards the development of new functional materials for coatings, structural elements, wound-dressings, and fabrics.

POLYMER CHEMISTRY PROGRAM – CURRENT SCIENTIFIC OBJECTIVES

- ▶ Create polymers with precise control over molecular structure and composition, and explore how molecular structure impacts morphology and properties.
- ▶ Devise strategies to control polymer assembly to render complex functional materials.
- ▶ Create polymeric materials that exhibit precise, programmed responses to external stimuli.

RESULTS

- ▶ Laser-based photothermal curing method enabled heating of monomers by over 1,000 degrees in less than one second, resulting in an enhanced rate of polymerization by a factor of one billion versus a traditional thermal curing process
- ▶ Investigators started a small business Actinic LLC to transition this photothermally driven chemistry method to industry, with initial efforts focused on how this method could be scaled for use in additive manufacturing methods.

REACTIVE CHEMICAL SYSTEMS PROGRAM



Dr. Dawanne Poree

Program Manager, Polymer Chemistry
Program Manager (Acting), Reactive Chemical Systems
Chemical Sciences Division
ARO Physical Sciences Directorate

Dr. Poree completed her undergraduate studies at Nicholls State University, receiving her B.S. in Chemistry in 2004. She trained as a polymer chemist at Tulane University, receiving her Ph.D. in Chemistry in 2010.

She came to ARO in 2011 as a SETA Contractor to support the Polymer Chemistry Program and was hired as the Program Manager in 2014. In addition, Dr. Poree has served as the Program Manager (A) for Reactive Chemical Systems since 2014.



Dr. Jennifer Becker

Basic & Applied Research Team Lead
US Army CCDC-Atlantic

Dr. Becker completed her undergraduate studies at Gettysburg College, receiving her B.S. in Chemistry in 1997. She trained as an organic chemist at the University of North Carolina at Chapel Hill, receiving her Ph.D. in Chemistry in 2002.

She came to ARO in 2005 as a SETA Contractor to support the Organic and Inorganic Chemistry Program and was hired as the Program Manager in 2008. Dr. Becker is currently completing an assignment with the US Army CCDC-Atlantic.



Dr. Stephen Lee

Chief Scientist, ARO

Dr. Lee completed his undergraduate studies at Millsaps College, receiving his B.S. in Chemistry and Biology in 1991. He trained as a physical organic chemist at Emory University, receiving his Ph.D. in Chemistry in 1996.

He came to ARO in 1998 as the Program Manager for the Organic and Inorganic Chemistry Program, and was named ARO's Chief Scientist in 2007.

This success supports these ARL Core Technical Competencies



Protection Sciences



Computational Sciences

Supersoap: Development of a Non-Reactive Decontaminant

Challenge

Decontamination technologies capable of detoxifying and eliminating toxic hazards, including chemical and biological warfare agents, are an essential requirement for the Department of Defense, law enforcement, fire departments and hazardous materials response teams (HAZMAT). In addition to being highly reactive and effective, decontaminants must also be stable so they can be stored for long periods of time and easily transported so that numerous prepositioned stockpiles are not required. While traditional reactive decontaminants including oxidants such as bleach or hydrogen peroxide have demonstrated efficacy against a range of threats, they are corrosive and are not compatible with all military relevant materials.

Action

To address the military's need for novel decontaminants effective against a range of chemical and biological agents for diverse operational environments, previous ARL-

ARO Program Managers, Dr. Stephen Lee and Dr. Jennifer Becker, devised topics for the Joint Science and Technology Office for Chemical and Biological Defense (CBD) Small Business Innovation Research (SBIR) Program. Specifically, the two related but distinct topics focused on a readily portable system to rapidly decontaminate interior spaces (CBD05-108), and exterior and interior surfaces of forward deployed vehicles and associated infrastructure (CBD07-102), with minimal logistical burden and minimal hazardous by-products. Under both solicitations, TDA Research, Inc. (Wheat Ridge, CO) was awarded Phase I and II contracts to develop an electrochemical-based solution. The original electrochemical decontamination (eClO₂) technology consisted of a battery powered and operated sprayer integrated with an electrochemical cell, sodium chlorite and sodium bromide salts, and buffer/additives. The salts and additives were dissolved in water, and when the solution was sprayed, it passed through the electrochemical cell to generate the active decontaminants, chlorine dioxide and hypobromite, directly onto the contaminated surface. The decontaminant solution is very reactive and has been shown to deactivate live chemical and biological agents including VX, HD, G-agents, and bacterial spores.

During the development process, the firm discovered that decontamination efficacy improved by simply adding a mixture of commercially available surfactants to the base formulation. More specifically, the surfactant emulsified and rapidly lifted hydrophobic chemical agents, including thickened agents, from military relevant surfaces without requiring any mechanical agitation.

Results

Based on the decontamination efficacy improvements achieved with the eClO₂ surfactant formulation, a standalone, non-reactive, surfactant-based decontaminant was developed. In a joint development effort between TDA Research, Proctor & Gamble, CDC-Chemical Biological Center (CBC) (Dr. Lawrence Procell), and ARL-ARO, TDA Research was awarded Phase III funding (FY10) from the Defense Threat Reduction Agency (DTRA) (Dr. Charles Bass) and the Joint Program Executive Office (JPEO) for Chemical and Biological Defense, Office of the Joint Program Manager-Decontamination (Mr. Victor Murphy), to develop an advanced detergent formulation, SSDX-12®, that enhances removal of chemical agents from contaminated surfaces and improves materials compatibility, enabling use on sensitive equipment. The detergent is a stable emulsion and keeps chemical agents in solution, preventing re-deposition. In addition, the formulation is non-reactive, pH neutral, non-hazardous, biodegradable, has no shipping restrictions, and does not require a special applicator. Based on the success of this spin-off project, the firm has achieved commercial sales of the surfactant component as a non-reactive detergent solution qualified for use in routine aircraft cleaning per MIL-PRF-87937 and in facilities exposed to heavy metals such as aircraft maintenance facilities.



Figure 1. (Left) SSDX-12® product image with FDNY training in the background; **(Right)** SSDX-12® being used to clean a Blackhawk.

SUCCESS

Optimization of a reactive-based decontaminant formulation has resulted in the discovery of a non-reactive, surfactant-based decon product for the removal of chemical agents.

RESULTS

- ▶ Transitioned SSDX-12® technology to the FDNY Haz-Mat Battalion as an all-hazards, non-reactive decon
 - ▶ Approved for use on US military aircraft per MIL-PRF-87937
 - ▶ TDA's eClO₂ product is the only chem-bio decontaminant that is EPA registered for anthrax
-

This success supports these ARL Core Technical Competencies



Protection Sciences



Materials and Manufacturing Sciences

SUCCESS

First time discovery of long-range catalytic communication in non-biological nanocatalysts

In FY18, the New York City Fire Department (FDNY) Hazardous Materials (Haz-Mat) Battalion has acquired and is implementing within their teams the use of SSDX-12® as their primary all-hazards decontaminant for removal of gross contamination and pre-cleaning prior to reactive decontamination, and as a general cleaner for facilities, equipment, and fire trucks. In addition, other users across a range of units including Weapons of Mass Destruction Civil Support Teams (WMD CST), the Marine Corps Chemical Biological Incident Response Force (CBIRF), the Navy Explosive Ordnance Disposal Training and Evaluation Unit 2 (EODTEU), and local Drug Enforcement Administration teams have adopted this advanced detergent product as an all-hazards, non-reactive decontaminant for use on personal protective equipment.

Way Ahead

TDA is continuing to expand their SSDX-12® and eClO2 commercial and military capabilities by exploring cleaning for removal of other hazardous compounds, skin decontamination, and efficacy against emerging chemical and biological hazards. Continued collaborative efforts among ARO, CCDC-CBC, DTRA, and the Joint Program Manager-Protection will be sought and leveraged to develop and transition new capabilities to the Soldier.

Nanocatalyst Communication

Challenge

Enzymes are efficient natural catalysts that can carry out numerous transformations with extraordinary selectivity and specificity. A key feature of enzymes is catalytic allostery, or cooperative chemical communication, where reactions occurring at one site of the enzyme can influence reactions at another site. Synthetic nanoscale catalysts, similar in size to enzymes, can also catalyze various transformations on their surfaces. While tools have been developed to account for the location and time of each reaction on individual nanoparticles, “chemical communication” has not been considered in non-biological nanocatalysts.

Action

To address one of the program’s objective of understanding reactivity on nanostructured surfaces, previous ARL-ARO Program Manager, Dr. Jennifer Becker, strategically supported researchers at Cornell University to develop a method to resolve individual reactions spatially on single nanocatalysts in real time. A subsequent mapping technique dissects the nanoparticle and its catalytic product positions into segments along its long axis. For each segment, the catalytic product molecules can be arranged in a sequence of catalytic events according to when each product molecule was detected. For each sequence, the correlation of the microscopic reaction time (τ) for reactions that neighbor in time but occur at different segments or nanoparticles is analyzed and quantified. Using single-molecule super-resolution fluorescence microscopy, the research team has imaged and mapped reactions on single catalysts including palladium and gold nanorods and gold nanoplates. The Principal Investigator, Professor Peng Chen, who has an enzyme background, extended his investigation to probe whether reactions at different surfaces sites on the same nanoparticle could communicate with each other, similar to what is observed with enzymes.

Results

By analyzing the correlation between individual, temporally neighboring reactions, in FY18, the research team discovered long-range catalytic communication within and between single, non-biological nanocatalysts and defined possible mechanisms that support the observed phenomena.

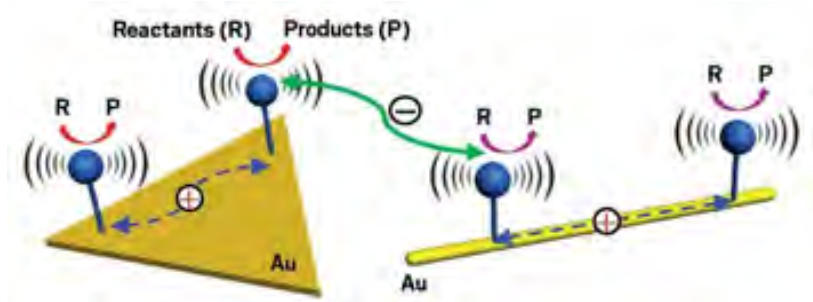


Figure 1. Active sites on metal nanoparticles can communicate (blue antennas) via two mechanisms. Positively charged species carry messages within a particle (dashed blue line). Negatively charged species drive communication between nearby particles (green line) (Courtesy of Chen Group/Cornell).

It was found that the intra-particle and inter-particle catalytic communication follow different mechanisms because of their distinct communication distance and temporal memory. Intra-particle catalytic communication was observed with Pd- and Au-based nanocatalysts in three distinct model systems including a photo-induced disproportionation reaction, an oxidative deacetylation reaction, and a reductive deoxygenation reaction. It was determined that communication extends up to 100 nanometers with a temporal memory of a few to tens of seconds, exemplifying positive cooperativity among surface sites within the same nanocatalyst. Intra-particle catalytic communication likely involves the movement of positively charged "messenger species", or surface holes. Communication distances between distinct nanocatalysts were observed over greater distances (up to many microns), and occur via molecular diffusion in which a negatively charged reaction product molecule from one nanocatalyst diffuses around in solution and impacts the rate of reaction on a different nanocatalyst. Inter-particle communication was limited to using Au-based nanocatalysts for the deacetylation and deoxygenation reactions, for which both model systems produce negatively charged reaction products (acetate and nitrite, respectively).

Way Ahead

Understanding biological-like phenomenon in a non-biological catalyst will lay the foundation towards designing novel catalysts with superior activity and selectivity for the detection and destruction of toxic industrial chemicals and chemical threats. While the technique allows observation of chemical reactions in real-time, it is limited to fluorescent reactions. With additional investment from ARO (Dr. Dawanne Poree), Cornell researchers are developing a method that can image non-fluorescent catalytic reactions, broadening the range of systems that can be explored. Collaborative efforts among ARO, ARL-WMRD, CCDC-CBC, and DTRA will be sought and leveraged to transition key knowledge products toward the advancement of new protection capabilities for the Soldier.

REACTIVE CHEMICAL SYSTEMS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Create chemically and biologically functionalized surfaces with precise control of structure and function that if successful is anticipated to lead to novel decontaminants, sensors, and coatings for Soldier protection.
- ▶ Attain a mechanistic understanding of mass transport, adsorption, and reactivity on surfaces and at interfaces that if successful is anticipated to lead to novel materials for degrading chemical threats.
- ▶ Design and synthesize chemical systems that sense and respond to external stimuli that if successful is anticipated to lead to intelligent materials for Soldier protection.

RESULTS

- ▶ Demonstrated "chemical communication" within the same nanocatalyst and between different nanocatalysts
- ▶ Proposed two distinct mechanisms for observed catalytic communication

LIFE SCIENCES DIVISION: FY18 SUCCESS STORIES

NEUROPHYSIOLOGY OF COGNITION PROGRAM



Dr. Fred Gregory

Program Manager, Neurophysiology of Cognition
Life Sciences Division
ARO Physical Sciences Directorate

Dr. Gregory completed his undergraduate studies at Morehouse College, receiving his B.S. in Biology in 1999. He training as a Neurobiologist at University of California, Los Angeles receiving his Ph.D. in Neurobiology in 2006.

He came to ARO in 2013 as the Program Manager for Neurophysiology and then took on the additional role of International Program Manager for Human Dimension in 2016.



Dr. Virginia Pasour

Program Manager, Biomathematics
Mathematical Sciences Division
ARO Information Sciences Directorate

Dr. Pasour completed her M.S. in Biostatistics at UNC – Chapel Hill in 1995. She trained as an Applied Mathematician at Cornell University, receiving her Ph.D. in Applied mathematics in 2007. She came to ARO in 2009 as the first Program Manager for the Biomathematics Program.

Accelerating Learning by Defining the Neural Basis of Expert Performance

Challenge

We appreciate the performance of the concert pianist or the star quarterback throwing a touchdown without much thought to how they became experts at their skill.

Scientific studies over decades have identified the psychological profiles and psychophysical advantages afforded to experts in many fields of sports and the arts when they performed, compared to novices. Results of these efforts led to popularization of concepts such as 'being in the zone' and the '10,000-Hour Rule,' claiming that world-class expertise in any skill requires around 10,000 hours of deliberate practice. The uprising of functional magnetic resonance imaging in the late 1990s and early 2000s led to hundreds of studies that sought to identify features of expert's brains that afforded advantages over the rest of the population. Comparisons showed correlations between metabolic changes in brain regions associated with controlling motor and sensory functions involved in the skilled performance as well as other regions associated with the decisions to act. Around this same time there was also a revolution in the understanding of cellular and molecular mechanisms underlying learning and memory. By the early 2010's, a large body of evidence pointed to synaptic plasticity as the candidate mechanism for mediating all learning and memory. These bodies of work naturally pointed to synaptic plasticity as a vital component of learning to become an expert, but there remains a gap in understanding how synaptic plasticity (at the cellular scale) enables mind-body control of expert performance (at the systems

This success supports
these ARL Core Technical
Competencies



Human Sciences



Protection Sciences

and organism level). This lack of understanding phenomena across size scales is a general impediment in neuroscience and limits the extent to which neuroscience will directly impact Army Human Sciences challenges associated with Accelerated Learning for a Ready and Responsive Force. Is the '10,000-Hour Rule' a biological necessity? Can neurophysiology generate an opportunity to reduce the amount of time it takes to train expertise for military-relevant tasks? The Army Research Office initiated actions, beginning in 2014, to address these outstanding issues by exploring opportunities for Army research and strategic extramural basic research.

Action

To identify grand challenges for the Army of 2050, ARO Neurophysiology of Cognition program manager, Dr. Frederick Gregory, co-organized the Human Dimension Basic Research Concept Exploration meeting for ARL. The meeting enlisted the expertise of an academic panel to identify research gaps in quantifying human behavior, and other topics in cognitive sciences that included training expertise. Our conclusions, published in the 2014 Army Science Planning and Strategy Report, included a recommendation that the Army should invest in multidisciplinary studies to enhance education and training for optimal decision-making. As a result, Dr. Gregory helped to devise a research initiative submitted to ARL POM 16-20 focused on the Neurobiology of Simulation and Training. The objective is to uncover the mechanisms of cognitive adaptation during simulation and training in order to assess when learning is optimized. The initiative was funded as part of the Congressional budget and is currently a 6.1 scientific opportunity for ARL researchers to uncover and exploit links between neurophysiology and biosignals that are synonymous with effective human performance and learning during simulation and training.

Dr. Gregory also identified fundamental scientific barriers that must be addressed to augment skill learning. The state-of-art in psychology, neuroscience, human factors and human performance typically compared an independent variable between a group of novices and a group of experts. After hundreds of journal articles identifying correlative relationships between a study's independent variable and performance, conclusions emerged that expertise is mediated by distinct changes in the structure and function of the brain. In 2014, Dr. Gregory explored the potential for a new multidisciplinary approach to identify brain and body state variables that transition as an individual journeys from novice to expert. In 2015, the Executive Director of the National Institute for Mathematical and Biological Synthesis (NIMBioS) was interested in this idea and invited Drs. Gregory and ARO Biomathematics Program Manager Dr. Virginia Pasour to propose a cutting-edge workshop to address the scientific challenges associated with understanding expertise. As a result, they identified key researchers in the field and initiated the 2015 Neurobiology of Expertise investigative workshop. The meeting brought together leading mathematicians, neuroscientists and psychologists. This included the psychologist whose research led to coining of the '10,000-Hour Rule.'

Drs. Gregory and Pasour leveraged the results from the workshop to devise a novel multidisciplinary basic research challenge. They identified that a major aspect of physical expertise involves seamless decision-making, and formulated a MURI topic to define expertise by discovering the underlying neural mechanisms of decision-making during skill learning. The MURI topic was one of the eight ARO topics selected by OSD for public release in the FY16 MURI Broad Agency Announcement. Dr. Scott Grafton's proposal from University of California, Santa Barbara was awarded in late 2016. The focus on learning expertise in a decision-making task combined with experimental and theoretical approaches from psychology, neuroscience, network sciences and mathematics was an ideal approach to develop a novel multiscale modeling framework to identify causative neural mechanisms. The MURI facilitated an approach that involves expertise from neuroscience, mathematics, network science and human performance. Together, a suite of experimental and analytical tools are used

SUCCESS

Strategic multidisciplinary investments to advance knowledge of learning and the development of expertise is leading to focused initiatives that are expected to enable future accelerated learning, opening the door new simulation and training platforms of the future.

to probe and model similar decision processes in human, non-human primates and rodents; since they all show similarly involved brain structures, learning processes and behaviors. This approach will have the potential to develop a novel neurocomputational description of expertise based on neuroscience.

Results

Recent experimental results in non-human primates from Massachusetts Institute of Technology identified specific neuronal features and brain states directly involved in repetitive poor decision-making. Microstimulation and recording electrical activity demonstrated that a subset of neurons in the striatum are selectively active in, and causally necessary for, cost-benefit decision-making under behavioral conditions known to evoke anxiety in humans. Interestingly, electrical stimulation consistently biased animals toward high-cost low-reward decision choices, which would be considered poor decisions (see Figure 1).

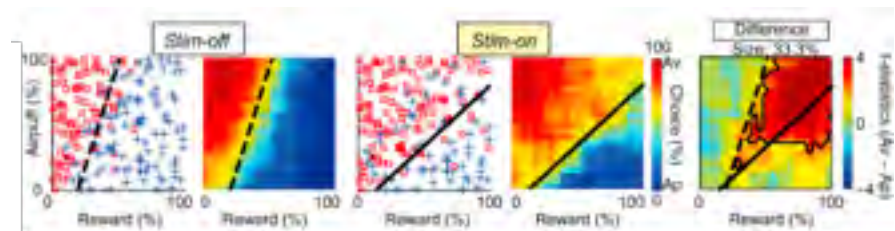


Figure 1. Monkeys made a decision between acceptance and rejection of a combined offer of reward and punishment. The decision was reported by choosing targets (cross for acceptance; square for rejection) that appeared on screen during the response period. Approach (blue cross) and avoid (red square) choices in the Stim-off (left panels) and Stim-on (middle panels) blocks in the same session and difference between these blocks (right panels). Microstimulation of basal ganglia neurons shifted the decision boundary toward higher-risk and low reward. Dashed and solid lines denote decision boundaries. (DOI: 10.1016/j.neuron.2018.07.022)

Stimulating these same regions, separately, resulted in abnormal beta-band brainwave oscillation patterns (12.5 to 30 Hz), which was predictive of when high-cost low-reward decisions would be made. Stimulation of other nearby circuits did not affect decision-making or beta band activity, highlighting that cognitive and emotion-related functions are compartmentally-organized. This could be a step toward identifying causative relationships between specific neuronal populations (cellular-scale) and brain signals (systems-scale) that are predictive of choice; highlighting a new biomarker to inform human studies and potentially hasten translation to Soldiers.

Way Ahead

This scientific accomplishment lays a foundation for uncovering underlying bases of human decision-making by strengthening the potential to translate information from primate behavioral tests, brain states and computational models to human data. This research helps uncover underlying neural features in addition to trait and state features of human decision-making performance that are likely to be engaged during training and simulations. This research may ensure fidelity of future Synthetic Training Environments by offering biomarkers, computational models and mechanistic understanding that will help optimize training of decision accuracy.

RESULTS

- ▶ New ARL collaborations with U Santa Barbara, and U Penn
- ▶ Based on this area ARL made intramural investments in the Accelerated Learning for a Ready and Responsive Force Essential Research Program beginning in 2018.
- ▶ POM increase supports ARL intramural investments in the Neurobiology of Simulation and Training

NEUROPHYSIOLOGY OF COGNITION PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Map, measure and model structural and functional neural components of multisensory synthesis and modulate human multisensory information processing bandwidths.
- ▶ Determine how brains structure, process and refine biological neural networks to generate efficient decisions and behaviors.
- ▶ Determine underlying neurobiological mechanisms mediating the vulnerability of the brain to mild injury under high-rate loading conditions.

MICROBIOLOGY PROGRAM



Dr. Robert Kokoska

Program Manager, Microbiology
Life Sciences Division
ARO Physical Sciences Directorate

Dr. Kokoska completed his undergraduate studies at Villanova University, receiving his B.Ch.E. in Chemical Engineering in 1978. He trained as a biochemist at Duke University receiving his Ph.D. in Biochemistry in 1995.

He came to ARO in 2006, as the Program Manager for Biochemistry, has served as the University Affiliated Research Center (UARC) Program Manager and has been the Microbiology Program Manager since 2014.

Prof. Frances Arnold, ARO-Funded Investigator For 20 Years, Awarded The 2018 Nobel Prize in Chemistry

Challenge

Living cells rely on a constellation of protein enzymes to rapidly catalyze the many reactions that occur in a cell that keep organisms alive and healthy. Each enzyme is evolutionarily finely tuned by its protein sequence to have optimal activity driving the formation of specific products. Because protein sequences are optimally selected, small random changes to this sequence usually results in degraded performance, but that does not preclude instances in which sequence changes can result in enhanced performance (e.g., higher catalytic activity or improved performance over a broader range of temperatures), or interestingly, the ability to catalyze the formation of different products.

If one wishes to improve or alter enzyme activity by changing its sequence, how would one go about doing this? Given that proteins sequences typically comprise a few hundred individual amino acid “building blocks,” the challenge has always been identifying which individual or combination of amino acids need to be specifically changed out of the literally millions of possible combinations that can be made that result in the desired activity.

This success supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Computational Sciences



Ballistics Sciences



Propulsion Sciences



SUCCESS

Over 20 years of strategic investments has led to discoveries that have transformed how biologists can create new enzymatic functions leading to unprecedented and revolutionary capabilities in expanding the reach of what biology can deliver including the ability to produce cost-effective biofuels for the Army.

Action

In the early-to-mid 1990's Prof. Frances Arnold, a chemical engineer at Caltech, was interested in this challenge: how can we engineer enzymes to perform functions that nature does not provide. Based on known enzyme structures, she hypothesized that there were specific amino acids embedded in the sequence and structure of the protein that should alter its reactivity and/or specificity. Upon identifying the likely identity of those amino acids, she constructed rationally-chosen amino acid substitutions (by making directed mutations in the DNA encoding these proteins) at those locations and assayed the effects of these variants for altered properties. To her disappointment, she was not successful in engineering an enzyme that had the desired properties.

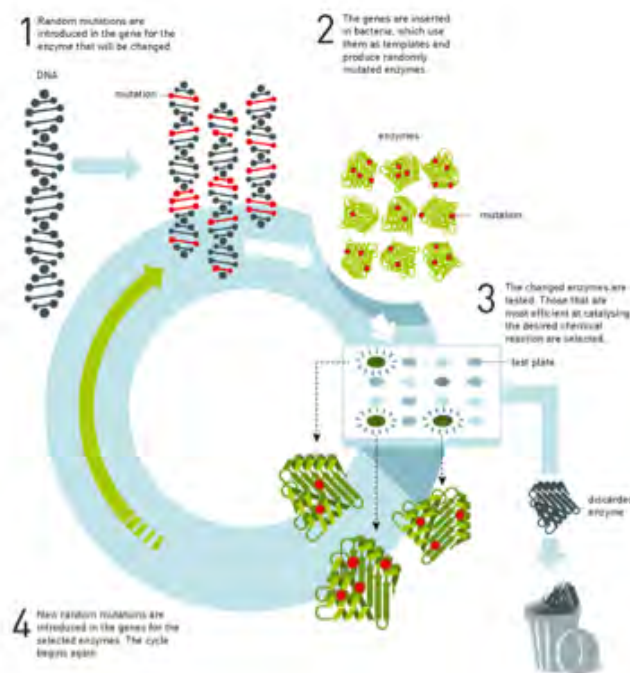


Figure Legend: Schematic of directed evolution process where millions of randomly generated genetic variants are screened for desired properties. This process is iteratively repeated to further enhance enzymatic properties.

In the late 1990's, Prof. Arnold engaged in discussions with the ARO Life Sciences Division to pursue a different approach. Rather than painstakingly construct directed individual mutants, Prof. Arnold proposed a system called directed evolution, where one can randomly mutate the gene encoding the enzyme of interest producing literally millions of non-natural variants that can be iterated and screened to identify the enzymes that will catalyze a desired reaction. Based on this idea, ARO Life Sciences awarded Prof. Arnold a modest single investigator grant to pursue this approach. Through this methodology, she demonstrated the ability to modify an enzyme that provided robust native activity but at higher temperatures. During this grant period, she also developed a computational algorithm called SCHEMA which provides a means of improving molecular evolution searches toward targeted protein sequence alterations. Through SCHEMA, the sequences of distantly-related homologous proteins from different organisms are recombined to generate thousands of chimeric sequences; based on known 3-D protein crystal structures, SCHEMA predicts which fragments of the native homologs can be recombined without disturbing the stability of the chimeric protein structure. She demonstrated that this algorithm can be successfully used to design variations of a model protein that confer functional diversity including enhancements in activity and thermal stability and altered substrate specificity.

In his role as Program Manager for the Army's Institute for Collaborative Biotechnologies (ICB) UARC, Dr. Kokoska continued to sponsor Prof. Arnold's basic research in directed evolution and worked toward awarding a 6.2 effort to the AICB

program that provided initial funding to Gevo, a start-up company. Gevo's business goal was to scale-up processing systems that utilize SCHEMA-designed enzymes incorporated into microorganisms for the cost-effective synthesis of biofuels. From rather humble beginnings where Gevo's facilities consisted of modest rented bench space in Pasadena and a lab-scale fermenter, Gevo developed into a business that is the world's only commercial producer of renewable isobutanol and in 2013, the US Army successfully flew the Sikorsky UH-60 Black Hawk Helicopter on a 50/50 blend of Gevo's ATJ-8 (Alcohol-to-Jet) fuel.

Results

Prof. Arnold has utilized SCHEMA to design novel activities for a broad host of enzymes including activity and stability improvements in enzymes capable of degrading cellulosic biomass toward renewable fuel synthesis and has developed new machine learning tools to enhance the selection of novel engineered enzymes. Based on the success of the process of directed evolution originally funded through the ARO Single Investigator Program and later advanced through the AICB 6.1 and 6.2 programs, she was awarded the 2018 Nobel Prize in Chemistry. As only the fifth woman to receive this distinction, she is also the only woman who is a member of all three National Academies (National Academies of Science, Engineering and Medicine). Notably, the graduate student in Prof. Arnold's lab who developed the SCHEMA computational algorithm is Prof. Chris Voigt of MIT, who is now one of the world's leaders in the field of synthetic biology and an investigator at the AICB. As Prof. Voigt embarked on his beginnings with the AICB, Dr. Kokoska introduced him to the Army Research Laboratory during a visit and a seminar to ARL's Adelphi Laboratory Center in 2014. From this introduction, Prof. Voigt has become one of the most pro-active collaborators with ARL's Biotechnology Branch. Most notably, he has established a productive collaboration through one of ARL's Directors Research Initiatives, has served as an advisor for both the DoD Applied Research for Advancement of priorities (ARAP) program in Synthetic Biology and the ARL Transformational Synthetic Biology for Military Environments (TRANSFORME) ERP and has heightened his visibility with ARL as a DoD Vannevar Bush Fellow.

Way Ahead

Prof. Arnold's remarkable success is a prime example of how pro-active identification of creative ideas by ARO PMs can seed effective 6.1 level efforts and how this patient and rigorous funded research can lead toward more applied systems and ultimately toward a valued Army capability. With current ARO funding, she continues to utilize the same combinatorial principles that provide altered enzyme function toward the design of new biocatalysts for abiological reactions, specifically catalysts that drive stereo- and region-specific modular synthesis of functionalized bicyclobutanes. She will be pursuing collaborative efforts with ARL-WMRD to transition this technology toward the biological synthesis of energetic and protective materials.

Study of the Human Microbiome – Army Leadership within the Tri-Service Research Community

Challenge

One of the most impactful and potentially disruptive research ventures in the field of Life Sciences is the study of the human microbiome. It is known that humans provide a favorable environmental landscape for the growth of complex microbial communities; in fact there are more bacterial cells on and within the human body than there are human cells. More importantly, from the standpoint of biological function, there are a few orders of magnitude more microbial genes harbored within us than there are human genes! Broadly, this field of study is focused on gaining a fundamental understanding

RESULTS

- ▶ Development of a laboratory technique to engineer new enzymatic properties now routinely used within the bioengineering research community.
- ▶ Transition of a graduate student from Arnold lab to scientist at Army Research Laboratory Biotechnology Branch.
- ▶ New collaborations and transitioning of materials research to ARL-WMRD.
- ▶ Applied research from ICB led to development of Army-fielded biofuels.
- ▶ ARO-sponsored research recognized by Nobel committee (Prof. Arnold awarded 2018 Nobel Prize in Chemistry).

This success supports these ARL Core Technical Competencies

Computational Sciences



Human Sciences



Protection Sciences



SUCCESS

The first three years of the TSMC has brought together scientists from all three services, and OXR-sponsored academic investigators, including two complementary MURI teams from ARO and ONR, who are engaged in the science of the human microbiome. Discussions during annual meetings and program reviews have already led to a number of working collaborations between the academic and DoD communities to further the health, well-being and performance of the Warfighter.



Figure Legend: The Tri-Service Microbiome Consortium (TSMC) was chartered by the Office of the Assistant Secretary of Defense for Research and Engineering Human Performance, Training and Biosystems Directorate in December 2016. The TSMC was tasked with establishing a forum for collaboration and coordination among DoD research performers, research sponsors, policymakers and stakeholders on microbiome-related projects.

of the collective activity of complex species-diverse families of microorganisms that colonize different regions of the human body and the effects of the metabolic output of these microbial communities on human physiology. While microbiome research guided by other federal agencies, such as the NIH, are rightfully geared toward

aspects of human health, the DoD has a unique interest in the effect of the human microbiome on Warfighter protection and performance. In recognition of this benefit, and in response to growing interest in the study of the human microbiome among the services including within the ARO Life Sciences Division, OASD chartered the Tri-Service Microbiome Consortium (TSMC) in 2016 as part of the DoD Biotechnologies for Health and Performance Council. The purpose of the TSMC is to enhance collaboration, coordination and communication of microbiome research among DoD organizations. Since the inception of the TSMC, Dr. Robert Kokoska, the ARO Microbiology Program Manager, has been a leading member of the TSMC steering committee by planning and organizing an annual DoD-wide TSMC workshop to discuss technical challenges and identify collaborations within the DoD as well as more targeted workshops, symposia and seminars between TSMC members and the academic community.

Action

To address the technical challenges and provide a significant contribution to the TSMC goals, Dr. Kokoska has started to devote a significant percentage of resources available through the ARO Microbiology Program toward funding extramural basic research in the study of the human/mammalian microbiome. One of the most significant challenges in attaining a meaningful understanding of the activity of a microbiome is the sheer complexity and diversity of the microbes that form a stable community. Indeed, there are hundreds to thousands of different species of microorganisms that can inhabit a specific region of the human body. Even with continued rapid advances in genomics and computational capacity, the analysis of the contributions of the microbial components within these complex communities as drivers of community activity is intractable. To date, the productivity of the research community in this field has provided valuable working knowledge on the role of specific microbes within a natural community in generating specific metabolic outputs and how those outputs affect physiology, but the issue of complexity has rendered many of these interpretations to be more correlative than causative. In recognition of this challenge, the ARO Microbiology Program has focused on: (a) “top-down” approaches that look toward mathematical modeling or ecological approaches to develop predictive frameworks for understanding the complexity of interactions within microbiomes and their downstream effectors; this approach will help provide the tools for formulating specific hypotheses that can establish more definitive causative effects in microbiome activity; and (b) “bottom-up” approaches that utilize more tractable model microbial community systems that can establish “design rules” for the assembly, activity and sustenance of microbial community function and can thus provide rational approaches toward studying communities of ever-increasing complexity.

Results

Among the “bottom-up” extramural efforts recently funded through the ARO Microbiology Program that forward the study of model systems that can help inform the activity of complex microbiomes: Ophelia Venturelli (University of Wisconsin – Madison) is developing a high throughput microfluidic system that can identify stable pairwise interactions and their relative fitness from a synthetic community of 100 microbes from the human gut. This collective data will be used to develop a model-guided approach to dissect dynamics within this model community. Karsten Zengler (University of California – San Diego) is exploiting the specificity between glycans and species-specific lectins on the bacterial surface to systematically and selectively remove individual species from a skin microbiome community to enable the effect of that species on community composition and robustness of the microbiome. Steve Lindemann (Purdue) is examining the response of the gut microbiota and its compositional trajectory to structurally-distinct dextrins (breakdown products of starch). Julie Biteen (University of Michigan) is initiating a study using single-cell and single-molecule biophysical imaging techniques to monitor the effects of spatial patterning between two commensal gut bacteria – one of which breaks down resistant starch and the other feeds off the by-products of that digestion.

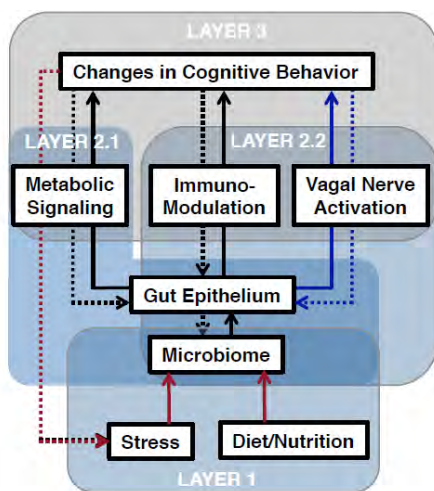


Figure Legend: Multi-layered Modeling Framework of the Gut-Brain Axis Pursued by ARO-sponsored MURI Team: Through iterative in vivo, in vitro and in silico experiments with cross-referenced testing of predictions across experimental systems, the team will extract fundamental biological insights for how nutrition and physical stress modify microbial community structure and function (Layer 1), how microbial products biotransformed through the gastrointestinal tract modulate metabolic (Layer 2.1), immune and vagal signaling (Layer 2.2), and how metabolic, immune and vagal activity determine cognitive performance (Layer 3).

The “top-down” approaches are embraced largely through two MURI efforts. The first is a study of the ecology of the skin microbiome led by David Karig (Johns Hopkins University/Applied Physics Laboratory) and co-managed by the ARO Biomathematics Program. This MURI team has gathered 4000 clinical skin microbiome sample and have started to generate a trait database that identifies specific trends in taxonomic inter-personal variation that can be explained by environmental factors including local temperature, pH, moisture and sebum. The gathering and taxonomic cataloging of a publicly available isolates collection from this effort is being used to design in vitro experiments to better understand the interactions between species based on the ecological analysis derived from the trait database. The second recently initiated MURI effort is led by Elaine Hsiao (UCLA) and is co-managed by the ARO Neurophysiology Program designed to develop a predictive modeling framework for the two-way gut-brain axis. This model will in large part utilize control theory to describe the dynamics between different nodes of this axis as a function of nutritional input and physical stress (specifically, hypoxia) and how those perturbations influence cognitive performance. The model will be informed by data that describes the dynamics of the gut microbiome, neurophysiological responses, behavioral measurements and the immune response. It is envisioned that the initial modeling framework developed through this MURI can be further embellished and validated by the microbiome research community as a

RESULTS

- ▶ Two active MURIs co-managed through the ARO Microbiology Program address the challenges of understanding the ecological underpinnings of the human skin microbiome and the modeling of the gut-brain microbiome.
- ▶ CCDC-ARL, CCDC-Soldier Center, USARIEM and AFRL research groups leveraging output of ARO Microbiology Program-sponsored scientists (Single Investigator and MURI) studying various aspects of the human microbiome.
- ▶ In its third year, the Tri-Service Microbiome Consortia has successfully brought together scientists from DoD intramural labs and academic community to work together toward addressing Warfighter challenges that can be met through the study of the human microbiome.

predictive tool – one that can elucidate testable hypotheses that can clearly delineate causative effects between the activity of different nodes that define the gut-brain axis that lead to reliable predictions of cognitive performance and microbiome health.

Through Dr. Kokoska's leadership within the TSMC, the Consortia has started to identify new collaborative research efforts between DoD labs and academic investigators, many of whom are among the aforementioned investigators funded through ARO. Dr. Kokoska hosted Prof. Venturelli at the CCDC Soldier Center to discuss strategies for designing synthetic gut microbial communities with scientists at the Soldier Center, ARL and AFRL. These meetings led to a direct collaboration with ARL to link her observations on pair-wise growth of gut microbes with ARL's capabilities in metabolic modeling. Proactive coordination between Dr. Kokoska and DoD scientists at annual MURI review meetings have led to productive engagement between MURI efforts and the DoD. Some of the in vitro skin model systems developed through the MURI led by Karig have been transitioned to studies at the CCDC Soldier Center. Other members of this MURI team have opened discussions with AFRL about transitioning some of the bioinformatics and visualization tools developed through the MURI into AFRL's bioinformatics infrastructure. In collaboration with the gut-brain MURI, CCDC Soldier Center's Human Performance team and USARIEM have coordinated a transition of human microbiome data from a USARIEM high altitude study to compare against Prof. Hsiao's rodent models.

Way Ahead

Dr. Kokoska co-organized a TSMC workshop scheduled in June 2019 at the CCDC-Soldier Center that will brought together the Hsiao gut microbiome team, a separate ONR MURI team studying the effects of circadian disruption and sleep deprivation on the performance of the gut microbiome and other OXR-funded investigators studying different aspects of the gut microbiome to identify new collaborative efforts between different extramurally funded efforts as well as with DoD labs. From this gathering, the two MURI teams identified data sets and models that can be shared between the teams to further the goals of each MURI. From discussions with Army scientists in attendance, the academic researchers gained a clearer understanding of the DoD's own intramural research in this area providing starting points for building trust among the attendees and for additional discussion toward collaboration. The TSMC will holding its 3rd annual meeting in October 2019 where discussions will range between from the biology of the skin and oral microbiomes, the challenging faced in dissecting environmental microbes (including soils and microbial communities found in the built environment) and transition points to warfighter solutions – what does the science inform toward the development of new therapeutics and dietary supplements to enhance and maintain healthy microbiomes. Dr. Kokoska's own program will continue to pursue new research ideas focused on the study of model microbial systems that can identify key features of microbial interaction that can inform studies of more complex microbiota and the development of new in vitro platforms to enable these studies.

MICROBIOLOGY PROGRAM – CURRENT SCIENTIFIC OBJECTIVES

- ▶ Discover the dynamics and communication mechanisms that drive robustness and function within bacterial communities that if successful, is expected to lead to the effective design of microbial-based platforms for on-demand fielded material synthesis.
- ▶ Develop and test experimental strategies to better understand the physiology of complex microbial communities that if successful, will provide reliable new platforms for the study of the human microbiome.
- ▶ Identify and characterize bacterial metabolic programming under harsh environmental conditions that if successful, will provide new approaches in the field of synthetic biology toward fielded living material systems.

BIOCHEMISTRY PROGRAM



Dr. Stephanie McElhinny

Program Manager, Biochemistry
Life Sciences Division
ARO Physical Sciences Directorate

Dr. McElhinny completed her undergraduate studies at Gannon University, receiving her B.S. in Chemistry in 1999. She trained as a biochemist at the University of North Carolina - Chapel Hill, receiving her Ph.D. in Biochemistry in 2004.

She came to ARO in 2009 as the Program Manager for Biochemistry.

Artificial Cells for Novel Synthetic Biology Chassis

Challenge

The field of synthetic biology aims to achieve design-based engineering of biological systems. Toward this goal, researchers identify and characterize standardized biological parts for use in specific organisms, which serve as the chassis for the engineered biological systems and devices. However, even the relatively simple single-celled organisms that are typically used as synthetic biology chassis are highly complex and present significant challenges to achieving robust and predictable engineered biological systems. Biological organisms, even those comprised of only a single cell, have evolved over millions of years to perform specific functions in specific environments in response to specific signals. Engineering these organisms to perform a human-directed function must effectively override the natural reaction networks in the cell or effectively run "in the background" without impacting the natural functions of the cell. To facilitate engineering of biological systems, a simplified chassis that supports robust and predictable human-designed functions is needed.

Action

As a potential solution to this challenge, ARO Biochemistry Program Manager Dr. Stephanie McElhinny and the ARO Reactive Chemical Systems Program Manager (at that time) Dr. Jennifer Becker co-developed a MURI topic in 2011 to explore the potential of artificial non-living cells to serve as a stable and predictable chassis for synthetic biology designs. The goal of the MURI program was to assemble a non-living artificial cell that was capable of executing human-designed synthetic biology "programs" while also demonstrating several functions inherent in natural biological systems, including transport into and out of the cell. Drs. McElhinny and Becker actively coordinated this MURI topic with Army and DoD scientists working in the area of synthetic biology and cultivated active engagement in program reviews by scientists at ARL-SEDD, CCDC CBC, ERDC, AFRL and NRL. In FY2018, this program demonstrated significant technical achievements that were recognized by the greater scientific community, as well as successful transition of knowledge products to Army and DoD laboratories.

Due to the exciting potential impact of artificial cells for the Army and DoD, Dr. McElhinny and Dr. Stephen Lee, ARO Chief Scientist, contributed a chapter on Artificial Cells for the 2017 report of the ARL Projections Committee, "Potential Science and Technology Game Changers for the Ground Warfare of 2050: Selected Projections Made in 2017" (ARL Technical Report ARL-TR-8283). Anticipating several additional breakthroughs for the artificial cell field over the next 30 years, Drs. McElhinny and

This success supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Protection Sciences



SUCCESS

Artificial non-living cells were developed that demonstrate several functions akin to living cells and have potential to serve as a novel chassis for Army and DoD engineered biological systems enabling materials production, sensing and therapeutics.

Lee project that artificial cells will revolutionize logistics for the ground warfare of 2050 by enabling on-demand, on-base production of high-value molecules (e.g., pharmaceuticals, fuel sources, or material precursors), significantly reducing the logistics tail and associated transport and storage costs. An artificial cell platform could be programmed with the capacity to produce a large library of different pharmaceutical molecules, with the specific program that is executed in a given scenario triggered upon exposure to a blood sample from an infected Warfighter. Biomarkers in the blood would trigger the production of the appropriate medical countermeasure or treatment, significantly reducing the need for cold chain storage in the field and providing a capability akin to a “pharmacy on a chip.” Artificial cells could also be programmed to produce inorganic materials that serve as precursors for additive manufacturing, supporting the vision of self-sustaining field operations that no longer require transport of replacement parts for engineered systems

RESULTS

- ▶ Development of a non-living artificial cell with synthetic analogs of the cell membrane and nucleus
- ▶ Demonstration of communication between distinct artificial cell populations driven by engineered biological programs effectively executed by artificial cells
- ▶ Transition of knowledge products to Army, Air Force and Navy laboratory scientists for intramural synthetic biology applied research efforts

Result

The MURI team, led by Prof. Neal Devaraj at the University of California-San Diego, achieved a major aim of the program in FY2018 by demonstrating successful assembly of an artificial cell in which the membrane (outer shell) and an internal organelle (the cell’s nucleus) were replaced with synthetic analogs, while maintaining complex biological functions including the operation of synthetic genetic circuits (synthetic biology “programs” that drive the production of specific protein products) and transport of these protein products between distinct artificial cell populations, enabling “communication” between the cells. This significant technical achievement, which was

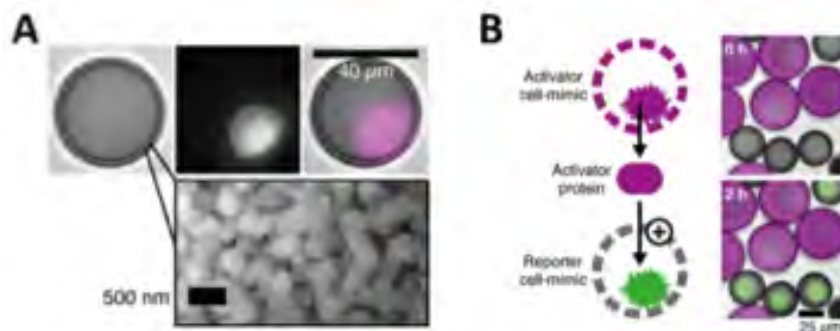


Figure 1. Artificial cells with synthetic replacements of natural cellular structures and active biological functions. (A) Optical micrographs (top) of an artificial cell with GelRed stained hydrogel nucleus (merge of brightfield and red fluorescence) and scanning electron microscopy of porous cell-mimic membrane (bottom). (B) Communication between two distinct artificial cell populations via a diffusive genetic activator protein. The larger “producer” artificial cells (magenta) contain DNA in their hydrogel nucleus that encodes the production of an activator protein. This activator protein diffuses out of the porous cell membrane and through the porous membrane of the smaller “receiver cells” (gray), which contain a DNA sequence in their hydrogel nucleus to which the activator protein specifically binds, resulting in production of a green fluorescent protein that is captured in the nucleus, producing a green signal. (DOI: 10.1038/s41467-018-07473-7)

the culmination of several years of effort under the MURI program, was published in the prestigious journal *Nature Communications* in November 2018, and was prominently featured in a full page news story in the journal *Science* (<http://www.sciencemag.org/news/2018/11/biologists-create-most-lifelike-artificial-cells-yet>), in which a prominent synthetic biology researcher posited: “This may be the most important paper in synthetic biology this year.” In this seminal work, the MURI team created a synthetic cell membrane using a porous polymer shell and encapsulated within this membrane

a synthetic cell nucleus composed of a clay hydrogel that sequestered DNA into a discrete structure, akin to the nucleus within living cells (see Figure 1A). The team then demonstrated that their artificial cell was capable of operating synthetic genetic circuits encoded within the DNA sequestered in the artificial nucleus. Moreover, the porous polymer membrane of the artificial cell supported transport of the protein generated as a product of this circuit out of the producer cell and into a receiver cell that was not programmed to produce the protein on its own (see Figure 1B; efficient transport of the protein product out of the magenta producer cells and into the gray receiver cells (top right image) results in the production of a green fluorescent signal in the artificial nucleus of the gray cells (bottom right image)).

As further recognition of the scientific impact of this MURI program, the PI, Prof. Devaraj, was recognized as the 2018 Blavatnik National Laureate in Chemistry (<http://blavatnikawards.org/honorees/profile/Neal-Devaraj/>). This is the largest unrestricted scientific prize offered to faculty-level scientific researchers aged 42 or younger. The MURI-funded artificial cell research was prominently featured in national press releases and in videos posted by the New York Academy of Sciences announcing the 2018 Blavatnik National Laureates.

Way Ahead

In addition to the significant technical achievements of this MURI program, the research team has also transitioned specific knowledge products from this program to Army and DoD laboratories. As part of this effort, the MURI team developed a novel approach for the preparation of highly active bacterial cell lysates for cell-free gene expression that is three times faster than traditional methods and highly reproducible. This protocol was transitioned to Army, Air Force, and Navy laboratory scientists working together under the Synthetic Biology for Military Environments (SBME) Applied Research for the Advancement of S&T Priorities (ARAP) Program. A major thrust of the SBME ARAP is focused on advancing cell-free synthetic biology, and this protocol is expected to enhance experimental efforts in this thrust area. In addition, a synthetic genetic circuit that produces a mercury biosensor was developed by the MURI team and demonstrated to be highly sensitive in cell-free lysates. Due to the demonstrated activity in cell-free lysates (as opposed to living biological cells) and the detection limit aligning very closely with operational parameters, this mercury biosensor was also transitioned to the SBME ARAP team for implementation in a cell-free heavy metal sensor suite that is being developed under the ARAP program in an attempt to meet water quality testing needs at CCDDC Soldier Center.

As the MURI program comes to a close in 2020, elements of this program are transitioning to funding support under the National Science Foundation (NSF) Design and Engineering of Synthetic Cells and Cell Components (DESYN-C3) Program, which was initiated in 2018.

Biologically-derived Targeted Antimicrobials for Improved Warfighter Health

Challenge

Antimicrobial treatments are being utilized by the U.S. Army in a number of textile systems including T-shirts, socks, and sleeping bag liners in an effort to control odor and reduce skin irritation, thus improving quality of life for the Warfighter.

This success supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Protection Sciences



Human Sciences



Current chemically-derived antimicrobials including metals (silver- and copper-based compounds), polyphenols, halamines and quaternary ammonium compounds have proven effective as antimicrobial treatments for textiles. However, the processing and use of these compounds results in production of environmental hazards, and these compounds suffer several deficiencies including lack of durability, deleterious impact on textile physical properties and high costs. Most importantly, the current chemical-based treatments possess broad-spectrum antimicrobial activity, which may contribute to the development of dangerous bacterial resistance. Moreover, textiles treated with broad-spectrum antimicrobials non-specifically kill beneficial bacteria required to maintain skin health. The normal skin flora helps prevent pathogenic microbial colonization and growth by providing competition for space and resources and maintaining an acidic skin pH (pH ~5).

SUCCESS

A highly selective non-chemical-based textile coating effectively kills > 99.9% of pathogenic bacteria while sparing beneficial skin bacteria, paving the way for an effective antimicrobial treatment for a variety of Army materiel, including next-to-skin clothing, combat surgical shelters, and medical/hygiene wipes.

RESULTS

- ▶ Co-development of a research topic with CCDC SC to specifically eliminate pathogenic bacteria while sparing beneficial skin bacteria
 - ▶ Demonstration of highly targeted biologically-derived antimicrobial that kills > 99.9% of *S. aureus* within 1 minute of contact
 - ▶ Development of a textile coating process that maintains targeted antimicrobial killing activity after laundering
 - ▶ 2017 Defense TechConnect Innovation Award
-

Action

As a potential solution to the challenges presented by chemical-based broad-spectrum antimicrobials, ARO Biochemistry program manager, Dr. Stephanie McElhinny, partnered with Mr. Jason Soares and Mr. Steven Arcidiacono of CCDC Soldier Center (SC) to conceive a research topic for the Small Business Technology Transfer (STTR) Program to explore the potential of biologically-derived molecules to serve as targeted environmentally-friendly antimicrobials for textiles. Targeted bacterial killing to eliminate pathogenic microbes while maintaining beneficial bacteria could improve overall Soldier health and quality of life. Many biologically-derived molecules (e.g., bacteriocins, bacteriophage, and phage lytic enzymes) have demonstrated effective antimicrobial activity with increased specificity relative to chemical-based systems and no associated environmental hazards, representing a potential new generation of selective antimicrobials.

The goal of the STTR topic was to develop biologically-derived antimicrobials that demonstrate efficacy against the primary bacteria responsible for skin irritation and/or odor, while maintaining the viability of bacteria required for skin health when applied to military textiles that have direct contact with the skin. Healthy skin is colonized by consortia of bacteria consisting of mainly Gram-positive bacteria from the genera *Staphylococcus*, *Micrococcus*, *Corynebacteria* and *Propionibacteria*. For this topic, the antimicrobial technology was to selectively kill *Corynebacteria*, which is primarily responsible for malodor associated with sweat and/or *Staphylococcus aureus*, which is associated with atopic dermatitis. The antimicrobial technology was to have no effect on *Staphylococcus epidermidis*, *Micrococcus* and *Propionibacteria*, to maintain beneficial skin bacteria.

Result

Giner, Inc., a small business located in Newton, MA, partnered with Texas A&M University to develop a promising biologically-derived targeted antimicrobial technology under this topic that is compatible with textile coating and robust to laundering. The research team has identified a bacteriophage (viruses that infect bacteria) that specifically targets and kills *S. aureus*, while having a negligible impact on beneficial skin bacteria. The team has demonstrated effective targeted killing of *S. aureus* by > 99.9% (> 3 log) after only 1 minute of contact time with no significant effect on the commensal beneficial skin bacteria. The team has also developed a novel textile coating that maintains the activity of the bacteriophage after laundering.

Based on the research team's significant achievements thus far, this effort was selected for a Subsequent Phase II award in FY2018 (\$1M investment over 24 months) to further optimize and expand testing of the bacteriophage coating and to demonstrate safety and efficacy in preclinical animal models. The team will also focus on refining the coating process to attain a commercially viable product pipeline. The significant potential impact of this research effort for the DoD was recognized with a Defense TechConnect Innovation Award in October 2017 (<https://defensetechconnect.com/awards/>), which is awarded to the top 15% of technologies presented at the Defense TechConnect Summit based on their potential positive impact for the Warfighter and national security.

Way Ahead

The development of a biologically-derived antimicrobial textile coating with selective killing efficiency will prevent complications inherent with broad-spectrum antimicrobial compounds used for odor reduction and/or prevention of skin irritation and will support commercially-viable antimicrobial textiles with negligible environmental hazards associated with production and usage. A variety of military textile materials would benefit from development of targeted antimicrobials including Army combat T-shirts, medical/hygiene wipes, ballistic boxers, Army combat socks, Army combat boots, combat surgical shelters, and combat sleep systems (linens, sacks, etc.). This targeted biologically-derived antimicrobial coating technology is well-positioned to transition into existing programs at CCDC SC and PEO Solider, and the Defense Threat Reduction Agency (DTRA) has recently expressed interest in this effort due to a focus on antimicrobial technologies for next-to-skin applications.

BIOCHEMISTRY PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Develop approaches to engineer and control mechanisms underlying biomolecular specificity and regulation that if successful is anticipated to lead to novel biosensing reagents and responsive materials.
- ▶ Design self-assembled biomolecular architectures to support functional organization of biological molecules that if successful is anticipated to lead to novel power and energy systems and on-site manufacturing capabilities.
- ▶ Understand sequence-structure-property relationships in biological and biohybrid materials that if successful is anticipated to lead to rationally designed materials with tailored properties.

This success supports these ARL Core Technical Competencies



Protection Sciences

GENETICS PROGRAM



Dr. Micheline Strand

Program Manager, Genetics
Life Sciences Division
ARO Physical Sciences Directorate

Dr. Strand completed her undergraduate studies at Oberlin College, receiving her B.A. in Biology in 1985. She trained as a geneticist at the University of North Carolina - Chapel Hill, receiving her Ph.D. in Genetics and Molecular Biology in 1995.

She came to ARO in 2000 as the Program Manager for Genetics.

Elemental Reducing Agents to Modulate Mitochondrial Activity and Reduce Warfighter Mortality

Challenge

Bacteria spores are well known suspended animators; when times are tough they transform into tough dried out spores and they can survive in this metabolically inactive state for years and even centuries. Similarly, many Americans may remember buying “sea monkeys” as children: dehydrated brine shrimp eggs that could be rehydrated into instant living pets. Even more interestingly, there are numerous cases of human beings being buried by avalanches or snow or falling into icy water – whose bodies are recovered having neither a pulse nor a heartbeat – but nevertheless revive when being warmed up and go onto to lead normal, productive lives. In fact, doctors are trained not to declare a cold body dead unless it remains dead when warmed up!

Action

ARO’s involvement in elemental reducing agents began in 2001 when the Genetics Program Manager read an article in PNAS from Mark Roth’s lab about putting zebra fish into suspended animation (Padilla and Roth, Oxygen deprivation causes suspended animation in the zebrafish embryo, Proc Natl Acad Sci USA 2001 19;98(13):7331-5). When she was asked by the past Director of ARO’s Life Sciences division to recommend some deep thinking scientists for the brainstorming session for what would eventually lead to the Army Institute of Collaborative Biotechnologies (AICB), she recommended Mark Roth. Mark Roth accepted the invitation and came to ARO’s biotechnology/pre-AICB brainstorming session. Although the AICB ended up focusing on biomaterials, not 6.1 biology, and did not include the Fred Hutchinson Cancer Research Center or research on suspended animation, discussions at this meeting were the catalyst for DoD support that enabled Mark Roth to pursue this research.

Normal air on this planet is 21% oxygen. Eight minutes at 8% oxygen is 100% fatal for humans. Nematodes also die at these lowered oxygen levels. However, Dr. Roth noticed that at 100-fold lower concentrations of oxygen, 10 parts per million, the nematodes did not die, they instead entered a state of suspended animation, and that furthermore they could be brought back to life and suffered no detectable long-term effects. He also discovered that when he put his nematodes into cold they died, but if he put them into suspended animation first (via exposure to very low levels of oxygen) they survived being very cold for long times just fine.

However, many humans cannot be woken back up after being buried by avalanches or falling into icy seas. Dr. Roth was motivated to find a way to put humans into a state of suspended animation. After many failures he realized that hydrogen sulfide – found naturally in some caves – was already known to cause exposed people to collapse and appear dead, but that they could be reanimated if removed from the hydrogen sulfide – as long as one didn't wait very long. Having a solid background in biochemistry, he also knew that mitochondria burn oxygen to generate energy, which is what enables humans to move and to think, and that hydrogen sulfide could bind the mitochondrial cytochrome c oxidase in the very same binding site. So the question then was: would this work in something bigger than a nematode?

Dr. Roth went on to test hydrogen sulfide in mice, and discovered that indeed, exposure to hydrogen sulfide blocked mitochondrial activity and the mouse became unable to produce energy. However, and this was unexpected, the mouse also stopped moving, became cold, and appeared dead (with no heart beat or brain activity). After six hours of exposure to hydrogen sulfide and apparent lifelessness the mouse could be brought out of the chamber, placed on the lab bench, and it would warm up, come back to life, and go on to live an apparently normal mouse life.

Result

Dr. Roth founded a company at this point, Ikaria, which went on to test hydrogen sulfide in pigs and then humans as an agent to prevent deaths from heart attack and strokes. Hydrogen sulfide turned out to be too dangerous for human use (the therapeutic index is too narrow) however the company did use this technology to develop a therapy for newborns with hypoxic respiratory failure, this is now a FDA approved drug that is used to save newborn babies that would otherwise die from an inability to be able to properly oxygenate their tissues. This therapeutic saves thousands of babies every year from certain death.

However, there is still the unresolved issue of adult humans. Dr. Roth then went on to look at other chemically similar compounds that could also bind cytochrome c oxidase and block energy production in humans. He found one that is chemically similar and is already part of the normal human diet. He is convinced that our daily consumption of this mineral is massively too low. Phase I human safety trials have been completed and demonstrate that elevated levels of this compound in human beings is very safe. His company has been approved to begin multi-center trauma clinical trials in the summer of 2019. Mark's results have been replicated by Army scientist Dr. Mike Morrison and discussions are ongoing with other Army scientists at the Army Medical Command to test efficacy in burn and sepsis patients. Levels of this compound are naturally variable in individual humans, however higher concentrations are strongly correlated with better outcomes after stroke and trauma. Further work is needed to conclusively establish that supplemental dosing would reduce mortality in Soldiers and Civilians.

Way Ahead

In summary, this research has demonstrated a completely new approach to reducing human deaths from hemorrhagic shock, trauma, sepsis, heart attack, and stroke. Although not finished, the work has attracted approximately thirty million dollars in co-funding from DARPA and venture capital funds. Dr. Roth has consistently affirmed that his work could not have occurred without DoD support; it is simply too high risk to be funded in NIH's peer reviewed group decision making process. ARO's enthusiastic support for high-risk high-payoff research is the only possible model by which such innovative, ground-breaking, and paradigm shattering research could have occurred.

SUCCESS

ARO-funded research led to characterization of metabolic mechanism and new therapeutic to potentially extend the time for treatment after severe blood loss. With external funding, the safety of this therapeutic has now been established in human clinical trials, and human clinical trials to validate the efficacy are underway.

This success supports these ARL Core Technical Competencies



Protection Sciences

SUCCESS

ARO-funded research led to the first successful breeding pairs of pouchies in captivity at Cornell University.

Pouchies, Social Biology and the Detection of Unexploded Ordnance

Challenge

Unexploded ordnance contaminates 78 countries and kills 15,000 to 20,000 people a year. Eighty percent of these casualties are civilians and most of them are children. Mines are a cheap and asymmetric form of warfare; placing them is easy but removing them is time consuming and expensive. Low-cost, highly-effective unexploded ordnance detection capability is a humanitarian and a DoD priority.

Although earlier generations of mines could be detected with metal detectors, there is an increasing move towards plastic encased non-metallic mines and IEDs that must be directly detected by trace odors. Direct smelling of explosive vapor is done either by explosive trace detector equipment or with animals. Although not rigorously quantified, it is apparent that trained animals are capable of detecting explosives at levels lower than abiotic systems such as GC/MS.

Action

In 2010, ARO assembled a task force of experts to travel to Tanzania and directly investigate whether the reported use of giant African pouched rats by Anti-Persoonsmijnen Ontmijnende Product Ontwikkeling (APOPO), a Belgium based non-profit, to find unexploded mines is a reliable method and whether this would be a useful capability to bring into the Army. The investigative team consisted of a combat engineer and a cadet from West Point, three chemists with expertise in explosives, one canine physiologist, one person who trains dogs full-time to find explosives, one rodent behavioral scientist, and the ARO Genetics Program Manager.

The goal of this task force was to determine whether rats are capable of detecting mines and to determine whether the rat has potential utility for the U.S. DoD in demining operations and/or explosives detection. The team traveled to Mozambique and Tanzania to first hand observe and evaluate the training and demining operations done by APOPO.

Result

The site visit to APOPO in Tanzania and Mozambique confirmed that the African giant pouched rat has a robust ability to detect land mines. Despite their small size, these rodents' ability to detect and report the presence of mines is on par with trained dogs. Although there is considerable emotional resistance from warfighters to replacing military working dogs (MWDs) with military working rats (MWRs), ARO's intent was not to replace the military working dogs with trained rats, but instead to create an additional capability. Rats have benefits and capabilities that dogs do not: rats are light and small, their logistical support needs are minimal, they don't bark, they can travel unnoticed through most environments, they can climb trees, and (most) warfighters will not risk their life to save their trained rat.

The current cost of an IMAS-accredited mine detecting rat is somewhat lower than a comparably-accredited dog, however this is primarily due to low labor costs in East Africa. Compared to dogs, pouched rats appear to have simpler logistical needs, potentially making them an economical alternative to the use of dogs in selected situations. Small animal based detection systems have potential value in exploring spaces too small for people to get into, or otherwise difficult for humans or dogs to access. In addition, Warfighters could carry rats in their backpack, they would be more covert than dogs, and could be left behind at the end of the mission.

However it is the social science of rats that makes them a compelling potential capability for the Army. Dogs are motivated by human interaction. They train with a particular soldier and training a dog consumes considerable soldier time. A Soldier must train with his or her dog a month before deployment; dogs are not an off the shelf capability. The \$30K per trained mine detecting dog cost is primarily due to the time required by the human trainer. In contrast, the rat is motivated by food. Thus it should be possible to remove the human from the training loop altogether, and reduce the cost from ~\$20K per trained rat to a few hundred dollars. ARO has been working with two small U.S. businesses, with some assistance from scientists at the Defence Science and Technology Laboratory (DSTL) and demining experts at the State Department, to automate rodent training. Significant progress has been made however large scale production for field use is still several years away.

A more immediate and scientifically interesting problem is defining and understanding the biology of these giant African pouched rats. APOPO is sorely lacking in scientific expertise, scientific equipment, and funds for scientific research; this species is essential unstudied. APOPO catches their animals in the wild, and even releases trained animals back to the wild when funds for rodent chow run low. APOPO says that they are "difficult to breed" but has no information on why.

ARO initiated a research project with Dr. Alex Ophir, now at Cornell University, to import some of these animals from east Africa to the United States so that modern scientific equipment and expertise could be used to examine their social, molecular and genetic biology. This turned out be considerably more complicated than expected. First permits had to be obtained from the CDC and U.S. Fish and Wildlife, then in 2011 the Prime Minister of Tanzania banned the export of all live animals from Tanzania. Finally in 2012, eighty giant African pouched rats left Ghana on a direct flight on Delta to Atlanta. Upon arrival in Atlanta, 76 of the 80 of the animals were dead. A second shipment was arranged and permitted but multiple airline crashes in Ghana led to further delays. Finally, in early 2013 fifty rats left Tanzania and arrived alive at Cornell University.

After this, multiple unexpected and surprising scientific discoveries followed in quick succession. The whole genome was sequenced and the genome analysis revealed that the Giant African Pouched Rat is not a rat at all; it is more closely related to hamsters than rats. Giant African Pouched Hamster would be a more accurate name but instead they are now being called Pouchies.

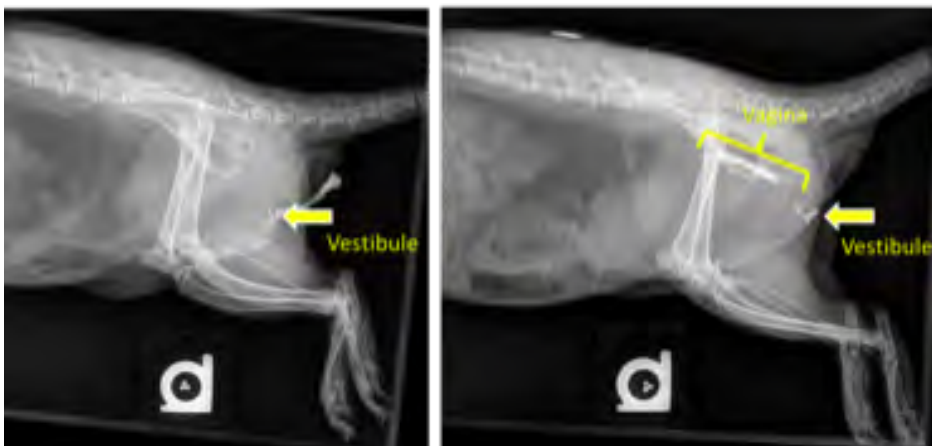


Figure 1: Vaginal patency refers to the opening of the vaginal canal to the vestibule (which allows for intromission). The adult female on the left has a non-patent vagina, the adult on the right has a patent vagina.

At the same time, the graduate students at Cornell were realizing that the pouchies were not behaving like rats. Pouchies reproduced for the first time in the U.S. at Cornell and the students – expecting these animals to behave like rats – removed the animal that was not taking care of the pups (i.e., presumably the father, from the cage, so that there would be no risk of him eating the pups (as male rats will do). Unfortunately it turned out that the male pouchie had been taking care of the pups and it was the mother that was napping by herself in the corner, and by the time the students realized their error, the pups were dead. When the second and subsequent litters were born, both parents were left with the pups, and the pups thrived.

Even more surprising was the discovery that some fully grown female pouchies did not have vaginal openings. This has never been observed in mammals before. As the scientists at Cornell noted: “To say that the lack of vaginal patency presents a barrier to mating is a tremendous understatement.”.

Even more shockingly, it turned out that mature females with vaginal openings could lose them, and close back up again. Clearly, something unusual was going on.

In brief, after considerable research, it is becoming clear that colonies of pouchies do not act like humans and other mammals (in which males and females pair up temporarily or permanently, with most individuals successfully reproducing) but rather that a group of pouchies more closely resembles a honey bee colony; one female reproduces and emits chemical signals to keep the other females from reproducing (and, like honey bees, the asexual females can become patent and reproduce if the dominant female dies or is removed).

Way Ahead

In summary, ARO initiated and enabled the establishment of the first U.S. breeding colony of pouchies, initiated work to automate pouchie training, sequenced the pouchie genome leading to the discovery that Giant African Pouched Rats are not really rats, and determined that pouchies have a most unique social biology that governs who may and who may not reproduce. Further work is ongoing to understand their learning and motivation (also very different from rats) in order to explore the value of trained explosive detecting rodents as a new Army capability.

GENETICS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Identify and characterize the molecular and genetic mechanisms regulating mitochondrial integrity and activity in order to transform warfighter protection and performance capabilities.
- ▶ Create a high throughput technology for rapidly characterizing human polymorphisms in order to be able to remediate suboptimal enzyme levels for enhanced warfighter protection and performance.
- ▶ Understand and characterize the drivers and signatures of DNA mutations at a whole genome level and across species for enhanced stability of engineered genomes, for better warfighter protection and for intelligence applications.
- ▶ Create new platform technologies to rapidly identify the provenance of mixed microscopic samples.
- ▶ Understand and characterize learning and performance in *Cricetomyces ansorgei* in order to create new smart autonomous sensing capabilities.

SOCIAL AND BEHAVIORAL SCIENCES PROGRAM



Dr. Lisa Troyer

Program Manager, Social and Behavioral Sciences
ARO Physical Sciences Directorate
Life Sciences Division

Dr. Troyer completed undergraduate studies in 1989 at the University of Washington, receiving her BA in Sociology. She trained at Stanford University, earning her M.A. in 1990, and Ph.D. in Sociology in 1995.

She came to ARO in 2013 as a SETA Contractor to support the development of programming in the social and behavioral sciences. In 2015, she was appointed as Program Manager of the Social and Behavioral Sciences Program, Life Sciences Division.

Path-Breaking Research in Collective Biometric Dynamics Generates New Capabilities to Identify and Track Adversarial Groups

Challenge

Existing research in the social and behavioral sciences does not objectively measure human behavior or social dynamics such as collective influence, aggression, affective diffusion, and performance. While emerging biometric technologies are affording new ways to objectively measure individual states, extending them to the level of collective action has remained a challenge; and as a result, advances in social dynamics have been hobbled. In 2015, the Army Research Office initiated a program to investigate how combining methodologies from individual-based biometric measurement with theories of social dynamics could address both human-level and collective-level dynamics. The program develops a new strategy of collective biometrics to predict collective behavior.

Action

Starting in FY15, Dr. Troyer, the program manager for Social and Behavioral Sciences, began crafting a new program to overcome deficiencies in measuring and modeling social dynamics focusing on pathways from individual action to large-scale social processes. The approach Dr. Troyer developed is two-pronged. First, it requires developing unbiased measurement of individual and collective behavior. Existing research has relied on inappropriate sampling, self-report, and observation – all of which tend to generate biased data and inaccurate analyses, leading to faulty conclusions. Second, accurately determining the relationship between individual and population dynamics requires recognition that the large-scale action is not a simple aggregation of action by individuals. Aggregation is a longstanding fallacy in social and behavioral science. Consequently, new measurement methods and techniques to capture the dynamic nature of collective action need to be developed to accurately capture collective action.

As a first step, Dr. Troyer used her 20+ years of prior research expertise on developing objective measures of collective action in the domains of influence, opinion formation, credibility, and decision sciences. The work leverages biometric measurement at individual levels with iterative modeling strategies to track the relationship of individual states to collective outcomes. She encouraged researchers working on such techniques to submit proposals, beginning in 2015. In 2016, Dr. Frederick Gregory (ARO), Dr. Justin Brooks (CCDC ARL-HRED), and Dr. Amar Marathe (CCDC ARL-HRED) invited her to join

This success supports these ARL Core Technical Competencies

Human Sciences



Network and Information Sciences



Computational Sciences



SUCCESS

In only four years (FY14-FY18), ARO has crafted a new strategy in collective biometrics that leverage advances in human biometrics to predict social dynamics, paving the way for less obtrusive ways that Warfighters and decision-makers can use to identify adversarial groups, predict risk of collective conflict, and enhance operational decision-making

in planning a workshop on individual states and traits. Dr. Troyer suggested adding expertise on collective dynamics in human groups and offered to recruit scientists to share their research. The workshop was convened at Johns Hopkins University on 24 Mar 2016.

She asked researchers who were pioneering different methods to detect collective dynamics to participate. They included scientists developing: (1) facial thermography to track emotion diffusion in groups, (2) methods to trace brain patterns across group members involved in collective decision-making; and (3) vocal spectrum analysis techniques to influence dynamics. The contribution to the workshop was to demonstrate that biometrics could be used to explain more than individual states at a point in time. Combined with social theory and dynamic modeling, biometric approaches could capture collective outcomes and pave the way for a new approach to social science. From the workshop, additional avenues for advancing these methods became apparent and Dr. Troyer encouraged the PIs already working with her to leverage the new insights and invited other PIs to submit proposals. Another line of work that emerged from this effort was work on epigenetic theories of collective aggression, leading to a proposal that Dr. Troyer also selected for funding.

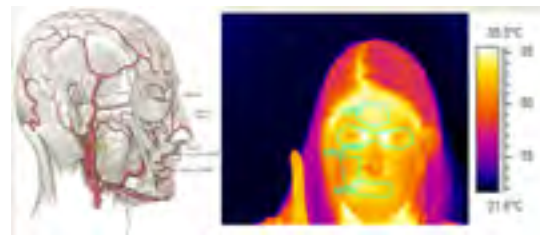


Figure 1. Facial thermography examines the relationship between blood flow to facial muscles and specific emotional states. Different configurations of muscles correspond to different specific emotions (Emotion Review, 7:157-162)

In the facial thermography component of Dr. Troyer's collective biometrics thrust research shows that fine-grained emotion can be detected by thermographic tracking of facial muscles. Dr. Troyer selected a proposal by Dr. Dawn Robinson (Univ. Georgia) to pursue facial thermography. Traditional self-report methods for capturing emotion can at best detect coarse states (e.g., positive vs. negative affect), and even then with substantial bias and variability. This is because people tend to report what they want others to think they feel (e.g., to deceive or conform to social norms), rather than what they actually feel. More objective methods, such as thermography, could provide less-biased fine-grained distinctions (e.g., anger vs. frustration; happiness vs. satisfaction). This is because different configurations of muscles are involved in expressing different emotions and these muscles are difficult for individuals to control.

Importantly, not only does thermography enable dynamic tracking of an individual's emotional state; if used in a collective setting, it can detect the diffusion of emotion within a group. By combining thermographic sensors and network analytics, non-intuitive patterns of emotional diffusion occur. For example, in an experiment a "cheater" was planted among a group of test-takers who thought their test scores would be rewarded by a commensurate share of a pool of money. Counterintuitively, once the cheater became known, spatially proximate actors were less likely to reflect anger sooner in the thermographic results, compared to less-proximate actors. Also, Dr. Robinson found that thermography detects guilt when an individual is over-rewarded. This research led to the development of a new coding system that integrates theoretical perspectives on norms of emotion with facial muscle groups.

Another project aimed at tracking affective states involves the genetic bases for aggression. Research shows heightened aggressive tendencies in response to environmental stressors. Dr. Troyer reasoned, that social stressors may generate similar tendencies. She chose a proposal by Dr. William Reed (Univ. Maryland) to test the effects of social stressors on aggression, including political violence. This

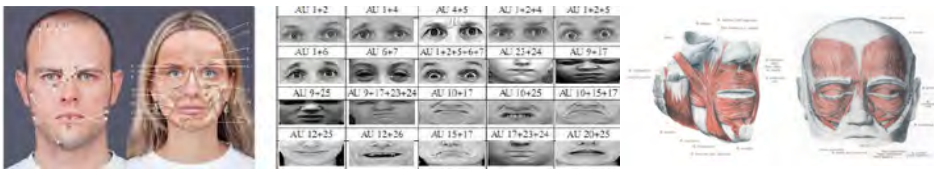


Figure 2. Facial Action Coding System identifying key facial areas and associated muscle groups for fine-grained differentiation of emotions. Left panel shows regions of face corresponding to muscle groups in the right panel that define key muscle groups for emotion detection (Advances in Group Processes, 2018, Stanford Univ. Press)

research focuses on the MAO-A gene. This is a gene affects the production of an enzyme, monoamine oxidase A. This enzyme regulates social behavior through neurotransmitters related to self-regulation. Researchers have found that the low variant of MAO-A results in significantly lower levels of this enzyme. Consequently, the low MAO-A variant has been associated with higher aggressive tendencies, while the high-MAO-A variant is associated with lower aggressive tendencies. Surveys, validated through public records, were used to determine if individuals enrolled in the study had participated in political violence. Additionally, experiments were conducted that expose the enrollees to social injustice, (i.e., by denying them earned rewards). The experiments allowed subjects to elect the degree to which they would punish the actor they believed imposed the injustice. Results showed a tendency for individuals with the low MAO-A variant to have a greater probability of engagement in political violence, as well as heightened aggressive tendencies when experiencing social injustice.

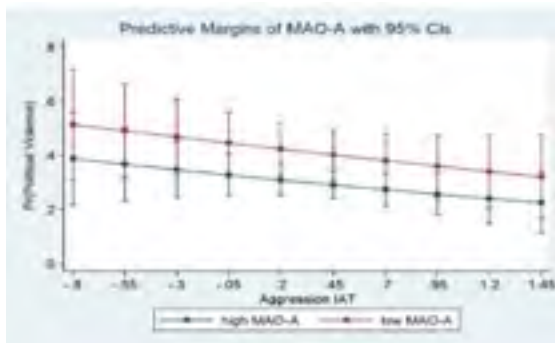


Figure 3. The low variant of MAO-A is associated with greater aggressive tendencies, both in the form of probability of engaging in political violence and aggressive responses to social injustice.

Aggressive tendencies are a sign of the emergence of dominant actors in groups. As Dr. Reed's research proposes, this is traceable to neurological functioning. To further this research program on collective biometrics, Dr. Troyer selected a proposal submitted by Dr. William Kalkhoff (Kent State Univ.) that investigates the neurodynamics of dominance and influence in social groups. This work draws on expectation states theory, which traces the emergence of influence hierarchies to subconscious stereotypes that elicit expectations for performance (independent of relevance to the task). Dr. Kalkhoff reasoned that the subconscious nature of influence dynamics suggests that a neurological process is at play and set out to identify it. This project was developed in tandem with another ARO-funded effort Dr. Troyer had selected led by Dr. David Melamed (The Ohio State Univ.). This project used fMRI to identify brain regions that are activated when influence hierarchies come into play in groups. After discussing this with Dr. Troyer and Dr. Melamed, Dr. Kalkhoff leveraged the work to focus on the same regions Dr. Melamed had discovered. Dr. Kalkhoff used EEG technologies, which have high temporal resolution and permit more mobility, compared to fMRI, which requires subjects to remain prone in close quarters in a scanner. A key premise of expectation states theory is that the actions of other members of a collective will be processed by a focal actor as indications of whether others accept the focal actor's attempts at influence. If the focal actor believes influence is warranted, but others reject the influence attempt, the focal actor is theorized to experience both emotional

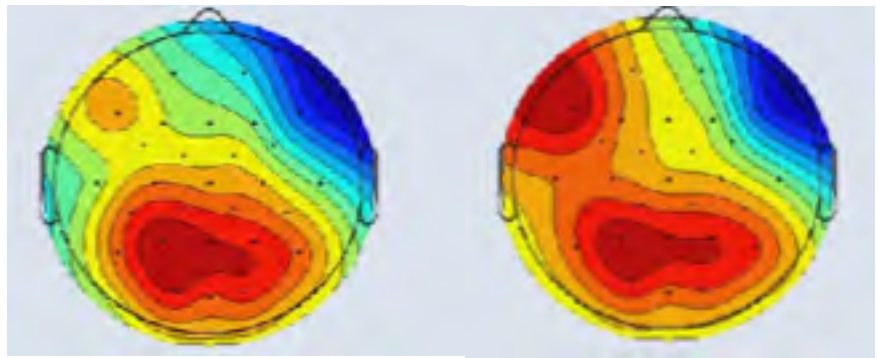


Figure 4. Neurological patterns reflecting influence dynamics in collectives working on decision-making patterns when influence is accepted or rejected by group members. Left panel shows influence acceptance pattern; right panel shows influence rejection, characterized by drastic increases in Dorsolateral Prefrontal Cortex activity (Social Psychology Quarterly, forthcoming)

and cognitive reactions, such as anger and confusion. To date, however, the cognitive reactions have remained a black box. Drawing on existing research, Dr. Kalkhoff reasoned that the feedback-related negativity (FRN) event-related potential component (ERP) occurs around 250 milliseconds post-stimulus. Thus, the hypothesis was that this slice of the spectral analysis was key to detecting impact of influence behaviors by the focal actor and responses of other group members.

Dr. Kalkhoff's research demonstrates distinct neurological patterns for actors whose groups disregarded their influence. This activity is particularly pronounced in the Dorsolateral Prefrontal Cortex, a region associated with problem-solving and cognitive adjustment. Moreover, the results are more robust, with less variation, than conventional self-report of influence dynamics. Self-report may reflect egocentric biases (i.e., disregarding what actually happened, instead reporting what should have happened). This breakthrough is the first evidence of how collective influence dynamics reflect neurological functioning.

The fourth project comprising Dr. Troyer's initial steps in the path-breaking program on collective biometrics to capture social dynamics also focuses on dominance and influence using vocal spectrum analysis. In an experimental test of patterns in the low voice spectrum, Dr. Dippong was able to document the emergence of dominant actors. Early in the interaction, actors who are initially undifferentiated share this vocal range. As the interaction progresses, however, one actor will cede dominance of this range to the other, who also is identified as the more influential actor (both by behavioral measures and observer assessments). The deferring actor, however, continues to follow the trend of the dominant actor. The work by Dr. Dippong is the first to isolate this dynamic, demonstrating its potential to serve as an objective dynamic indicator of influence in collectives.

Result

Early detection of adversarial groups and understanding their dynamics is critical to the decision-makers and Warfighters. These groups may not be easily identifiable, but by understanding the relationship between social dynamics and biomarkers that can detect those dynamics, the Army can more swiftly intervene to mitigate risk and retain overmatch. The Army Research Office is using a systematic approach to identify objective methods to detect risks within collectives and accurately model collective biometric dynamics to predict large-scale collective action that threatens national security. The starting point is collective biometrics as an objective measurement of social states that feed into models of collective action, with improved reliability, as demonstrated by these projects, to avoid significant disadvantage in operational decision-making. The Army Research Office investment in Social and Behavioral Sciences is driving this research agenda forward. The program's objective is to aid the U.S. in maintaining overmatch in non-kinetic conflict. It has played a key role in advancing Multi-Domain Operations, which include developing regional sociopolitical awareness and defeating challenges by near-peer powers (e.g., China, Russia) that are already gaining a foothold in non-kinetic domains.

Way Ahead

The next steps for the collective biometrics thrust of ARO's Social and Behavioral Sciences Program involve continuing to develop and refine measurement and modeling strategies; and integrating the measurement strategies described here. In addition, the program will incorporate strategies to measure the emergence of pro-social collective action, including cooperation, social facilitation, cohesiveness to further, in addition to continued focus on asocial dynamics related to influence, dominance, and aggression, fundamental concerns systems to enable enhanced capabilities to distinguish adversary from allied collectives and identify when collectives are transitioning from one to the other.

SOCIAL AND BEHAVIORAL SCIENCES PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Identify and validate measurement methods to detect shifts in human behavior and collective action that if successful will lead to new tools to identify emergent conflict, violent extremist individuals and groups, and deception attempts by adversaries.
- ▶ Generate and validate predictive approaches to causally model emergent risks from individual to population levels that if successful will provide decision-makers with improved operational effectiveness.
- ▶ Investigate interdependencies among social, natural, and physical systems to determine the spatial and temporal evolution of dynamics that if successful will enable long-term prediction of precursors of conflict.

RESULTS

- ▶ Invited briefings to key policymakers (Joint Staff, J9; National Security Agency, Defense Intelligence Agency)
 - ▶ One scientist appointed to American Academy of Arts and Sciences
 - ▶ ARO program manager invited to participate on red-blue teaming exercise in information warfare strategies and biological ethics
 - ▶ Nine peer-reviewed publications in scientific journals/edited volumes.
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PHYSICS DIVISION: FY18 SUCCESS STORIES

ATOMIC AND MOLECULAR PHYSICS PROGRAM



Dr. Paul M. Baker

Program Manager, Atomic and Molecular Physics
Physics Division
ARO Physical Sciences Directorate

Dr. Baker completed his undergraduate studies at Wright State University, receiving his B.S. in Physics in 2002 with honors. He trained as a physicist at Tufts University receiving his Ph.D. in 2009.

He came to ARO in 2010 as the Program Manager for atomic and Molecular Physics and has served as USASOC Liaison since 2013.

Superradiance: Strong Interaction Provide Improvements in Metrology

Challenge

A major DoD priority is to provide sustained accurate navigation and timing in the absence of external aiding, such as GPS. Quantum systems provide a potential solution due to their extreme sensitivity and non-classical error rates. Recent scientific progress has focused on control and isolation, because of the general sensitivity of quantum systems to local environments. For quantum systems to be effective for many U.S. Army applications laboratory control and isolation will be challenging to engineer. Therefore, ARO Atomic and Molecular Physics program made strategic investments in strongly interacting quantum systems that increased the robustness, while maintaining non-classical sensitivity.

Action

In 2010, ARO Atomic and Molecular Physics program manager, Dr. Paul M. Baker began funding Professor Murray Holland at the University of Colorado. The project began as a nine-month Short Term Innovative Research (STIR) grant titled "Development of a Superradiant Collective Optical Laser." At the time Professor Murray was not sure that his idea would work, and this high-risk theoretical effort was to provide evidence that could be supported and confirmed experimentally. This theoretical effort provided enough evidence for ARO to pursue experimental confirmation. Dr. Paul M. Baker contacted Professor James Thompson and encouraged him to submit a proposal to experimentally confirm the theoretical result. Within nine months, an experimental demonstration was achieved under the ARO grant titled "A superradiant laser: Toward a mHz linewidth laser." This experimental proof of principle effort was so successful it resulted in \$5M DARPA DSO program titled Advanced Timing and Navigation (ATN)/ ARO managed grant "Extreme sensing using collective quantum physics" and has paved the way to achieving a critical DoD technical capability in assured Position, Navigation, and Timing (PNT).

The superradiant laser efforts have resulted in a new sub-field of engineering collective quantum states for enhanced metrology. This effort pioneered a new paradigm of narrowing laser linewidth by relying on atomic ensembles trapped within the cavity. This

This success supports these ARL Core Technical Competencies



Network and Information Sciences



Computational Sciences

novel insight provided a new scientific path for discovering non-classical sensors that are robust to local environment noise. ARO's ability to identify, execute, and advocate on behalf of the U.S. Army's Modernization Priority are resulting in new capabilities in assured position, navigation, and timing in the absence of GPS.

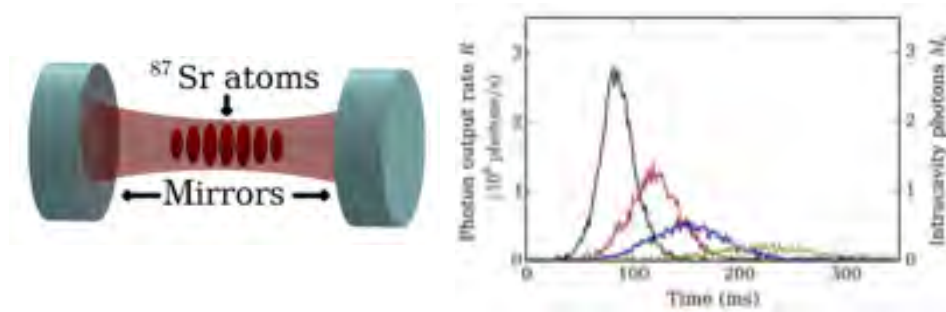


Figure 1. (Left) Strontium atoms confined in an optical lattice within a high Finesse optical cavity. (Right) Time traces of photon output rate of superradiant emissions at different atom number, (green) $N=100 \times 10^3$, (blue) $N=125 \times 10^3$, (red) $N=150 \times 10^3$, (black) $N=200 \times 10^3$.

Results

What has emerged from this effort is a transformative branch of quantum optics utilizing superradiance and more broadly the establishment of using collective states of quantum matter. Superradiance is a phenomenon that occurs when a group of atoms collectively and coherently emits light in a high intensity pulse. In the form that it was first proposed by professor Holland and has since been realized by Professor Thompson, atoms are trapped in a one-dimensional optical lattice that is contained within an optical cavity as shown in Figure 1 (left). The resulting array of atoms interacts with the cavity field to produce a superradiant pulse of light, Figure 1 (right). The rate of collectively enhanced emission per atom increases proportional to N^2 , for higher atom numbers the pulses appear sooner, have shorter duration, and have a higher peak power than for lower atom numbers.

The frequency stability of a superradiant laser is dependent upon the collective coherence properties of the strontium atoms. The better the collective coherence the more stable the laser frequency. (^{87}Sr) has a quantum state with a long decay lifetime of roughly 150 s. The inverse lifetime of this state corresponds to a frequency linewidth of 1 mHz, which is more than 109 times narrower than typical optically excited states. In a normal laser the cavity mode linewidth is much narrower than the gain profile linewidth of the lasing medium which in this case is the strontium atoms. Thermal and mechanical fluctuations in the cavity mirrors which effect the cavity length will cause fluctuations in the frequency of traditional lasers. In contrast, a superradiant laser's linewidth depends upon the coherence of the gain medium. The effect depends upon a "bad cavity" or a cavity with a broad linewidth, much broader than the gain profile. The resulting frequency is insensitive to fluctuations of the cavity length.

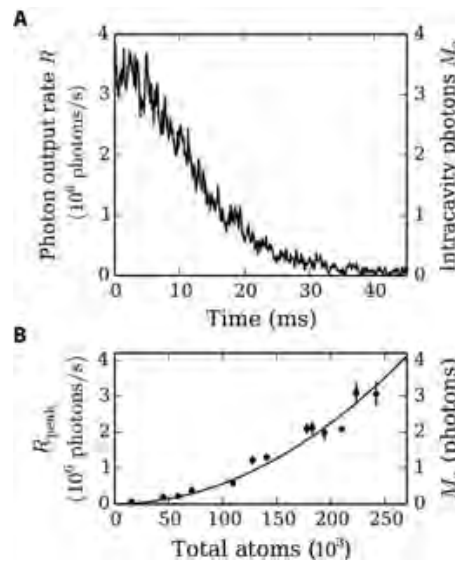


Figure 2. (A) Time trace of the photon output rate. (B) Peak photon output rate as a function of atom number.

RESULTS

- ▶ FY21 MURI on Quantum State Engineering for Enhanced Metrology
- ▶ Sub-mHz laser linewidth for precision navigation and timing
- ▶ Success led to a new DARPA program on ATN

In order to initiate a superradiant pulse on demand, the atoms are prepared in superposition of the excited and ground states. This leads to the immediate onset of superradiant emission as can be seen in Figure 2. If the atoms were prepared in the excited state superradiant emission and collective behavior would depend upon quantum noise and there would be a delay between state preparation and the onset of photon emission as is observed in Figure 1 (right). Collective enhancement lead to an emission rate into the cavity mode over two orders of magnitude greater than that of the same number of independently emitting atoms.

A Lorentzian fit to the peak in the average power spectrum returns a FWHM linewidth of 11 Hz, primarily reflecting the finite length of the pulse. In the future, in order to operate in a continuous manner, with pump lasers applied to return the atoms to the excited state. An important property of a continuous superradiant laser is that the linewidth of the emitted light is not limited by the collectively enhanced decay rate, as would be the case for single-atom decay. A second key promise of a superradiant laser is its reduced sensitivity to fluctuations in the length of the laser cavity. Expanding on the methods demonstrated here a millihertz stable laser may be achievable. This work demonstrates that marked effects can result from collective interactions with an optical field, even when mediated by an optical transition so weak that it takes roughly 150 s to decay without stimulation.

Way Ahead

The U.S. Army Research Office continues to drive this emerging field of collective states of matter for Extreme Sensing by managing a DSO DARPA program established to capitalize on ARO discovery. The ARO Atomic and Molecular Physics (AMP) PM manages the grant and is active in helping determine the scientific direction resulting in \$1M add-on to the original grant to explore inertial sensing. In addition, ARO AMP has championed and successfully achieved funding for a new FY21 MURI titled "Engineering Quantum States of Matter for Enhanced Metrology," where collective states will be used to further push the precision and protection needed to realize new U.S. Army capabilities.

Time Crystals: Scientific Investment in Many-Body Physics Provides New Possibilities for Future Materials

Challenge

In 2012, it was proposed by physicist and Nobel laureate Frank Wilczek that symmetry breaking in time could result in a new form of matter coined time crystals. Symmetries lead to laws of conservation. Translational symmetry results in the conservation of momentum and rotational symmetry requires conservation of angular momentum. Spontaneous symmetry breaking occurs when system becomes less symmetric than its parent system. The classic example of spontaneous symmetry breaking are crystals. The continuous spatial symmetry is broken and only discrete spatial symmetry remains (i.e., when you translate along a principle axis the crystals periodicity becomes apparent). In Floquet time crystals, periodicity exists in both space and time. Breaking of the discrete time translational symmetry has implications regarding the conservation of energy. The Army Research Office began an initiative in 2013 that strategically pursued to demonstrate the existence of Time-Crystals.

Action

In 2013, ARO Atomic and Molecular Physics program manager, Dr. Paul M. Baker, recognized an opportunity to investigate non-equilibrium phenomena, specifically at strongly interacting many-body dynamics using laser-cooled atoms trapped optical

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lattices. Discoveries made over the program's five years would result in promising new insight into the phenomena of Time-Crystals.

For discrete time symmetry to exist, a time crystal would have to be in a non-equilibrium state where the balancing of forces would lead to a constant periodic cycling. This implies that there must be some periodic driving potential as well as an out of equilibrium ground state associated with the lowest energy of the system. Further, the ground state would have to be independent of the driving potential. This leads directly to the time crystal requirements proposed by Army Research Office (ARO) funded researchers Norman Yao and Chetan Nayak who have helped define and invigorate the research in this field. These requirements are:

1. The system will exhibit spontaneous symmetry breaking by oscillating with a ground state frequency slower than the driving potential;
2. The system will generate no entropy by its oscillations (in ground state); and
3. The system will exhibit long range order; that is, oscillations will remain in phase over long distances and times.

Not only did ARO funding assist in the development of the theory behind time crystals, in fact, two separate ARO funded researchers were the first to demonstrate that time crystals could be realized in specific periodically driven systems. The U.S. Army Futures Command and ARO generated a Multidisciplinary University Research Initiative (MURI) titled Fundamental Issues in Non-equilibrium Dynamics which helped focus the physics community to look at non-equilibrium many-body dynamics. These demonstrations of time crystals are important to our understanding of foundational physics under specific symmetry breaking of time. In two separate publications in Nature Letters, investigators Mikhail D. Lukin, a professor at Harvard University, and Chris Monroe a professor at the University of Maryland present their observations of time crystals.

Time Crystals in Nitrogen Vacancy (NV) Diamond

Like its name implies, the nitrogen vacancy defect consists of a substitution of nitrogen and a vacancy site situated next to one another in a diamond matrix. The energy states of the NV site are determined by the combined effective system of the electrons in the dangling bonds of the vacancy and have an electronic $S=1$ spin. NV centers in diamond have some special qualities. Electronic levels are resonant with visible light, and hyperfine levels are addressable via microwave radiation. Spin state energy levels are magnetic field tunable and spin lifetimes are long even at room temperature.

Professor Lukin and his team at Harvard University use a diamond sample with a high density of NV centers. As shown in Figure 1, green laser light is used during state preparation and state readout, and microwave radiation manipulates the spin state. Microwaves induce interactions and excite global spin rotations. In order to probe the existence of time-crystalline order, the team uses two orthogonally polarized microwave pulses. The first induces interactions between NV centers and the second rotates the spin state. The duration of the pulses determines the strength of the interaction as well as the angle of rotation. The pulses are then repeated many times providing a periodic driving potential.

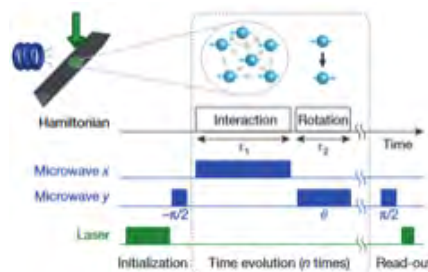


Figure 1. Experimental set-up, Nitrogen–vacancy centers (blue spheres) are illuminated by a focused green laser beam and irradiated by a microwave source.

Recall the three requirements of time crystals stated above. The smoking gun experimental evidence would be to observe a response oscillation at a subharmonic of the driving potential. Indeed, the researchers see such a response, and the response is robust only when strong interactions are applied to the system to induce long range order. Consequently, the system demonstrates the third requirement of long-range order.

Figure 2 shows the spin response. The spin polarization is plotted as a function of time and a Fourier spectra shows the frequency of the response (top). A perfect $\theta=\pi$ rotation is applied and the response is half the floquet cycle as expected (middle). When a rotation angle of $\theta=1.034 \pi$ is applied the spectra shows a disordered response (bottom). When interactions are increased, the subharmonic response is restored. This robust locking to the subharmonic of the driving potential only in the presence of strong interactions raises important questions regarding the role of long-range order and how systems can be isolated and coupled to their outside environment.

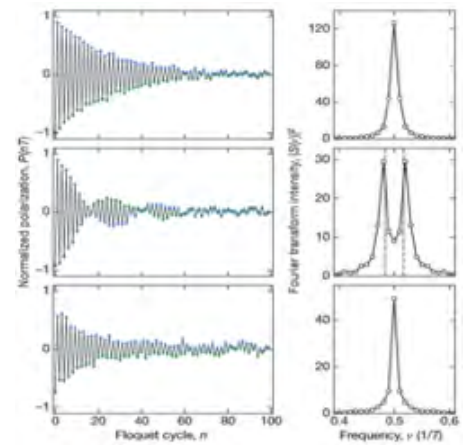


Figure 2. Spin response and observation of discrete time crystalline order.

Time Crystals in Ion Traps

Chris Monroe and his research team at the University of Maryland have conducted a similar experiment to the one described previously. Here the team has assembled a system out of trapped ions. A one dimensional array of $(^{171}\text{Yb}^+)$ ions is assembled in a linear radio frequency Paul trap. Spin rotations are driven by optical Raman transitions while spin-spin interactions are generated by spin-dependent optical dipole forces. The spin-spin interactions give rise to long range coupling. Disorder is applied to the system in a controlled way through the ac Stark shift arising from tightly focused laser beams.

A three-step sequence is developed to observe the spontaneous breaking of discrete time translational symmetry that is a signature of the Floquet time crystal. First a global spin rotation of nearly π is applied. Next, long range interactions are generated. Finally, disorder is introduced. These steps are shown pictorially in Figure 3. The steps are repeated many times and the time for each cycle is the Floquet period.

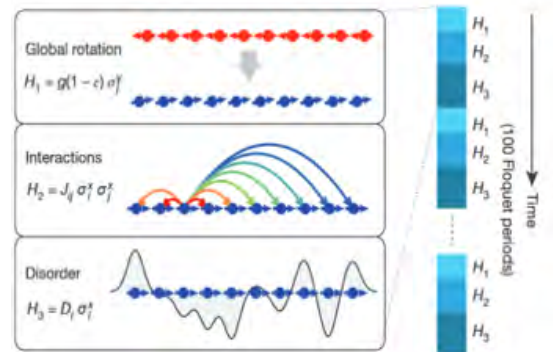


Figure 3. Floquet evolution of a spin chain.

Again, experimental evidence for discrete time symmetry breaking and observation of floquet time crystals would be to demonstrate a robust subharmonic response that depends upon long-range interactions. As can be seen in Figure 4, this is just what is observed. Shown is the time-evolved magnetization of each spin and their Fourier spectra. The subharmonic response is clear, centered around half the driving frequency: (a) When only the global rotation is applied the spins oscillate with a subharmonic response that beats owing to a small perturbation from a perfect π pulse; (b) When both

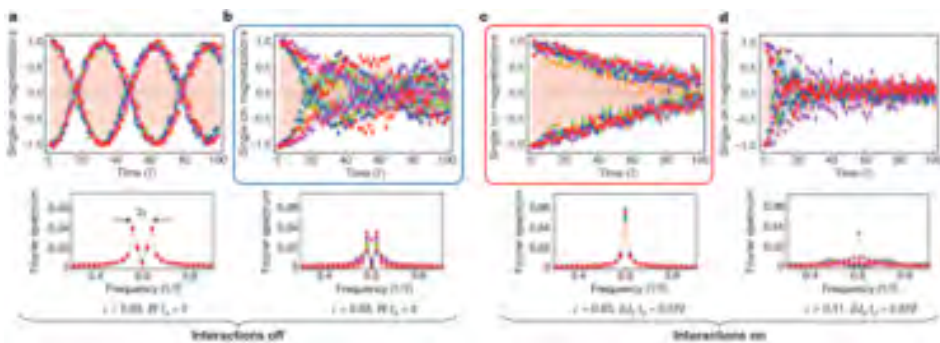


Figure 4. Spontaneous breaking of discrete time translational symmetry.

the global rotation and disorder is applied each ion rotates at a different frequency and the Fourier spectra shows significant spreading; (c) Adding the spin-spin interaction term, the spins all lock together at the subharmonic frequency of the drive period - here the Fourier spectrum merges into a single peak even in the face of the perturbation on the global rotation; and (d) when the perturbation is too strong a boundary is crossed from a discrete time crystal to a symmetry unbroken phase.

Result

These experiments demonstrate the existence of a new form of matter, a discrete time crystal. The observation of discrete time symmetry breaking raises questions with regard to the conservation of energy. This does not mean researchers have created a perpetual motion machine as the system is out of equilibrium as well as externally driven. However, it does have shed light into the nature of out of equilibrium ground state systems, which researchers have termed in “crypto-equilibrium” where no entropy is generated in an oscillating system.

Out of equilibrium many-body systems with strong interactions are a class of theoretical problems that are intractable. These theoretical difficulties make finding materials with novel properties, which could provide revolutionary capabilities an important research challenge. Many future capabilities that can impact low power electronics and agile frequency switching will rely on material properties that may not be found in the ground state, therefore this experimental effort provides critical insight into studying driven systems with strong interactions.

Way Ahead

The next objective in this effort is to target desirable driven states of matter that support properties that are conducive to precision metrology. Collaborative efforts among ARO, AFOSR, ONR and DARPA will be sought and leveraged to more aggressively address those questions.

ATOMIC AND MOLECULAR PHYSICS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Discover the emergent properties of many-body systems, which are challenging to analyze computationally.
- ▶ Determine if strongly interacting non-equilibrium matter can be used to enhance metrology by mitigating environmental noise.
- ▶ Observe new non-equilibrium states of solid state matter induced by coherent light that if successful is anticipated to lead to new forms of matter with novel properties that are dynamically controlled by lasers.

QUANTUM INFORMATION SCIENCES PROGRAM



Dr. Sara Gamble

Program Manager, Quantum Information Science
Physics Division
ARO Physical Sciences Directorate

Dr. Gamble completed her undergraduate studies at the University of Florida, receiving her B.S. in Physics in 2003.

She trained as a physicist at Stanford University, receiving her Ph.D. in Applied Physics in 2010. She came to ARO in 2017 as the Program Manager for Quantum Information Science.



Dr. Joe Qiu

Program Manager, Solid-State Electronics and Electromagnetics
Electronics Division
ARO Engineering Sciences Directorate

Dr. Qiu completed his undergraduate studies at the State University of New York at Stony Brook, receiving his B.S. in Physics in 1991. He trained as a Physicist at the State University of New York at Stony Brook, receiving his Ph.D. in Physics in 1997.

He came to ARL in 2008 as an Electronics Engineer and then to ARO in 2013 as the Program Manager for Solid-State Electronics and Electromagnetics.

Hidden Within Quantum Devices

Challenge

Quantum information science (QIS) is an interdisciplinary field which leverages concepts in areas such as condensed matter physics, materials science, computer science, electrical engineering, and network science in its attempt to realize capabilities not attainable through traditional, classical, means. Optical photonics is an area which is also attractive to leverage in QIS work, and early investments in the field were pursued through ARO's QIS program lead by Dr. T.R. Govindan. This work, however, is extremely challenging. One of the key difficulties is that optical photons have very weak nonlinear interactions, which are crucial in the physics of quantum information.

One promising platform for large scale quantum information implementations relies on superconductivity. Qubits are the quantum analog of classical bits in QIS, and superconducting qubit systems have extremely large nonlinearities in the microwave regime. T.R. Govindan's QIS program recognized this and steadily invested in superconducting qubits and the architectures which may ultimately make the technology scalable for quantum computation applications.

While the optical photonics and superconducting qubit communities were empirically relatively siloed, in 2013 T.R. Govindan along with Joe Qiu recognized that there may be an incredible opportunity to bring these disciplines together. Could the nonlinearities attained in the microwave regime with superconducting systems be exploited to explore regimes in quantum optics simply not obtainable with optical photons?

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Action

Drs. Govindan and Qiu delved into the idea and ultimately crafted a MURI topic aimed at leveraging recent progress in superconducting qubits and the high-quality microwave cavities used in their implementations to open new regimes in quantum optics. At the time of topic formulation, there had been no experiments in this area and the novel pairing of the two disciplines is attributed to the ARO PMs connecting their deep knowledge in both fields to see a truly unique, emerging opportunity.

The MURI topic was selected in the 2015 cycle. The team ARO ultimately selected to pursue the work is led by Andrew Houck from Princeton University and consists of co PI's David Schuster and Jonathan Simon from the University of Chicago, Mohammad Hafezi and Vladimir Manucharyan from the University of Maryland, and Michael Hatridge from the University of Pittsburgh. One interesting feature of this group is that all participating PIs are at the beginning of their careers; every participant was less than 10 years out from their advanced degree at the time their proposal was received. While evaluators expressed concern regarding the relative youth of the team, Drs. Govindan and Qiu rather considered this an advantage. A young team with novel ideas, to them, seemed ideally suited to explore this novel topic. To date the energy, enthusiasm, and innovation these PIs have shown has demonstrated that, in this case, youth is absolutely an asset.

As of 2018 the team has produced cutting edge research on multiple fronts across multiple disciplines, and this write up highlights an exciting and high impact result obtained in 2018. In the following we discuss the development of "hyperbolic lattices" which has not only lead to excitement in the physics community, but has also garnered interest the math community as well.

Result

In superconducting qubit systems microwave photons mediate interactions between qubits by traveling through microwave resonators. There is a natural comparison of this system to a traditional cavity Quantum Electrodynamics (QED) system wherein an atom resides in and is coupled to an optical cavity. Similarly, in a circuit Quantum Electrodynamics (cQED) system, a qubit can be thought of as an artificial atom residing inside a microwave cavity formed by a transmission line resonator.

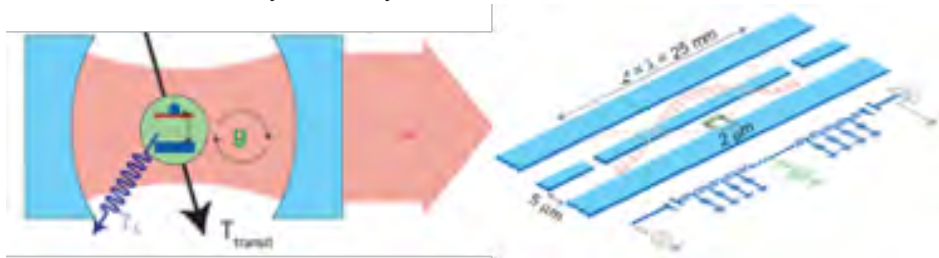


Figure 1. In cavity Quantum electrodynamics (QED) an atom (green circle) resides within and is coupled to an optical cavity. Similarly, in circuit QED a qubit (green box) can be thought of as an artificial atom residing in a microwave cavity formed by a transmission line resonator.

Microwave resonators come in multiple forms. The coplanar waveguide (CPW) resonator is one such form of relatively simple design. When constructed from superconducting materials and cooled, these resonators have minimized resistive losses. Further advantages are realized when advanced microwave circuit engineering is brought to bear to improve coherence and function, and materials science is employed to mitigate decoherence induced by defects in materials, surface chemistry, and interface quality.

Recognizing PI Andrew Houck's potential early, Dr. Govindan successfully nominated him for a Presidential Early Career Award for Scientists and Engineers (PECASE) in

SUCCESS

The MURI team has made progress across all research thrusts. This article highlights the effort to produce interacting photons in hyperbolic space. Unlike previous attempts at quantum simulation, lattices in circuit QED systems are not confined to Euclidean space. Through this effort lattices have been identified as maximally gapped with flat bands making them ideal candidates to conduct simulations with interacting photons.

2009. Some of the work Houck carried out through that grant explored how microwave photons in lattices of coupled resonators and superconducting qubits can exhibit surprising matter like behavior. While some lattice work related to this was addressed in the MURI proposal, it was not originally conceived of as a major focus of the work. Drs. Govindan and Qiu, however, consistently encouraged the team to be creative with the ideas emerging from their research and explore unanticipated opportunities, as long as they lie within the confines of exploiting the nonlinearities of the superconducting systems. Thus, when the team emerged with a very surprising idea ARO was extremely enthusiastic about supporting the team in pursuing it.

What Houck and his group uncovered was that the lattice sites explored in the PECASE are deformable and that they can permit tight-binding lattice structures that are unattainable in actual solid-state systems. Further, networks of CPW resonators can create a class of materials that exist on lattices in an effective hyperbolic space.

Hyperbolic surfaces are not easy to envision. A hyperbolic surface has negative curvature, which should be thought of with regard to the flat surfaces of Euclidean geometry and the positive curvature surfaces of spheres. While positive curvature surfaces exist in nature, research in hyperbolic space is mostly theoretical and informs the fields of general relativity, mathematics, and computer science. The difficulty of attaining negative spatial curvature in the laboratory (or really even visualizing it) has limited experimental work. Thus, the MURI's novel and strikingly elegant study of hyperbolic systems has drawn the interest of multiple groups. ARO PMs Gamble and Qiu have encouraged a collaboration with Princeton's mathematics department with whom the MURI team is working to bridge the language gap between material science and graph theory.

To a large extent our ability to emulate behavior in complex lattice systems is limited. Often we are confined with respect to the geometries in which we can configure these systems. Typically, crystallography deals with periodic lattices consisting of a unit cell and a tiling of that unit cell that fills all of space with no gaps and no overlaps. Euclidean geometry therefore strongly constrains the set of all possible unit cells. The lattices formed with the CPW microwave resonators being explored by the MURI team, however, are not nearly as heavily constrained. Lattices in these systems are formed by connecting many resonators together end to end (Figure 2), but a CPW resonator can be bent, and as long as the length of the resonator is fixed, its resonance frequency is unchanged. Thus, despite the differences in their physical layout, the resonators in Figure 2 are all identical regardless of the number of twists and turns. This deformation enables the team to map curved spaces (both negative and positive) onto planar geometries. Hyperbolic and spherical polygons are smaller and larger than their Euclidean counterparts, respectively, and the set of allowed lattices is different in curved spaces.

In order to characterize these lattices, the MURI team analyzes their band structure. The band structure illuminates the allowable energy range of a given material. Often, this describes the allowed energies of electrons in solids and it is thus a common descriptor in solid-state physics. While bandstructures are unique to a material and depend upon

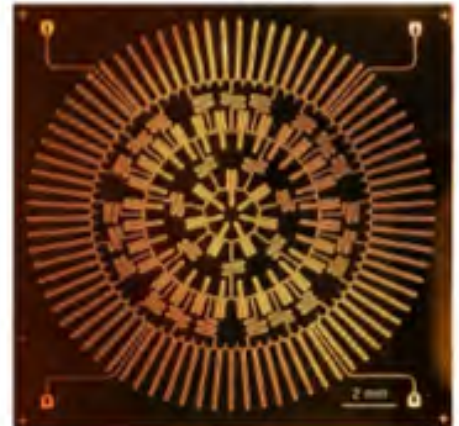


Figure 2. In cavity Quantum electrodynamics (QED) an atom (green circle) resides within and is coupled to an optical cavity. Similarly, in circuit QED a qubit (green box) can be thought of as an artificial atom residing in a microwave cavity formed by a transmission line resonator.

many factors, some broad generalities can be seen graphically and are easily intuited. Two of the features we look for are a flat band or a band gap. A flat band indicates a highly degenerate system typically associated with strong correlations like those found in high temperature superconducting materials. In contrast, a band gap is always found in a semiconductors, where electron energies associated with conduction are distinct and separate from the energies associated with insulation.

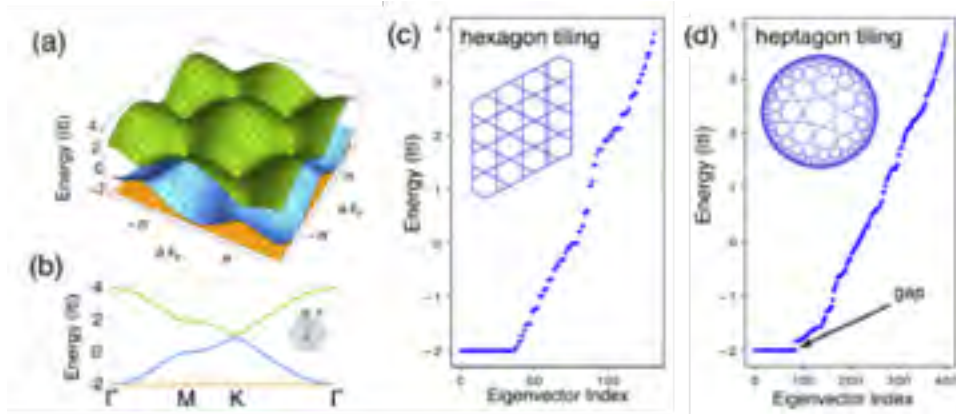


Figure 3. Band structures of a hexagonal and heptagonal kagome lattices. Band structures reveal intrinsic material qualities.

In Euclidean lattices, calculating the energy band structure is straight forward once a unit cell is defined and hopping rates are determined. In hyperbolic space, however, no equivalent theory yet exists, and brute force methods must be used to determine the energy spectrum of the lattice. Shown in Figure 3 is (a) the band structure of a hexagonal kagome lattice in Euclidean space calculated in the traditional way. The flat band is the lowest energy band (orange). Two dispersive bands (blue and green) touch the flat band at points. Part (b) shows a slice through the band structure indicating the band touch. Part (c) shows the Euclidean hexagon kagome lattice result obtained through brute force methods. Here the more complex features of the full band structure are lost, but some elements remain. For example, the flat band seen in (a) and (b) is present at the smallest eigenvector indices. Part (d) shows the analogous numerical eigenenergy spectra for a hyperbolic version of the kagome lattice using heptagons. In this case, a gap is visible. Additional calculations which are not shown indicate that in hyperbolic space odd number sided kagome lattices display a gap, while even ones do not.

In close collaboration with partners in the mathematics department Houck and his team have expanded on these insights, creating maximally gapped flat band lattices. These lattices will be used in quantum simulation, potentially providing insight into materials of interest to the DoD such as high temperature superconductors and optimal sensors.

Way Ahead

These circuit QED lattices represent artificial photonic materials which exist in an effective curved space. Currently the work is purely non-interacting, however interactions could be included by incorporating qubits in each resonator. As such, a new class of strongly interacting metamaterials may be produced using these methods. The new states of light established in this program provide tools for metrology, offer insight into non-equilibrium quantum systems, and are resources for quantum communication and sensing, which are central to many DoD goals. In particular, a focus of the proposed research will be on developing building blocks required for generating exotic states of microwave fields, beyond Maxwell's equations. Such improvements could lead to a new class of sensing devices with an unprecedented sensitivity due to many-body quantum effects.

ACCOMPLISHMENTS

- ▶ 23 published articles and dissemination at domestic and international conferences
 - ▶ Trained graduate students, undergraduates and postdoctoral researchers in quantum science and engineering, ultra-sensitive microwave detection, nanolithography, data analysis, and scientific communication
 - ▶ Fruitful collaborative effort between physics microwave engineering and mathematics departments across multiple universities.
-

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SUCCESS

Researchers at the University of Chicago have constructed a photonic reservoir. Absorbed photons can be immediately replaced from a reservoir. This technology may provide the basis for defeating decoherence.

The Chemical Potential of Light & Synthetic Quantum Matter

Challenge

Particle-wave duality, a central tenant of quantum mechanics, dictates that matter and light exist as particles and waves simultaneously. A key difference between light and matter is that particles of light known as photons, unlike particles of matter, do not obey number conservation. While light has many qualities that makes it an ideal carrier of quantum information, this is a considerable drawback for potential applications. If a photon is trapped in a box it will eventually be absorbed and the information it carries will be lost.

A consequence of this lack of number conservation in the presence of absorbers is that light does not have a chemical potential, which is the energy associated with adding or removing particles from a system. In situations where absorbing walls are absent, however, it was later discerned that non-zero chemical potentials can be associated with photons. Despite this, finding a general solution to creating a controllable chemical potential for light still remains an open problem.

Action

The MURI topic “New Regimes in Quantum Optics” was created with one objective aimed at exploring regimes of behavior not accessible with optical frequency photons. The ARO program managers T.R. Govindan and Joe Qiu recognized that developments emerging from the superconducting qubit and microwave photonics communities could potentially be leveraged in this effort and targeted the topic to these areas. They selected a MURI team with deep expertise in the circuit quantum electrodynamics, quantum optics, and microwave engineering disciplines necessary to explore the potentially novel systems.

The selected team was composed of Lead PI Andrew Houck from Princeton University and co PI’s David Schuster and Jonathan Simon from the University of Chicago, Mohammad Hafezi and Vladimir Manucharyan from the University of Maryland, and Michael Hatridge from the University of Pittsburgh. In their initial proposal, the team proposed a scheme for creating a controllable chemical potential for photons. In particular, PIs Hafezi, Hatridge, and Houck would leverage recent theoretical work by Hafezi and parametrically couple a circuit quantum electrodynamic system to a thermal bath. This challenging work is still in progress.

As with all MURI efforts, close collaboration amongst PIs is encouraged by ARO PMs and is necessary for maximizing the potential for reaching the topic objectives. In this case, discussions regarding the chemical potential work by Hafezi, Hatridge, and Houck unexpectedly lead to the team realizing the viability of an alternate approach based on a combination of work at Chicago and Princeton. While this idea would only lead to an artificial chemical potential, it could enable the exploration of quantum many-body phases. The ARO PMs enthusiastically supported the development of this parallel track, recognizing the potential of the disruptive approach as an addition to the MURI effort.

Result

Simon and Schuster chose to focus their attention on synthetic quantum materials. Quantum materials are rich systems which originate from the competition between quantum fluctuations arising from strong interactions, motional dynamics, and the topology of the system. Exploring how these systems order themselves under a Hamiltonian (a description of the energy of a quantum system) is often difficult because of efficient thermalization of the system. This difficulty can potentially be avoided, however, by studying synthetic quantum materials like those created with photonic systems.

The use of photonic systems as a platform for studying synthetic quantum matter is complicated, however, by the photon loss problem. Without an imposed chemical potential, the system will eventually decay to a vacuum state with no photons. The work-around Simon and Schuster leveraged in their research utilizes dissipative preparation and manipulation of quantum states via tailored reservoirs in which dissipative coupling to the environment serves as a resource.

Specifically, Simon and Schuster realized a Bose-Hubbard chain as their synthetic quantum material. A Bose-Hubbard chain is a one-dimensional chain of particles. In this case, the particles are photons. In the chain only two types of interactions are allowed: ones that involve a kinetic energy which allows particles to move between sites, and a potential energy which describes on-site interactions. In the experiment, the chain is realized with a line of capacitively coupled qubits. Each qubit serves as a lattice site, the kinetic energy comes from the capacitive coupling, and the potential energy from the anharmonicity of the qubits.

The team uses a single qubit to couple the chain to a lossy “bath” resonator. The resonator is shown as the red circle attached to qubit 1 in Figure 1. The bath resonator is first used in a scheme which allows driving and photon loss to stabilize a lattice site. Subsequently, the single stabilized site acts as a spectrally narrow-band photon source that is continuously replenished. Photons from this site can travel to, and gradually fill, the other sites until the addition of further photons requires an energy different from that of the stabilized source. This results in an ordering of the photons into the desired synthetic quantum matter state. It is this conditional addition or blocking of photons at different energies which provides the team with their effective chemical potential.

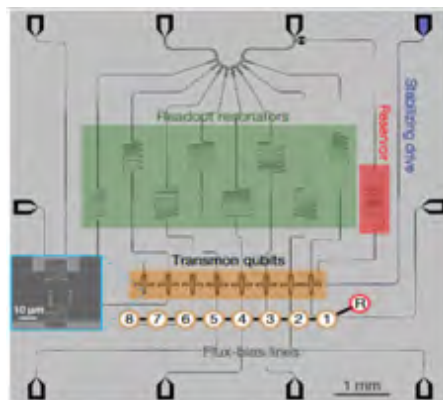


Figure 1. Circuit layout used in the experiment. Microwave resonator circuit elements are used to populate photons on qubit sites while clever engineering of a reservoir and stabilized drive system allows for steady state occupation of a single photon per qubit site.

An optical image of the circuit used in the team’s experiment is shown in Figure 1.

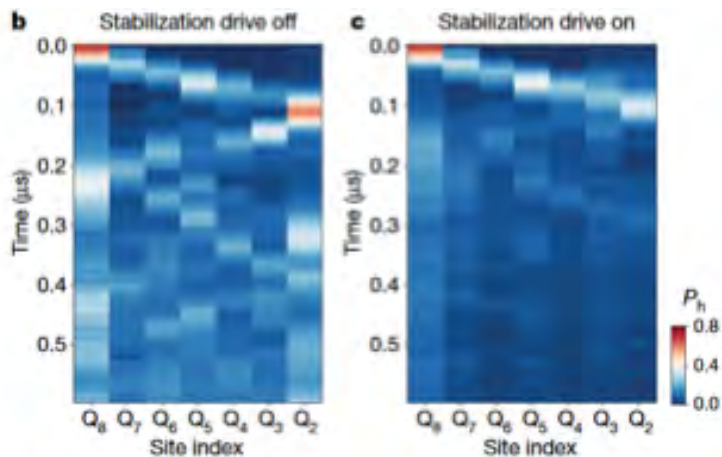


Figure 2. An experiment demonstrating the ability of the reservoir engineering to maintain photon occupation. When a single photon is removed from the system the hole that forms can be observed moving from site to site. When the stabilization drive is turned on the whole is filled with a photon from the reservoir after only 1 trip.

Figure 2 highlights the success of the MURI team's technique for robust stabilization as explained in the figure's caption.

In the work pursued by the team so far, they've utilized this approach to successfully stabilize a Mott insulator of photons against losses. Site and time resolved readout of their qubit lattice allowed them to investigate the microscopic details of the thermalization process through the dynamics of defect propagation and defect removal in the Mott phase. This is just the first of a plethora of experiments the team can now explore.

Way Ahead

The exciting possibilities pursued in this effort exist thanks to a combination of insight by ARO PMs, the ingenuity of the team, and the flexibility of the PMs and team to work together to tailor the direction of research as it progressed. In recognition of new bottlenecks which emerged in not only the areas discussed here but in other thrusts of the MURI as well, ARO PM Sara Gamble recently worked with the team to develop an add-on proposal to enhance their electronic feedback and control capabilities. The proposal was selected for award and the enhanced capabilities should enable the team to make more rapid progress going forward.

The team is now poised to use this approach as the starting point for exploring other strongly correlated phases of matter. Additionally, further study of this driven dissipation stabilization is also possible which may enable additional capabilities. Finally, these results provide a path toward realizing topologically ordered matter using related tools which could lead to advances in both our understanding of fundamental physics and our ability to advance applications such as quantum computing.

QUANTUM INFORMATION PHYSICS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Extend our understanding of multi-qubit and entangled quantum systems to ultimately enable advances in quantum computation and quantum networks. If successful, this could enable beyond classical capabilities in computation, communication, and sensing.
- ▶ Establish the limits of the advantages of qubit-based quantum systems over classical systems for sensing and measurement. If successful, this could enable sensitivities physically unachievable by traditional, classical, systems.
- ▶ Devise novel, primarily non cryptographic focused, algorithms to expand the application space of quantum information processing. If successful, this could enable breakthroughs in fields ranging from machine learning, to optimization, to chemistry and materials science.

OPTICAL PHYSICS AND FIELDS PROGRAM

A New Form of Matter and Energy, Optical / Plasma Filaments, Provide New Opportunities for Directed Energy Applications



Dr. Marc Ulrich

Division Chief, Physics
Program Manager, Condensed Matter Physics
Program Manager (Acting), Optical Physics and Fields
ARO Physical Sciences Directorate

Dr. Ulrich completed his undergraduate studies at Houghton College, receiving his B.S. in Physics in 1994. He trained as a physicist at Auburn University receiving his Ph.D. in Condensed Matter Physics in 2001.

He came to ARO in 2003 as the Program Manager for Condensed Matter Physics and was promoted to the additional role of Chief, Physics Division, in 2008.



Dr. James Harvey

Program Manager (Acting), Biontronics
Electronics Division
ARO Engineering Sciences Directorate

Dr. Harvey completed his undergraduate studies at the US Military Academy, receiving his B.S. in Engineering in 1964. He trained as a Physicist at Dartmouth College and at Lawrence Livermore National Laboratory, receiving his Ph.D. in Applied Science in 1990.

He served a postdoctoral fellowship at ARL in 1991 and then to ARO in 1994 as an Electronics Engineer and program manager for Electromagnetics and RF

Challenge

The Army has a long-standing interest in directed energy technology. However, until recently progress toward this goal has been sporadic, and while there have been many practical offshoots, realization of the idealized form has been elusive. Overcoming the problem of thermal blooming which has been well understood since the advent of high energy lasers has been particularly challenging. Thermal blooming is where a laser beam creates a plasma when it interacts with the atmosphere. The plasma then forms a lens which defocuses the laser and disperses the optical energy. A promising and exciting path forward is created by the advent of light filamentation. In 1995, the first observation in Europe of propagating terawatt, femto-second optical pulses, self-channeled in a plasma filament in air, presaged entirely new potential applications of directed energy. The optical pulse is coupled to the plasma filament, which it generates, by the stabilization of the natural optical diffraction and refraction from the plasma with the self-focusing due to the non-linear index of refraction. The propagation can be stable over distances from tens of meters to hundreds of meters and the plasma filament can form and reform over longer distances. A complex electromagnetic field extending well beyond the lateral limits of the pulse, accompanies it. The propagating beam structure can be very complex, with a single or multiple beams together. As the pulse propagates it generates a co-propagating white light optical continuum from the highly non-linear effects in the plasma filament. In high pressure rare gases, the optical pulse can produce high intensity, high energy, coherent X-rays. The detailed physics of the phenomena is still not well understood and an understanding of how to control the filament challenges the most sophisticated coupled propagation and quantum

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Ballistics Sciences



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Materials and Manufacturing Sciences



SUCCESS

ARO research is funding research into directed energy technology. If successful, light filamentation will be utilized to overcome the major obstacle of thermal blooming. This research has implications not only for directed energy weaponry but for high bandwidth communications, remote sensing, and fundamental materials science as well.

dynamical models available. It is still not clear what is the ultimate limit on the distance of propagation. The challenge is in understanding and then controlling this extremely complex state of coupled matter and energy.

Action

In 2004 ARO Program Manager Dr. Richard Hammond learned about this potential new form of energy propagation embodied by light filaments and, to find what research was needed, and what the applications were to the Army and DoD, he organized a workshop at Duke University to explore the existing knowledge on light filaments and future directions of research. The workshop was intense, led by Dr. Hammond working with Dr. Bob Gunther of Duke University, and the result of the two-day effort was the production of a document to serve as a blueprint the next steps. It was found there was much to learn and many potential applications. Following the guidance of the workshop, Dr. Hammond started a project with core single investigator funds.

Meanwhile, Dr. James Harvey was serving a foreign assignment exploring basic research breakthroughs in Europe. Independently he discovered the European filamentation research being conducted and worked to gain attention from the US military scientific community. On his return he worked with Dr. Hammond to establish a large scale Multi-disciplinary University Research Initiative (MURI) project at the University of Central Florida (UCF) to explore the new phenomena and to collaborate with Air Force Office of Scientific Research (AFOSR) MURI on the theory and modeling of the filamentation dynamics, which was designed to be complementary to the ARO MURI. Dr. Harvey also initiated some single investigator grants in his ARO Electromagnetics (EM) Program.

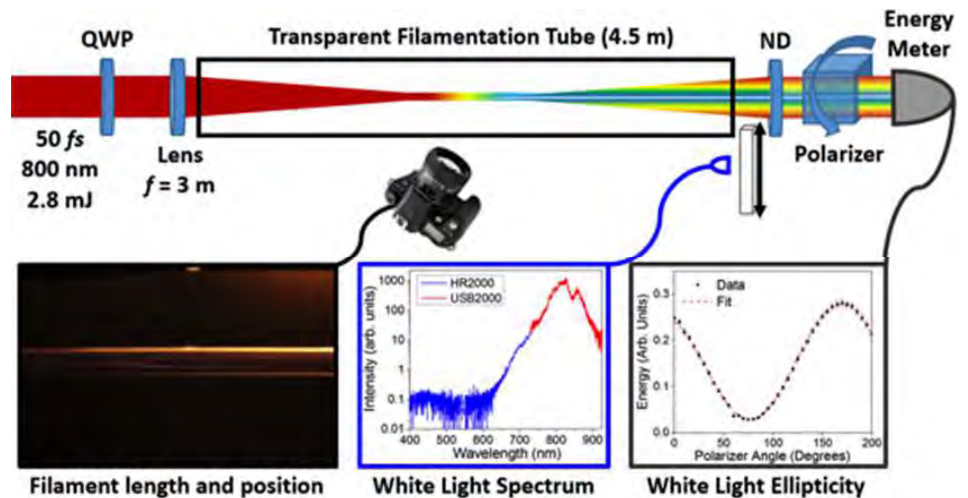


Figure 1. Experimental recording of the filament physical structure along with the spectrum of the white light continuum generated in the filament. a is a side view from the camera. The filament forms at the focus in the filamentation tube. b is the very broadband white light continuum formed in the filament and recorded from the end (energy meter). c records the polarization of the light.

During the ARO MURI, Dr. Hammond worked with NASA and Air Force to help the MURI PI, Prof. Richardson, secure vitally needed outdoor space on Merritt Island. With Dr. Harvey, Dr. Hammond was able to secure additional funding, via a DURIP (Defense University Research Instrumentation Program) grant, so the facility on Merritt Island can operate ultrahigh intense laser and measure light filamentation for a kilometer and more.

Result

Measurements taken at UCF and on Merritt Island showed some surprising and interesting effects. One was that light filaments create THz radiation at distance targets. This is exciting because THz radiation, a very important energy range for spectrographic analysis, does not propagate well in the atmosphere. With the light filament, the atmospheric loss is eliminated since it is created and detected at or near the target. This opens the way for applications in remote sensing and detection of chemical, biological, or explosive material.

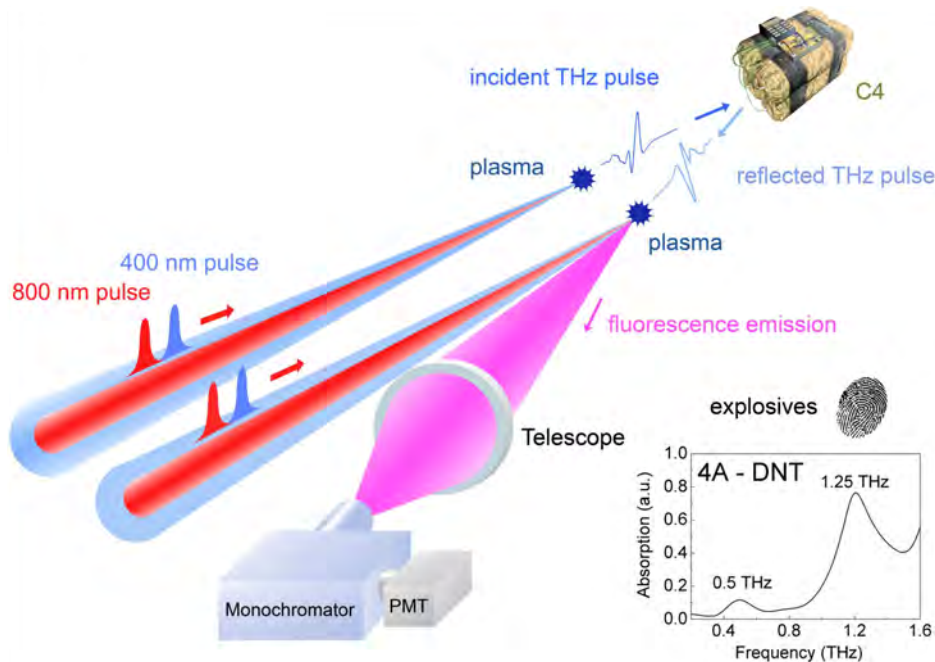


Figure 2. Notional schematic of remote spectroscopic THz detection. Shown is the THz spectrum of the explosive DNT. The key to this detection scheme is that the THz pulse is generated close to the target by laser plasma and is detected also close to the target by a second laser plasma, which produces optical fluorescence to be detected by the distant monochromator.

Another result of this research was the development of local EMP. The light filament, when hitting a structure housing any circuitry, will destroy or disable the electronics. Dr. Hammond worked with Richardson to develop a video showing these effects. The result was an exciting video showing a light filament knocking a drone out of the air. This video is being used to show the power of light filaments, and Dr. Hammond worked to involve other agencies to develop it further.

Supported by Dr. Harvey and Dr. Hammond in current and future research, Prof. Milchberg discovered for the first time that the femto-second laser beam creates an “air waveguide” for guided optical and electrical propagation. The gradient in the index of refraction can guide longer laser beams with higher energy, electrical discharges, and electrical currents.

Prof. Milchberg has also discovered for the first time that the optical beam collapse along the filament causes a spatial-temporal optical vortex in which the electromagnetic phase and energy circulate in a dynamic torus or “smoke ring” like structure around the propagating pulse (see figure below). This is fundamentally different than the much-studied Orbital Angular Momentum (OAM) vortex (e.g., a Laguerre-Gaussian beam). The STOV has a topological charge which protects the beam as it propagates from other propagating beams. He has shown theoretically that the STOV's are a general fundamental property of the collapse of non-linearly propagation of intense

pulses in many other systems as well, for example, in the relativistic self-focusing and filamentation of accelerated electron beams. His work is the first ever discovery of this important topological feature of nature in non-linearly propagating beams.

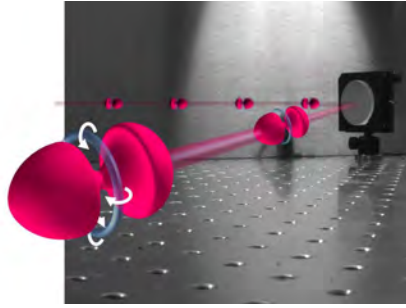


Figure 3. "Smoke rings in light." The electromagnetic phase and energy circulates in a torus shape around the point of collapse in the beam due to self-focusing and propagates with the pulse.

RESULTS

- ▶ Two professional society awards. Two prestigious foundation fellowships. Four honorary degrees from prestigious foreign universities. Elections to the US National Academy of Science, German Academy of Science, American Philosophical Society, Royal Irish Academy.
 - ▶ Pioneering research in understanding new optical / plasma phenomena.
 - ▶ Three breakthrough discoveries of new physical phenomena with wide range of applications.
-

Propagating the femto-second laser pulse through a high-pressure gas produces a laser filament in which the non-linear processes in the laser plasma support extremely high harmonic generation (HHG) of ultrashort pulses of extreme ultraviolet (EUV) radiation in a very bright, coherent, collinear, very broadband continuum. Support by Dr. Harvey and Dr. Hammond's ARO programs enabled the extension of the spectrum into the soft X-ray region up to several keV. ARO support resulted in the discovery that the HHG process was highly enhanced by using longer wavelength laser pulses and a high degree of phase matching between the driving laser field and the resulting X-ray field. Theory predicts that a 10 micron wavelength driving laser could extend the X-ray spectrum to 10 keV or more. ARO support also resulted in the discovery that an ultraviolet laser driving pulse provided highly enhanced conversion efficiency and a new phenomenon: the generation of well-separated narrowband peaks (~9 eV separation with linewidths of 70-700 meV). The discoveries in the HHG of coherent EUV and X-ray radiation open the way for table top sources with unique capabilities for the exploration of nanoscale magnetic, phononic, thermal, and phase-change phenomena in materials science. Although synchrotrons can produce coherent X-rays for materials science research, much of the range of phenomena are addressable with the much smaller and cheaper HHG sources, which can bring the capability within reach of every university, military, or industrial materials laboratory.

This research has over the years propelled Prof. Murnane to prominence in the Vannevar Bush Fellowship program, DARPA programs, and leadership of an AFOSR MURI. It has led to Prof. Milchberg being sought for the DARPA PULSE program. And has established Prof. Richardson and his collaborators as true pioneers of a new area of optical physics.

ARL-WMRD researchers are frequent collaborators in Prof. Milchberg's lab.

Way Ahead

These discoveries open the door to the development of new classes of electronic and structural materials with new properties. New insight into cellular biological processes will result from the ability to image living cells at the nanoscale in 3D. Military applications include controlled high voltage discharges for landmine/IED remediation, IR countermeasures, remote sensing of chemical and biological material, and directed energy for counter missile, counter UAV, counter-battery. The prospect to remotely discharge and shut down a town's electrical generation system has been demonstrated. There is a potential for plasma antennas for selective radar and communications. In the future, with larger systems, the Army may have important new capabilities from the application of light filaments. These include knocking out airborne missiles as well as ground platforms at standoff distances. It may be possible to destroy all electronics, or just temporarily suspend their operation.

Development and Application of Attosecond Pulsed Lasers



Dr. Richard Hammond (Retired)

Program Manager, Optics
Physics Division
ARO Physical Sciences Directorate

Dr. Hammond completed his undergraduate studies at New Jersey Institute of Technology, receiving his B.S. physics in 1973. He trained as a physicist at Rensselaer Polytechnic Institute, receiving his M.S. and Ph.D. degrees in optics in 1979.

He came to ARO in 2002 as the Program Manager for Optics and retired from ARO in June 2019.



Dr. James Parker

Program Manager, Molecular and Structure Dynamics
Chemical Sciences Division
ARO Physical Sciences Directorate

Dr. Parker completed his undergraduate studies at Marquette University, receiving his B.S. in chemistry in 1993. He trained as a physical chemist at the University of Mississippi, receiving his Ph.D. in physical chemistry in 1999.

He came to ARO in 2009 as the Manager for what was then called the Physical and Theoretical Chemistry Program.

Scientific Challenge

To develop and apply transient absorption spectroscopy in the attosecond time range for understanding the earliest time processes in electronic excitation in molecules and materials.

Action

In 2005, Richard Hammond, a Program Manager in Physics, submitted a MURI topic on the development of attosecond lasers (10-18 s). Professors Margaret Murnane (U. of Colorado), Henry Kapetyn (U. of Colorado), and Paul Corkum (National Research Council of Canada), had each contributed to the understanding of high harmonic generation, a process in which focused infrared radiation impinging on a noble gas sample causes the atoms to emit high-energy attosecond bursts of radiation. This discovery eventually brought laser pulse times from the femtosecond regime, where they had stalled since about the year 1980, into the attosecond regime (see Figure 1). At the time, Hammond's

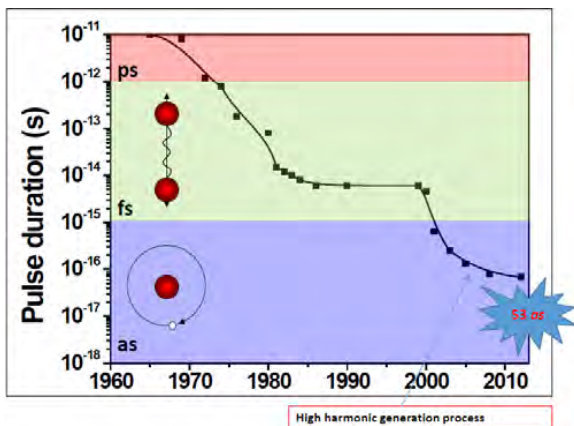


Figure 1. Shortest available laser pulse duration as a function of year.

This success supports these ARL Core Technical Competencies

Ballistics Sciences



Materials and Manufacturing Sciences



MURI topic was thought to be too ambitious, but Hammond argued aggressively for the topic and was able to get it approved. The award went to a relatively unknown physicist, Zenghu Chang at Kansas State University, and within the time frame of the MURI Chang had the world's record shortest pulse at 72 attoseconds.

Hammond was not satisfied yet, and he wanted to develop a whole new world of spectroscopy that would be allowed by these ultrashort laser pulses. Bringing together world's experts, Hammond held a workshop to determine the next steps. The conclusion was that the attosecond pulses needed more photon flux, and should be applied to the study of effects in solid materials. To achieve these goals Hammond funded a single investigator award to the University of Central Florida, where Chang was a faculty member by then, to produce high-flux, isolated attosecond pulses. Within a few years they set the world's record on making the shortest laser pulse, 53 attoseconds. By now Chang was an international leader in ultrashort laser physics. With the success of this program, everything was in place to use the high-energy, ultrashort pulse to open a new door in the study of molecules and materials.

At this time James Parker, a Program Manager in Chemistry, was looking for a way to study ultrashort electronic phenomena in molecules and recognized the need for attosecond lasers. Parker and Hammond jointly developed a MURI topic on Attosecond Electron Dynamics whose objective was to increase the power of attosecond pulses and to apply them to the study of molecular electronic processes. At the same time, Enrique Parra of the Air Force Office of Scientific Research independently proposed a MURI topic on studying the effects of attosecond pulses on materials. The two MURIs were awarded in 2014. The Army MURI went to the University of California, Berkeley with Professor Stephen Leone as the Principal Investigator and with Chang among the co-PIs on the team. The AFOSR MURI went to the University of Central Florida with Professor Zenghu Chang as the Principal Investigator and with Leone among the co-PIs on the team. A major accomplishment of the Army MURI was the development of the attosecond transient absorption spectroscopy technique (see Figure 2), which has been applied to study a variety of physical processes: probing dark states in oxygen, discovering signatures of light-induced conical intersections, observing electronic coherences in atomic ions, resolving surface crossing dynamics in ethylene,

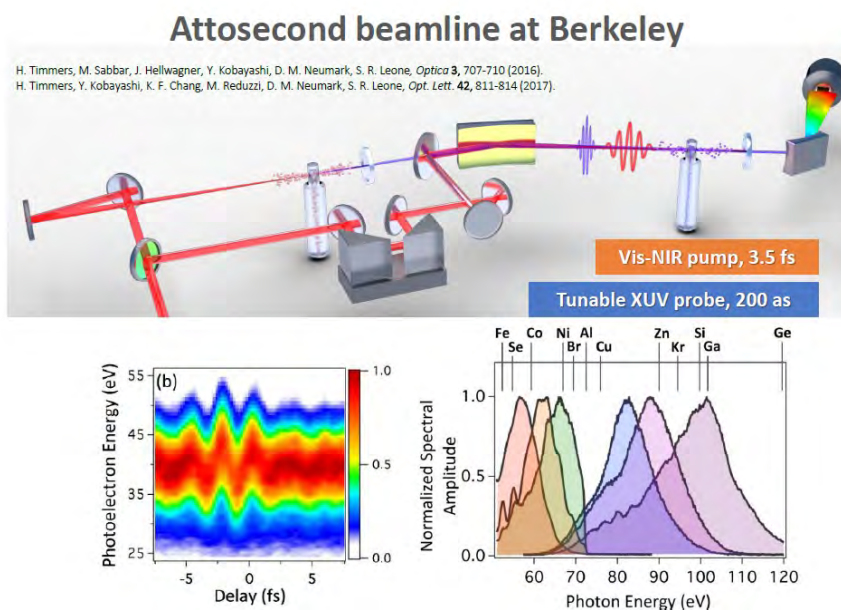


Figure 2. Schematic of the attosecond transient absorption spectroscopy technique showing the range of photon energies available, coinciding with numerous L, M, and N-edge electron binding energies of chemically relevant elements.

observing strong field-induced dynamics in methyl bromide, understanding how conical intersections can lead to branching in chemical reactions, studying Auger phenomena in real time, and understanding intramolecular charge migration at the moment a molecule absorbs a photon.

Result

The Army MURI topic on the development of attosecond sources and their applications to the study of molecules and materials have yielded a plethora of physical information about the electron dynamics in atoms and molecules at this timescale. Areas where significant progress has been made include development of attosecond transient absorption spectroscopy (ATAS) to probe valence reaction dynamics in atoms, molecules, and solids on timescales approaching the electronic domain, understanding charge migration in nanoparticles, development of velocity map imaging for studying electronic structure changes when a molecule absorbs a XUV pulse, driving laser development, new polarization gating techniques for attosecond pulses, extending theory for charge migration in molecules, and development of new theory for light-induced conical intersections.

As an example of a scientific result from ATAS, let us consider non-adiabatic molecular dynamics initiated by strong field excitation. The investigators have been studying the fragmentation of methyl bromide (CH_3Br) as the molecule relaxes through multiple conical intersections. In the experiment, a few-cycle NIR pulse is used for strong-field excitation of the molecule to the $5p$ Rydberg state (Figure 3a). As the Rydberg state relaxes and breaks apart through a series of conical intersections, the quantum state of the system is probed by resonantly exciting the Br $3d$ inner-shell electron with a time delayed attosecond pulse to fill the HOMO hole in the excited molecule. The resulting ATAS trace is depicted in graphic 3b. The non-stationary, energetic motion of the absorption features is representative of the non-adiabatic motion of the excited state wavepacket as it passes through multiple conical intersections. The superb temporal and energy resolution of ATAS is paramount for probing such a transient molecular reaction.

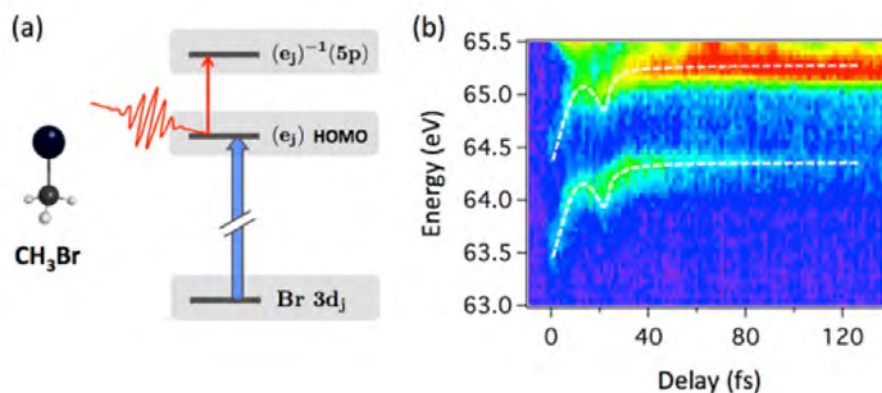


Figure 3. (a) Experimental probing scheme for probing non-adiabatic dynamics in methyl bromide. (b) Experimental ATAS trace in methyl bromide depicting non-stationary motion of Rydberg absorption lines.

The information obtained from this MURI has proven extremely valuable for understanding ultrashort time scale phenomena which occur on the timescale of the motion of bound electrons, and will continue to be of high value for future studies.

Way Ahead

It is possible that scientists at ARL/SEDD will adopt the attosecond techniques described here to study Army relevant problems in photovoltaics, energy storage, and detonation chemistry. These attosecond techniques require specialized training for their implementation, and it is likely therefore that ARL could hire graduate students or post-docs who graduate from this MURI.

OPTICAL PHYSICS AND FIELDS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Develop non-Hermitian optics to create more sensitive optical detectors.
- ▶ Apply supersymmetric optics to develop new capabilities, from eliminating optical loss to developing more powerful laser systems.
- ▶ Design, create, and understand the optics of epsilon near zero (ENZ) materials, which have very large nonlinear properties.

CONDENSED MATTER PHYSICS PROGRAM



Dr. Marc Ulrich

Program Manager, Condensed Matter Physics
Division Chief, Physics
ARO Physical Sciences Directorate

Dr. Ulrich completed his undergraduate studies at Houghton College, receiving his B.S. in Physics in 1994. He trained as a physicist at Auburn University receiving his Ph.D. in Condensed Matter Physics in 2001.

He came to ARO in 2003 as the Program Manager for Condensed Matter Physics and was promoted to the additional role of Chief, Physics Division, in 2008.



Dr. Joe Qiu

Program Manager, Solid-State Electronics and Electromagnetics
Electronics Division
ARO Engineering Sciences Directorate

Dr. Qiu completed his undergraduate studies at the State University of New York at Stony Brook, receiving his B.S. in Physics in 1991. He trained as a Physicist at the State University of New York at Stony Brook, receiving his Ph.D. in Physics in 1997.

He came to ARL in 2008 as an Electronics Engineer and then to ARO in 2013 as the Program Manager for Solid-State Electronics and Electromagnetics.

A Decade of Discoveries in Topological Physics Provides an Opportunity for Ultra-Efficient Electronic Technology

Scientific Challenge

Since the original electronic revolution, electronic materials were known to be only insulators, semiconductors, or conductors.

This success supports these ARL Core Technical Competencies



Materials and
Manufacturing Sciences



Computational Sciences

However, scientific breakthroughs in the mid to late 2000s revealed an electronic state in several materials could be “twisted” in such a way that new states and phenomena were discovered. Were materials with such states rare? Could they be engineered? Just how many different kinds of twists and unexpected phenomena were there to be discovered? Could anything useful be done with them? At what temperatures would they be relevant? The Army Research Office began an initiative in 2008 that strategically pursued answers to these questions.

Action

In 2008, ARO Condensed Matter Physics Program Manager Dr. Marc Ulrich recognized that an experimental validation of topological insulator physics presented a strong opportunity for new discoveries and began funding work to understand the physics of this novel family of materials. Topological materials are defined as those in which the material's characteristics are governed by a global property – such as the number of holes through a surface – rather than local properties – such as the curvature of a surface. In a topological insulator, such a globally-define property governs the behavior of electrons such that the bulk is not conductive whereas the surfaces and interfaces with other materials must be conductive independent of defects. The first topological phase (an electronic property within a material) discovered was the quantum Hall effect. It is called an ‘effect’ because it wasn't the material alone but how the electrons within the material behaved in the presence of a strong magnetic field. This and its cousin, the fractional quantum Hall effect, were the only known topological phases until the mid-2000s, and they were difficult to attain. These phases only exist in a handful of materials of exceptional high quality when held at a temperature of less than 5K while in a high magnetic field. During this time there were a pair of theoretical predictions, one developed for two dimensional and another for a three dimensional “topological insulator.” These were experimentally demonstrated in 2007 and 2008, respectively. Since then, and in part due to the ARO investment, it has been found that topological states may exist in as many as a quarter of natural materials with a fair number of those materials exhibiting unique properties arising from the topological nature of the material at room temperature and without the presence of a magnetic field.

While many dozens of topological phases have been discovered and hundreds of materials that host topological phases have since been found, the 3D topological insulator by itself is a noteworthy opportunity. The seminal 3D topological insulator, Bi₂Se₃, is technically an insulator with a 300 meV bandgap; in pristine form it should not conduct electricity. However, the parity of the atomic orbitals that comprise the conduction (empty of electrons) and valence bands (filled with electrons) are flipped in the material. This parity is opposite that of normal insulators such as glass, silicon, or even the vacuum, if one thinks of a vacuum as a material. Bands of opposite parity cannot mathematically connect in the same way that a cup cannot be both empty and not empty at the same time. Because the bands at the surface of Bi₂Se₃ are forced to connect to the bands of like parity of any atomic insulator, electrons at that surface can always move. Thus, while the bulk of the material is a bona fide insulator, the surface must conduct electricity regardless of its quality. In Bi₂Se₃, this parity flip is due to the coupling between electron spin and orbital angular momentum resulting in electrons that are spin-momentum locked at the surface, meaning spin up and spin down electrons must move in opposite directions.

Immediately after the discovery in 2008, Dr. Ulrich identified key researchers in the field and initiated a meeting with the researcher who led the discovery of the 3D topological insulator at a March American Physical Society meeting and with a leading theorist from Stanford. This meeting resulted in the development and submission of a proposal that combined theoretical and experimental work to advance the field. Dr. Ulrich conceived of and initiated workshop involving leading experts to assess the most strategic directions and approaches with the goal of driving this field forward. From

SUCCESS

A decade of strategic investments to advance knowledge of topological electronic states and device concepts led to tri-service and DoD-academic collaborations and focused initiatives that are expected to enable future electronics that exceed the energy efficiency of today's technologies, opening the door to ultra-low power electronics.

the results of this workshop, Dr. Ulrich along with Dr. Varanasi of the Materials Science division formulated a MURI topic on extending the quality of the topological materials and expanding the types of topological phases that may be experimentally available.

The MURI topic proposed by Drs. Ulrich and Varanasi was one of the eight topics selected by OSD for public release in the FY11 MURI Broad Agency Announcement. Dr. Bob Cava's proposal from Princeton University was awarded in 2012. The combination of theory, materials synthesis, and magneto-electrical characterization was an ideal approach for this nascent field. Many new and seminal topological states were discovered within this MURI as well as the guiding theoretical approaches that enabled them as well as other new materials to come. Two of the many notable advances gained by this initiative are achieving the most pristine 3D topological insulator known to date and the advent of Weyl semimetals which have now almost become a separate research field in their own right.

Prior to the MURI, 3D topological states were only observable at temperatures of about 4-5 K or less because the materials had not been well developed, though Dr. Cava had begun to make progress on this shortly before the MURI was awarded. The predominant difficulty with 3D topological insulators is that they aren't truly insulating. The materials naturally host enormous levels of defects causing the bulk to conduct electricity in parallel with the topological surface states (Bi₂Se₃, the quintessential 3D topological insulator, has been developed for thermoelectrics since the 1960s; for that application, bulk transport is desirable). Dr. Cava's MURI team worked through the solid state chemistry over several years and devised the most insulating topological insulator, Sn-doped BiSbTe₂S (Sn:BSTS). This material hosts topological surface states that predominate electrical transport up to a temperature of 150 K. While perfect bulk insulating character has not been observed at room temperature, this material provides access to the topological surface states at readily accessible conditions.

Weyl semimetals are also a unique topological material but one in which the 3D transport characteristics are as unique as the surface states. To picture the electronic structure of this material, consider the linear relationship between energy and momentum that shows up in graphene, but in three dimensions rather than two. This is a 3D Dirac cone and materials hosting this band structure are known as Dirac semimetals. The singular point (apex) of the Dirac cones, called Dirac points, host double-degenerate states. Whether broken by an external magnetic field or some internal symmetry of the crystal, the Dirac points can be split in momentum space. These are then called Weyl points. They always come in pairs and mathematically they are equivalent to momentum-space magnetic field monopoles of opposite sign. This gives a novel transport state in which electrons are pushed along a (real) external magnetic field rather than perpendicular to it.

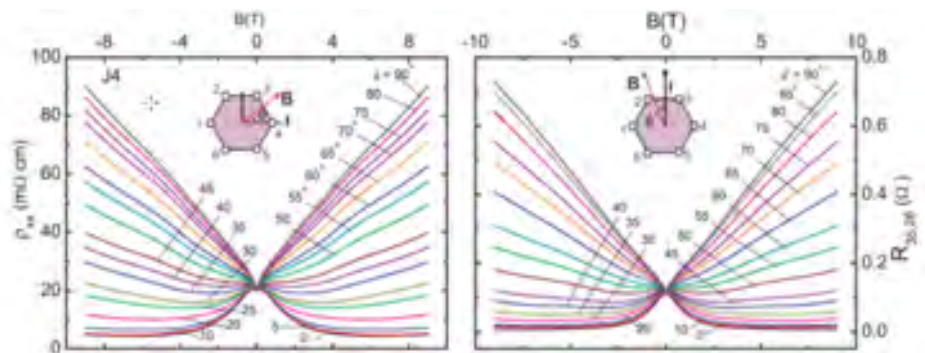


Figure 1. In a Weyl semimetal, electrons prefer to flow along the magnetic field. Regardless of the crystalline axis along which a current flows, the resistance reduces when a magnetic field is applied along the direction of the current (zero degrees in the figure). When perpendicular, the resistance increases as in normal materials. This data is from the Weyl semimetal Na₃Bi.

Drs. Bill Clark and Joe Qiu of ARO's Electronics Division recognized the importance of these findings. In 2013, they asked the question of whether or not the unique and unusual properties of the electrons in topological materials could be harnessed to create new devices that can significantly outperform those using conventional semiconductors. They initiated discussions with Professor Ki Wook Kim at North Carolina State University who is a world leading expert in electronic devices modeling, and eventually sought out and funded a theoretical effort to develop novel device concepts based on topological insulators. This single investigator effort revealed that topological insulators can potentially manipulate the magnetic order of a nearby magnetic film through the exchange mechanism. This enables device concepts ranging from switches several orders of magnitude more efficient than CMOS to IR detection to clocks.

Based on those results, those coming out of the physics-led MURI, and concurrent advances elsewhere in the field, Dr. Qiu initiated another MURI at UCLA led by leading magnetics researcher, Dr. Kang Wang, in 2016 on spin-orbit coupling in topological and magnetic heterostructures in concert with the Materials Science and Physics divisions. Among many advances in this MURI, several examples have been demonstrated in which a current through a topological surface state induces a change in a magnetic material (see Figure 2).

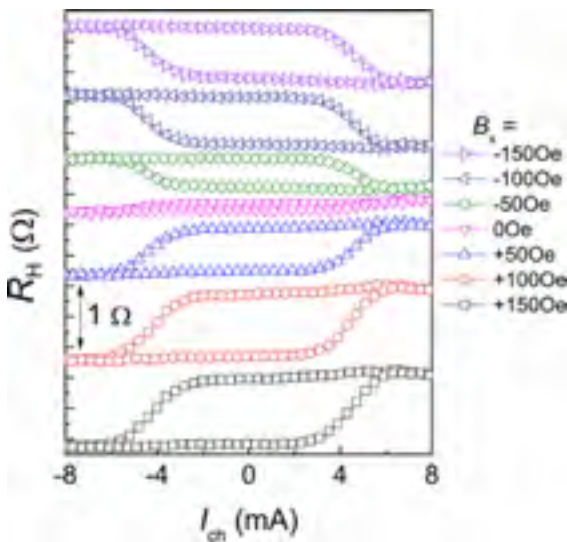


Figure 2. Switching a magnet with a current. A current through the topological insulator (BiSb)₂Te₃ causes a change in the magnetic order of a nearby 1 nm thin film of CoFeB. The different magnetic order affects the resistance through the device. The switching current density is 3×10^5 A/cm² which indicates that the spin-locked topological surface state current is relatively efficient at tugging on the magnetic order of the thin magnetic film. For this device geometry, an external in-plane magnetic field is necessary to produce the difference in resistance between the states of the magnetic layer. (DOI: 10.1109/IEDM.2018.8614499)

The strategy to push this field forward for Army technology involved three fronts: transitioning work into the laboratory, fostering an interest in topological materials at other DoD funding agencies and at USD(R&E), and fostering an environment that has enabled the service labs to begin collaborative work. With topological materials staged to potentially impact a wide variety of technologies ranging from low energy electronics to sensing, ARL has developed a series of research questions to guide efforts that will determine the level of opportunity and the approaches necessary to impact Multi-Domain Operations and Army functional concepts such as sustainment (through reduced logistical support necessary to maintain advanced electronics) and intelligence (through sensors platforms having adequate computational power at the point of use to reduce decision time).

The results obtained by ARO's strategic investments in this nascent field motivated researchers at the Army Research Laboratory to study this area. Scientists at ARL's Sensors and Electronics Device Directorate began work in this area in 2014 studying heterostructures between a topological crystalline insulator (here, the topological

state is mediated by a crystalline symmetry rather than time reversal symmetry) and a superconductor through a collaboration with an ARO-funded researcher at the University of Maryland. Though not focused on magnetic effects at that time, the work demonstrated the exceptional quality of ARL's topological materials and their ability to form pristine interfaces.

In 2018, the opportunity for advancing the field of topological device sciences was very clear. Several ARO PMs met to develop a strategy to push this forward and came up with the acronym, TEDs: Topological Electronic Devices. In May of 2018, ARL-SEDD sent Dr. Charles Rong to work with Dr. Ulrich as a Technical Advisor to the ARO Condensed Matter Physics program. Drs. Rong and Ulrich began working out a strategy for ARL to advance TEDs. On the extramural front, Drs. Qiu and Ulrich identified Dr. Moodera of MIT as a key TEDs device scientist for topological magnetic effects, encouraged him to pursue topological voltage control of magnetic anisotropy and began funding his work to enable it. Concurrently, Dr. Flagg of ARL-Northeast secured funding to hire an ARL postdoctoral scholar in Dr. Moodera's laboratory and another in Dr. Wang's laboratory at UCLA.

About this same time, USD(R&E) personnel visited ARO and during the visit indicated interest in learning more about topological materials. Dr. Ulrich offered to hold a workshop with AFOSR and ONR to provide USD(R&E) with the desired knowledge. This culminated in a workshop held July 2018 in which ARO, AFOSR and ONR program managers met along with ARL and NRL researchers working with topological materials. This workshop motivated a stronger interest in topological sciences at AFOSR and ONR and also initiated several interactions between ARL and NRL scientists and engineers. ARO, AFOSR and ONR program managers are currently working strategically together to advance the science and engineering in this space while ARL, NRL and AFRL researchers are collaboratively seeking resources to expand their initiatives.

Result

This novel phenomenon is the basis for ARL's new initiative for topological material-based energy efficient electronics. Because this and related topological materials are widely accessible and readily synthesized in an inexpensive laboratory (compared to the quantum Hall effect which required specialized molecular beam epitaxy and a dilution refrigerator), topological states suddenly became widely accessible to the community and exploded on the scene. Because of Dr. Ulrich's insight, the U.S. Army has been able to drive new knowledge in this area and transition it into a significant internal effort with exciting ramifications for implementing Multi-Domain Operations. Specifically, topological materials provide a path toward electronics that can be 1,000 times more efficient than the theoretical limit of CMOS technology and consequently the reduced heat generation will enable dramatic improvements in computational speed. With efficiency increases, mission length and reach can be extended dramatically or battery weight offloaded from advanced electronics for the dismounted soldier and small platforms. Furthermore, the speed may possibly enable artificial intelligence or machine learning at the point of collection, which would conserve available communications bandwidth.

The combined efforts of Drs. Ulrich, Qiu and Rong led to an ARL postdoctoral scholar being stationed in Dr. Moodera's research laboratory to enable a close ARL-academic collaboration in this area. Collaborations among the laboratory were established and researchers began considering ways to obtain external funding to advance in-house efforts.

RESULTS

- ▶ More than 120 peer-reviewed publications from ARO-funded efforts in this area
 - ▶ ARL postdoctoral scholar established in leading academic institution through ARL Open Campus
 - ▶ New ARL collaborations with U Maryland, MIT and UCLA
 - ▶ Success led to three MURI topic candidates from ARO, AFOSR and ONR for consideration in FY19
 - ▶ Based on these results, OUSD(R&E) selected topological electronic devices as a strategic research investment in ARL, AFRL and NRL beginning in 2019.
-

The DoD is now well positioned with the internal talent and extramural partnerships with world-leading experts to strategically direct and advance the science and engineering of topological materials and devices for TEDs and other concepts for Multi-Domain Operations.

Way Ahead

The next objective in this effort is to target magnetic phenomena within topological physics and electronics to address remaining key questions that will enable the development of TEDs. Collaborative efforts among ARO, AFOSR, ONR, and DARPA will be sought and leveraged to more aggressively address those questions. The collaborations with NRL and AFRL that resulted from SEDD participation in the ARO Tech Advisor program will be expanding their efforts and strategically addressing the basic and applied research questions directly associated with TEDs concepts.

Forty Years of Strategic Discoveries on Ferromagnetic Insulators Leads to Compact Communications and Radar Technology

Challenge

Magnetic effects have been long used to provide non-reciprocal effects for radio frequency technologies; out-going and in-coming signals are affected differently. Magnetic materials (or electromagnets) are bulky discrete elements that are added after the electronic circuits are fully designed and built. Since the 1980s, the Army Research Office Physics Division has invested in the physics of magnetic excitations in novel materials which would enable non-reciprocal effects to be captured in a greatly reduced form factor.

Action

In the 1980s, ARO Physics Division program manager, Dr. Charles Boghosian began supporting Dr. Carl Patton of Colorado State University for the investigation of magnetic excitations in hexagonal ferrites and other magnetic materials. In the 1990s, Dr. Mikael Ciftan, ARO Physics program manager for non-linear physics, took over this initiative. During this decade of continued study, Dr. Ciftan perceived an opportunity for simple magnetic metals to be utilized for high frequency responses and expanded the initiatives to include Dr. Robert Camley of the University of Colorado at Colorado State (UCCS) (which only offered Bachelors and Masters Degrees in Physics at the time) and Dr. Doug Mills of the University of California Irvine (UCI). During the early 1990s, work in this area was advanced by these theorists and some experimental collaborators to provide insight into magnetic interactions between multilayers and high frequency responses of heterogeneous magnetic systems. Much of the physical response of the material was associated with the microstructure of the metal films. Advancing the materials microstructure concurrent with the theoretical studies paved the way for engineering magnetic material structures to tailor high frequency magnetic excitations in waveguides. By the year 2000, the experimental and theoretical work had proven its value such that microwave filters and other device concepts could be demonstrated using thin magnetic films. This success was based on a combination of the theory of how magnetic materials interacted at high frequencies at the microscale and the experimental work necessary to enable the growth and integration of magnetic materials with standard semiconductors and dielectrics. For example, by integrating an ultra-thin magnetic metal into a standard waveguide, the ferromagnetic resonance of the magnetic film would absorb energy at a relatively specific frequency that could be engineered by the choice of material and its geometry within the waveguide.

This success supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Network and Information Sciences



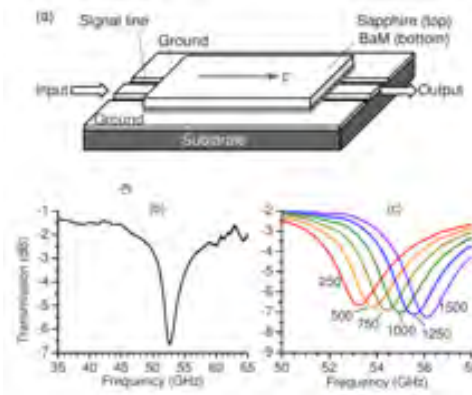


Figure 1. (a) A microwave notch filter in a coplanar waveguide results from spin waves generated in the magnetic barium hexaferrite (BaM) when the frequency of the incoming microwaves resonates with the natural frequency of oscillation of the magnetic moments in the BaM. (b) The high frequency response of the device shows significant attenuation at 52.5 GHz and can be tuned (c) with an external magnetic field. Curves in (c) labeled by the external field in Oersted. Taken from results from the MURI as published in *Appl. Phys. Lett.* 97, 173502 (2010).

This advance laid the foundation for a MURI on GHz-frequency physics and device concepts conceived by Dr. Ciftan and was given to Dr. Ulrich as the new Condensed Matter Physics program manager. The MURI began in 2004 with an award to UCCS as the lead institution. This MURI advanced our understanding of the physics of high frequency magnetic excitations, materials, and device concepts enabling filters, circulators and phased arrays in the 10 – 60 GHz frequency range. The MURI team was very responsive to the Army, taking cues from ARO as well as from Dr. Kokinski, a Chief Scientist at the former Communications and Electronics Research, Development and Engineering Center. Seeing the success and opportunity that this team had, Dr. Ulrich secured an add-on for this MURI to pursue device concepts that could transition readily to applied research programs. This add-on was to explore broadband device ideas as well as approaches for reducing insertion losses.

The success of this MURI was in large part due to the desire of the principle investigators to contribute meaningfully to the Army's mission and an informal advisory committee.

After the MURI came to a close in the Fall of 2010, there were some clear opportunities that were worth pursuing further. The ARO Physics and Electronics divisions recognized the opportunity for advancing device sciences in hexagonal ferrites and other materials and co-funded Drs. Celinski and Camley to pursue even higher frequency non-reciprocal device functionality. Dr. Celinski continues to effectively collaborate with defense contractors interested in the discoveries made under the ARO program.

Concurrent with these investments in the 1990s and 2000s was complementary work in the Materials Science of magnetic and multiferroic materials from Dr. John Prater's program. These strategic initiatives within the Electronics, Materials and Physics divisions and the results from them convinced Dr. Dev Palmer, former ARO program manager in the Electronics division, to move to DARPA to advocate for a program in this topic area.

Result

In 2017, based on the ARO-led advances, DARPA launched the Magnetic Miniaturized and Monolithically Integrated Components (M3IC) program with several contracts to defense contractors and related grants being awarded through the Army Research Office. The purpose of this program is to integrate magnetic materials directly into semiconductor substrates that are regularly used for microwave circuits, modeling the system-level impact of the magnetic materials on their characteristics, and optimizing frequency selective limiters and signal-to-noise enhancers in these integrated magnetic microwave materials. The effort to develop this technology continues. Phase I on this program succeeded in demonstrating that advanced magnetic materials can be integrated for radio frequency technologies with greatly reduced size.

RESULTS

- ▶ More than 200 peer-reviewed publications from ARO-funded efforts in this area
- ▶ ARO investments were the basis for the new \$20M+ DARPA M3IC program

Way Ahead

ARO has concluded its investment in this area and completely transitioned the work to DARPA which is supporting defense contractors' development of this exciting technology. ARL, AFRL, and NRL researchers are closely monitoring the progress of the M3IC program.

CONDENSED MATTER PHYSICS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Understand the physics governing the interaction between topological and magnetic states that if successful is anticipated to lead to ultra-efficient electronics.
- ▶ Unambiguously realize anyons and control them that if successful is anticipated to lead to novel electronic functions and a new highly scalable quantum information system.
- ▶ Observe new non-equilibrium states of solid state matter induced by coherent light that if successful is anticipated to lead to new forms of matter with novel properties that are dynamically controlled by lasers.

ELECTRONICS DIVISION: FY18 SUCCESS STORIES

OPTOELECTRONICS PROGRAM



Dr. Michael Gerhold

Program Manager, Optoelectronics
Program Manager (Acting), Electronic Sensing
Electronics Division
ARO Engineering Sciences Directorate

Dr. Gerhold completed his undergraduate studies at Purdue University, receiving his B.S. in Electrical Engineering in 1992, as well as a M.S. in Electrical Engineering in 1994. He received his Ph.D. in Electrical Engineering from the University of Michigan in 1999.

He came to ARO in 1999 as the Program Manager for Optoelectronics.

Pioneering Advances in Low Energy Information Processing

Challenge

The idea of on-chip optical interconnects has multiple components to it that are quite challenging due to the impact of Moore's law. In other words, the clock-speed of electronic CPUs became limited to 5 GHz or less due to the heat density created by ever increasing number of transistors on a chip. The heat is generated by the resistance of the wires and the net increase in current density for a given chip.

Action

ARO Optoelectronics Program Manager Michael Gerhold has established a major extramural research thrust in low-energy, high-speed optoelectronics which seeks to incorporate micro and nanophotonic devices onto integrated circuits to dramatically enhance computational performance. In 2015, Dr. Gerhold ventured into the thought realm of "On-chip Optical Interconnects" (OCOI) via a topical meeting he authored for the IEEE Photonics Society Summer Topical Meeting. This topic was selected by the IEEE Photonics Society and led to the first major discussion amongst thought leaders about the potential of incorporating photonics into an electronic "fabric" in a single chip-scale size (which could be completely monolithic or hybrid between two layers). Prior DARPA supported efforts had pursued levels of photonic integration that used off-chip lasers that were more concentrated on fundamental silicon photonics advances, but they had not tried to achieve competitive low energy/bit power consumption levels. This meeting was focused at gathering the leading nanophotonic device leaders from around the world to begin to ascertain this very goal to further IC communication performance at low energy levels – eventually low enough for true on-chip interconnects. The talks at the OCOI topical meeting were grouped into various headings aimed at showcasing the state-of-the-art in nanolasers, high-speed photodetectors, and high-speed optical modulators as well as relatively new integrated photonics platform approaches. Talks discussed advances and their potential to delve into the low femtojoule/bit regime needed for serious consideration of cm-scale or less interconnects.

In 2016, the DoD Integrated Photonics IMI, or Institute for Manufacturing Innovation known as AIM Photonics, was launched, and Dr. Gerhold's was selected to lead the Very High-speed Digital Data working group. He would participate in the near term goals of silicon photonics while continuing to assess how next generation photonic

This success supports
these ARL Core Technical
Competencies



Computational Sciences



Network and Information
Sciences

SUCCESS

ARO PM was able to motivate a large DARPA program with steps toward dense chip-scale photonic computing.

devices could be incorporated into needed packaging techniques and technologies of future electronic-photonic integration. Then, with about a dozen single investigator type programs, he put forth another topical meeting idea known as "Low Energy Integrated Nanophotonics" (or LEIN). This topical went forward in the summer 2017 topical series. It also brought together leading edge

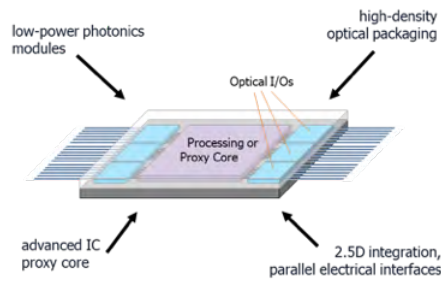


Figure 1. DARPA Photonics in the Package for Extreme Scalability (PIPES) Concept

researchers from the U.S. and abroad to look further at the state-of-the-art. Goals looked beyond the 5 year end-goal of AIM Photonics to reach 100 fJ/bit energy levels (by 2021) to what may be possible over the long-term. Discussions continued on current photonic device efficiencies such as Dr. Masaya Notomi's 1.6 fJ/bit optical modulator achievement (Nippon Telegraph and Telephone, Japan) using photonic crystal waveguide approaches, and also began a more thorough assessment of electronic circuit aspects related to true hybrid electronic and photonic integration scenarios. With the help of AIM Photonics, integrated photonics as field was greatly re-energized and brought life to the 2017 topical. Dr. Gerhold initiated panel discussions for the whole meeting (topical-wide) about the field looking both at the future of technology and the basic research required. Panelists from government labs including AFRL and NIST as well as leading groups from Stanford and UC-Berkeley were joined by recently selected DARPA PM, Dr. Gordon Keeler, who had come from Sandia. His participation in this topical meeting series was critical synergy for the field to see the need for programs asking what can truly be done with integrated photonics (outside of the more budding Si photonics based 100G transceiver work pursued at Intel) and it set the stage for pursuit of the DARPA Photonics in the Package for Extreme Scalability (PIPES) program announced just over a year later (a 6.2/6.3 investment aimed at technology transition by 2028 to provide new pathways to improve communication performance in such as a way as to be monolithically integrated with electronics).

Result

The topical meeting also led to a special issue of the IEEE Journal of Selected Topics in Quantum Electronics which Dr. Gerhold co-lead as editor. Integrated photonics advances over the past 5 years were all highlighted and brought together in one journal published as the November/December issue of 2018. ARO's program on low energy and high-speed optoelectronic was highlighted among other world leaders in the field and pointed to readiness of the field for a program announcement of DARPA PIPES.

The result of this story continues beyond PIPES. In 2019, Dr. Gerhold has refined his vision for further advances toward true intra-chip optical interconnects. DARPA has bought into the potential for photonics to outperform electronics at the chip-scale, but further advances in nanophotonic modulators, detectors, and possibly emitters (depending on the use of nanoscale light sources) are still needed for dense co-integration of photonics with electronics.

Way Ahead

Instead of looking at photonics merely as an improved way of transmitting data across a chip, photonic computing as a means of information processing apart from the transistor node of electronics is bring new perspective on the problem. While the goal of on-chip interconnects is still of interest, the motivation of new computing paradigms based more upon photonics than electronics has the potential to bring about the hybridization of the two and the introduction of even more disruptive photonic computing paradigms. These concepts are being pursued by the ARO Optoelectronics program in coordination with ARL-SEDD and CCDC AvMC.

RESULTS

- ▶ Workshop focus on "on-chip optical interconnect" concept moves into first major chip-scale electronic/photonic interconnect hybridization program.
- ▶ IEEE Journal of Selected Topics in Quantum Electronics focus issue borne from workshop.
- ▶ Lead role in DoD AIM Photonics institute garnered for Army.

This success supports these ARL Core Technical Competencies



Ballistics Sciences



Network and Information Sciences

SUCCESS

ARO PM was able to motivate a related DE-JTO program for ARL SEDD to partner with U. Central Florida. Potential DE System level advances are at hand.

RESULTS

- ▶ Dr. Gerhold's awareness of beam control technology led to new programs holding significant overmatch potential.
- ▶ Relationships with DE-JTO and ARL SEDD led to new patents partnered with ARO investigators
- ▶ ARL directed energy and free-space laser comm (ARAP) efforts enhanced.

Mitigating Atmospheric Turbulence with Modal Beam Control

Challenge

Directed energy research has long sought to achieve high intensity on target. In addition to the need for a high intensity laser source, atmospheric turbulence mitigation is the main challenge to achieving viable directed energy systems. Current approaches utilize wavefront sensors and deformable mirrors for adaptive optical beam control. Limitations of this approach are multifold, spanning both the technique of sensing and the adaptive beam control hardware.

Action

In order to achieve robust adaptive beam control goal, ARO Optoelectronics program manager Mike Gerhold was motivated by a decade of participation on the Advanced Concepts working group of the Directed Energy – Joint Transition Office (DE-JTO), where he served as one of the two Army representatives. As part of this effort, he led the 2012 Multidisciplinary Research Initiative (MRI) BAA for high energy laser research, and became highly engaged in current high energy laser efforts. One of those MRIs at the University of Central Florida's Center for Research in Electro-Optics and Lasers (CREOL), was making advances in fiber lasers and exploring ideas based on so-called "photonic lanterns" which generate an array of modes in a bundle of fibers that can be combined to form an orthogonal basis set. Each of the fiber contains one mode that can easily be switched in intensity at low power levels for high-speed agility to be later amplified within a fiber for multiple 10s of kW output levels.

A novel photonic lantern system with feedback mechanisms was formulated into a proposal as a result of Dr. Gerhold's prior relationship with Professor Guifang Li of CREOL. About that time, Dr. Jony J. Liu of ARL-SEDD was introduced to this research concept, as he had been the team leader for phased array beam control technologies pioneered at the ARL CISD Intelligent Optics Laboratory. However, ARL had never considered photonic lanterns or any mode basis set other than the commonly known idea of combining single lobed Gaussian type of beams coherently at a distant point from the laser array. Dr. Liu took a keen interest in the approach and discussed some of the nuances offering a possible direction for joint work with ARL. When DE-JTO was again interested in the research area of phased arrays, Dr. Gerhold was able to share the results of his recent investment in photonic lanterns, and discussions of the optical fiber field with Dr. Liu led to a new, but related idea based on Multi-Planar Light Control (or MPLC).

Result

As a result of these discussions and interactions, a proposal was formulated and submitted jointly by ARL-SEDD and UCF-CREOL to the DE-JTO. It was selected for funding to explore the MPLC and will be studied in parallel with the photonic lanterns. Dr. Liu also serves as the DoD's technical COR of a major beam control investment of the DE-JTO at Nutronics (Boulder, CO), which positions this research team to make tremendous strides for future Army directed energy systems.



Figure 1. Rendering of a 15-mode optical fiber photonic lantern

Way Ahead

The ARO Optoelectronics venture into atmospheric beam control research has led to new collaborative research efforts at ARL-SEDD with novel and uniquely promising approaches for the beam control field. Through these collaborations and their considerable collective expertise, ARL is well positioned to make significant contributions to the directed energy.

OPTOELECTRONICS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Explore the limits of low energy and high-speed optoelectronics to assess ways to surpass the performance of conventional electronics or consider hybrid integrated microsystems of the two. If successful, much faster and higher performance computing will be accomplished on mobile platforms with limited power supplies.
- ▶ Advance photonics capabilities through exploration of high intensity radiation generation within microscale systems. Chip-scale photonic light sources from UV to mid-infrared based upon novel materials, diffractive optical techniques for beam combining, shaping, and active control are aimed at Army surveillance, sensing, and communications.
- ▶ Power scaling methods and architectures along with adaptive optical control techniques to create directed energy solutions that reduce the size and power consumption of laser systems while revolutionizing beam control performance to mitigate the effects of atmospheric turbulence for greater power delivery.

ELECTRONIC SENSING PROGRAM



Dr. Michael Gerhold

Program Manager, Optoelectronics
Program Manager (Acting), Electronic Sensing
Electronics Division
ARO Engineering Sciences Directorate

Dr. Gerhold completed his undergraduate studies at Purdue University, receiving his B.S. in Electrical Engineering in 1992, as well as a M.S. in Electrical Engineering in 1994. He received his Ph.D. in Electrical Engineering from the University of Michigan in 1999.

He came to ARO in 1999 as the Program Manager for Optoelectronics.

Digital Alloys Based Upon Binary Semiconductors Produce Unexpected Noise Reductions

Challenge

Despite more than forty years of intense university and industrial research effort, no good III-V materials solution for avalanche photodiodes had been found. Specifically, the random nature of the multiplication mechanism in an APD results in gain fluctuations, a source of noise that is typically expressed as a multiplicative factor in the shot noise. The figure of merit is referred to as the excess noise factor. Could a disruptive materials solution be found? Could an engineering design be found that could overcome this barrier?

This success supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



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SUCCESS

ARO PMs were able to leverage DARPA co-funding to create a substantial program for achieving technical success.

RESULTS

- ▶ Recognition of a game-changing materials approach applicable to infrared systems as well as UV/Visible wavelengths.
- ▶ A long-term jointly funded basic research effort with DARPA/MTO.
- ▶ Identifies a path to explore for further device phenomena: highly order alloys, both digital and otherwise.

Action

Under ARO Electronic Sensing program manager William Clark, researchers were supported to artificially engineer the noise by building semiconductor alloys of InAsBi where hole transport was expected to be disrupted by the presence of the large bismuth atoms in the crystal. Professor John David's group at the University of Sheffield showed that, quite unexpectedly, InAs was itself a near perfect APD material from the perspective of low excess noise, since only electrons can trigger the impact ionization events that give rise to gain. The result was the first III-V material whose noise performance rivaled that of HgCdTe. The key advantage of InAs, a material where only electrons can impact ionize, is that the gain-bandwidth product is effectively infinite, permitting extremely high data throughput.

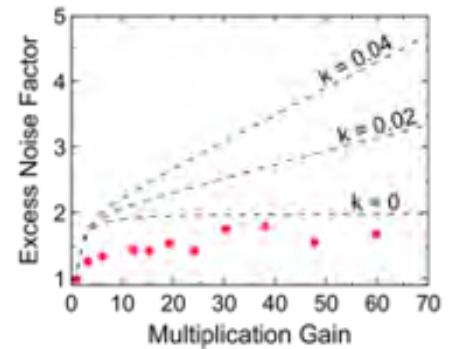


Figure 1. Anomalously low excess noise from InAs, as a function of multiplication gain.

The challenge with InAs is that the dark currents are high, due to the small bandgap. To combat this issue, Dr. Gerhold supported these researchers to investigate the AlInAsSb system (which includes InAs) on GaSb substrates in a follow-on effort. To prevent phase segregation, these alloys must be grown as a digital alloy.

Result

AlInAsSb soon was found to be the first III-V alloy system that exhibits low excess noise, independent of composition, enabling larger bandgap multipliers which exhibit lower dark currents than pure InAs. In 2018, these researchers demonstrated extremely high gains and low noise from these APDs, as shown in Figure 2. They have also demonstrated single photon counting at room temperature, an exciting opportunity for future practical quantum information processing systems.

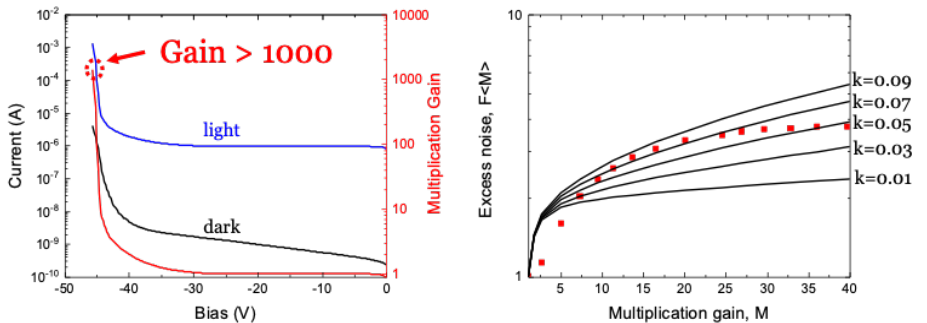


Figure 2. (Left) Multiplications >1000 at room temperature with (right) low excess noise demonstrated in 2018.

As an example of the potential flexibility of the digital alloy APD approach, as shown in Figure 3, ARO funded research also demonstrated in 2018 the first low-noise APDs on InP substrates. The digital alloy growth technique enables longer wavelength sensitivity, with sensitivity >2 μm , as well as low excess noise. Combining these two advantages would yield a revolutionary APD technology for LIDAR that is compatible with 2.039 μm fiber laser sources.

These results led to a joint effort between Dr. Gerhold and the DARPA Microsystems Technology Office to explore further enhancements of these approaches. With this joint support, Professors Seth Bank (UT-Austin) and Joe Campbell (University of Virginia) have developed new artificial semiconductor materials based on digital alloys that can manipulate high-field transport properties, enabling avalanche photodiodes (APDs) with record noise performance.

Way Ahead

The next steps are to apply this new capability to meet important future DoD needs, including: (1) developing arrays of these detectors to improve the sensitivity of future LIDAR systems; (2) combining these low-noise multipliers with smaller bandgap absorbers to access other technologically important wavelength bands, including the mid-wave infrared for high-sensitivity imaging systems; and (3) and demonstrating single photon counting with photon number resolution for quantum information processing at telecommunications wavelengths.

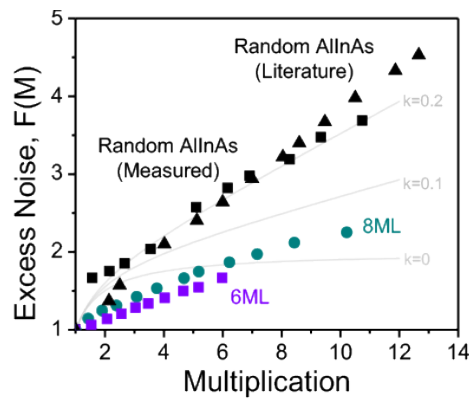


Figure 3. The excess noise of conventional InP-based AllnAs multipliers (black squares and triangles) can be dramatically reduced through the digital alloy growth method (green circles and purple squares).

Pb-Salt Based Detectors for Superior Uncooled Operation

Challenge

Mid-Infrared (IR) sensing and imaging have widespread military and industrial applications. The mid-IR detector system needs to be compact, portable, cost-effective, and have a fast response time. Thermal detectors, also known as bolometers, are based upon measuring a difference in temperature due to impinging infrared photons. They are the most widely used room temperature detector, but they offer a notably slow response time. Can a faster detector with room temperature operation be developed for superior mid-IR sensing and imaging?

Action

ARO Electronic Sensing program manager William Clark identified and supported a unique research team at the University of Oklahoma that developed an optimized fabrication process for Pb-salt uncooled photoconductive detectors. This research led to a record high detector performance, specific detectivity (D^*), in comparison with similar detectors developed by commercial companies (see Figure 1). Three patents were filed based on this ARO supported research, and the team has developed technologies that could grow PbSe detectors directly on Si read-out integrated circuitry (ROIC), making low-cost monolithic integration focal plane arrays possible.

After the ARO supported research demonstrated a record specific detectivity for PbSe as a mid-IR detector, Northrop Grumman reported a TE-cooled PbSe focal-plane array (FPA) monolithically fabricated on Si ROIC. These two results brought broad tremendous attention to the field and, in 2015, with expert guidance from ARO program managers, the DARPA Wafer Scale Infrared Detectors (WIRED) program was initiated to develop high-performance, low-cost mid-wave and short-wave infrared detector and imager. One of the key performers on the DARPA WIRED program was the University of Oklahoma team originally supported by ARO.

This success supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Network and Information Sciences



SUCCESS

ARO Electronic Sensing investment transitioned to DARPA, achieving record performance at mid-wave infrared wavelengths operating at room temperature

RESULTS

- ▶ ARO project resulted in the best uncooled mid-IR detector
- ▶ The ARO investment resulted in a DARPA/MTO FPA program.
- ▶ Dr. Gerhold identified a way forward by assessing the scientific understanding behind the record results.

Result

Uncooled, low-cost Pb-salt (PbS and PbSe) photoconductive detectors are now the preferred solution for many applications in the 1-5 μm mid-IR spectral range. In 2018, detectors were produced with external quantum efficiency (EQE) of 12% at room temperature. Researchers at Oklahoma University, in collaboration with a German research team, also revealed for the first time the complex oxide-semiconductor nanostructure that defines these materials due to the “sensitization” post-growth annealing process in oxygen and iodine atmosphere used to fabricate them.

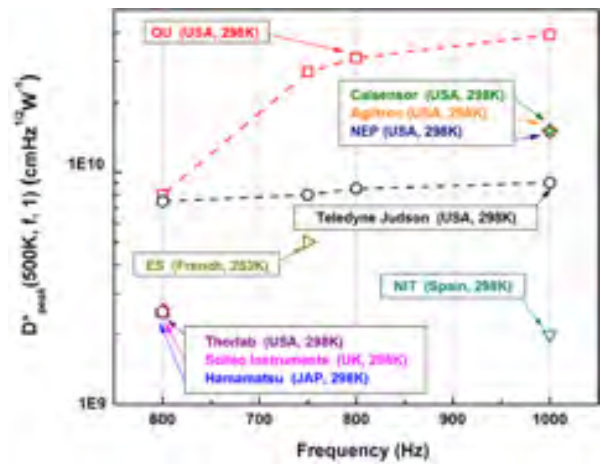


Figure 1. Room Temperature Mid-IR PbSe Detector Performance Comparison

Way Ahead

The detailed nanostructural characterization achieved in this recent effort has now enabled researchers to understand the fundamental properties, benefits, and limitations of Pb-salt detector materials, and how non-uniformity corrections need to be included in the ROIC. To overcome these problems, the ARO Electronic Sensing Acting Program Manager Michael Gerhold identified a new research effort, in coordination with ARL-SEDD, to use plasma assisted MBE with a well-controlled process to study, emulate, and improve PbSe thin film detectors with better uniformity and performance. The MBE deposition also opens doors to extend wavelength to long-wave IR and explore other heterojunction structure to further improve performance and reduce operating power.

ELECTRONICS SENSING PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Explore mid-infrared photodetector heterostructures, processing techniques, and architectures to enhance detectivity both for mid-wave and long-wave IR. Surpassing the high cost and low operating temperature of state-of-the-art HgCdTe detectors have been difficult objectives with continuing potential merit.
- ▶ Investigate promising photonic sensing techniques (UV to IR), usually involving intensity enhancements and possibly nonlinear interactions, to enhance the capabilities of both active and passive sensing modalities. Success will result in sensors with greater range, resolution, specificity, or other (often related) metrics for Army photonics-based systems.
- ▶ Other electronics sensing regimes that fall outside of photonics or utilize combined effects (e.g., electromagnetic, photoacoustic, etc.) have also been considered but often need de-conflicted with related ARO programs – particularly the Solid-State and Electromagnetics, Electronics Division program.

BIOTRONICS PROGRAM



Dr. James Harvey

Program Manager (Acting), Biotronics
Electronics Division
ARO Engineering Sciences Directorate

Dr. Harvey completed his undergraduate studies at the U.S. Military Academy, receiving his B.S. in Engineering in 1964. He trained as a Physicist at Dartmouth College and at Lawrence Livermore National Laboratory, receiving his Ph.D. in Applied Science in 1990.

He served a postdoctoral fellowship at ARL in 1991 and then to ARO in 1994 as an Electronics Engineer and program manager for Electromagnetics and RF



Dr. Richard Hammond (Retired)

Program Manager, Optics
Physics Division
ARO Physical Sciences Directorate

Dr. Hammond completed his undergraduate studies at New Jersey Institute of Technology, receiving his B.S. physics in 1973. He trained as a physicist at Rensselaer Polytechnic Institute, receiving his M.S. and Ph.D. degrees in optics in 1979.

He came to ARO in 2002 as the Program Manager for Optics and retired from ARO in June 2019.

A New Form of Matter and Energy, Optical / Plasma Filaments, Provide New Opportunities for Directed Energy Applications

Challenge

The Army has a long standing interest in directed energy technology. However, until recently progress toward this goal has been sporadic, and while there have been many practical offshoots, realization of the idealized form has been elusive. Overcoming the problem of thermal blooming which has been well understood since the advent of high energy lasers has been particularly challenging. Thermal blooming is where a laser beam creates a plasma when it interacts with the atmosphere. The plasma then forms a lens which defocuses the laser and disperses the optical energy. A promising and exciting path forward is created by the advent of light filamentation. In 1995, the first observation in Europe of propagating terawatt, femto-second optical pulses, self-channeled in a plasma filament in air, presaged entirely new potential applications of directed energy. The optical pulse is coupled to the plasma filament, which it generates, by the stabilization of the natural optical diffraction and refraction from the plasma with the self-focusing due to the non-linear index of refraction. The propagation can be stable over distances from tens of meters to hundreds of meters and the plasma filament can form and reform over longer distances. A complex electromagnetic field extending well beyond the lateral limits of the pulse, accompanies it. The propagating

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Materials and Manufacturing Sciences



beam structure can be very complex, with a single or multiple beams together. As the pulse propagates it generates a co-propagating white light optical continuum from the highly non-linear effects in the plasma filament. In high pressure rare gases, the optical pulse can produce high intensity, high energy, coherent X-rays. The detailed physics of the phenomena is still not well understood and an understanding of how to control the filament challenges the most sophisticated coupled propagation and quantum dynamical models available. It is still not clear what is the ultimate limit on the distance of propagation. The challenge is in understanding and then controlling this extremely complex state of coupled matter and energy.

SUCCESS

ARO research is funding research into directed energy technology. If successful, light filamentation will be utilized to overcome the major obstacle of thermal blooming. This research has implications not only for directed energy weaponry but for high bandwidth communications, remote sensing, and fundamental materials science as well.

Action

In 2004, ARO Program Manager Dr. Richard Hammond learned about this potential new form of energy propagation embodied by light filaments and, to find what research was needed, and what the applications were to the Army and DoD, he organized a workshop at Duke University to explore the existing knowledge on light filaments and future directions of research. The workshop was intense, led by Dr. Hammond working with Dr. Bob Gunther of Duke University, and the result of the two-day effort was the production of a document to serve as a blueprint the next steps. It was found there was much to learn and many potential applications. Following the guidance of the workshop, Dr. Hammond started a project with core single investigator funds.

Meanwhile, Dr. James Harvey was serving a foreign assignment exploring basic research breakthroughs in Europe. Independently he discovered the European filamentation research being conducted and worked to gain attention from the US military scientific community. On his return he worked with Dr. Hammond to establish a large scale Multi-disciplinary University Research Initiative (MURI) project at the University of Central Florida (UCF) to explore the new phenomena and to collaborate with Air Force Office of Scientific Research (AFOSR) MURI on the theory and modeling of the filamentation dynamics, which was designed to be complementary to the ARO MURI. Dr. Harvey also initiated some single investigator grants in his ARO Electromagnetics (EM) Program.

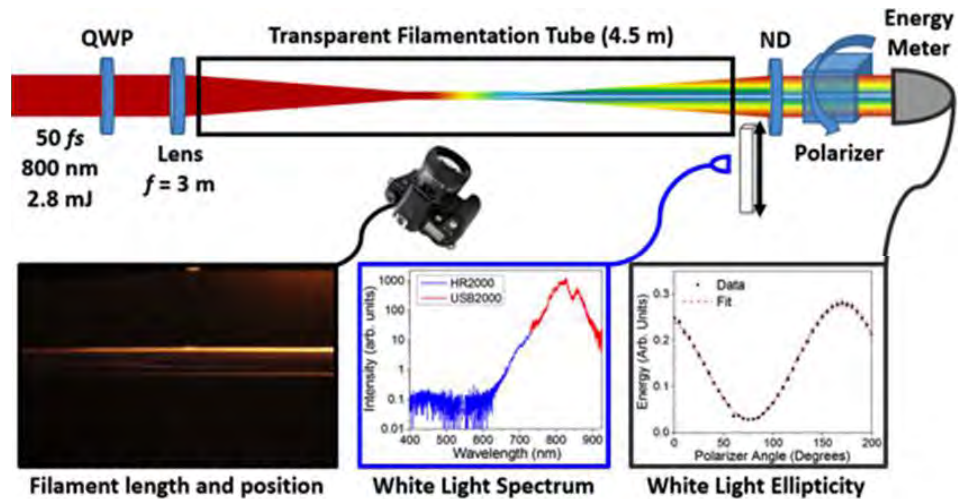


Figure 1. Experimental recording of the filament physical structure along with the spectrum of the white light continuum generated in the filament. a is a side view along the camera. The filament forms at the focus in the filamentation tube. b is the very broadband white light continuum formed in the filament and recorded from the end (energy meter). c records the polarization of the light.

During the ARO MURI, Dr. Hammond worked with NASA and Air Force to help the MURI PI, Prof. Richardson, secure vitally needed outdoor space on Merritt Island. With Dr. Harvey, Dr. Hammond was able to secure additional funding, via a DURIP (Defense University Research Instrumentation Program) grant, so the facility on Merritt Island can operate ultrahigh intense laser and measure light filamentation for a kilometer and more.

Result

Measurements taken at UCF and on Merritt Island showed some surprising and interesting effects. One was that light filaments create THz radiation at distance targets. This is exciting because THz radiation, a very important energy range for spectrographic analysis, does not propagate well in the atmosphere. With the light filament, the atmospheric loss is eliminated since it is created and detected at or near the target. This opens the way for applications in remote sensing and detection of chemical, biological, or explosive material.

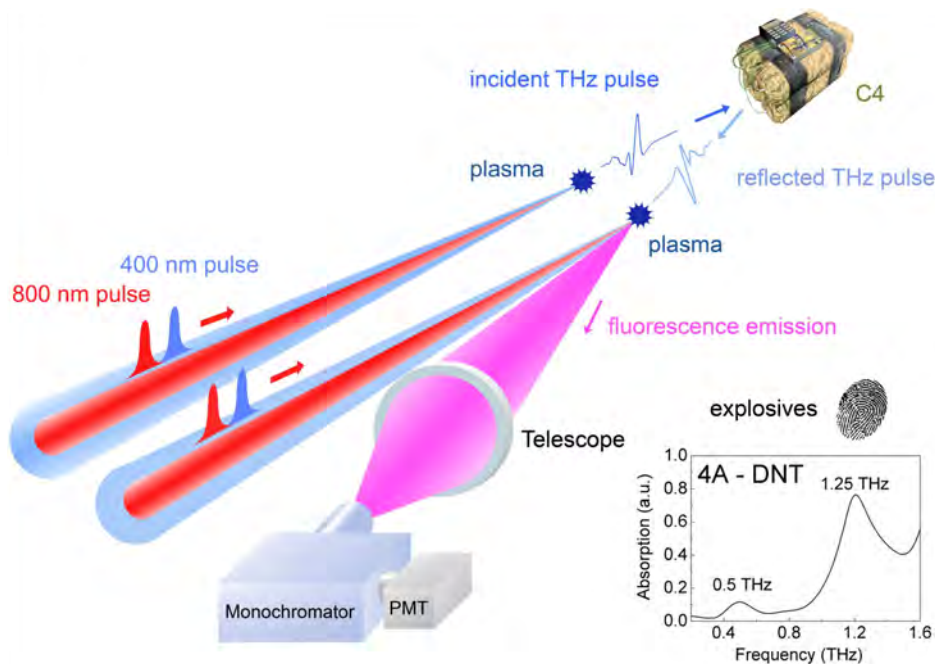


Figure 2. Notional schematic of remote spectroscopic THz detection. Shown is the THz spectrum of the explosive DNT. The key to this detection scheme is that the THz pulse is generated close to the target by laser plasma and is detected also close to the target by a second laser plasma, which produces optical fluorescence to be detected by the distant monochromator.

Another result of this research was the development of local EMP. The light filament, when hitting a structure housing any circuitry, will destroy or disable the electronics. Dr. Hammond worked with Richardson to develop a video showing these effects. The result was an exciting video showing a light filament knocking a drone out of the air. This video is being used to show the power of light filaments, and Dr. Hammond worked to involve other agencies to develop it further.

Supported by Dr. Harvey and Dr. Hammond in current and future research, Prof. Milchberg discovered for the first time that the femto-second laser beam creates an “air waveguide” for guided optical and electrical propagation. The gradient in the index of refraction can guide longer laser beams with higher energy, electrical discharges, and electrical currents.

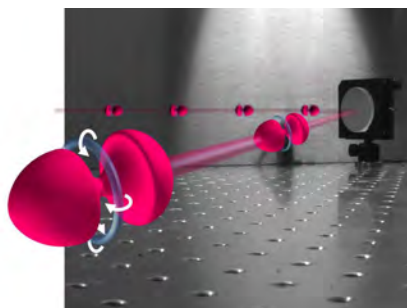


Figure 3. “Smoke rings in light.” The electromagnetic phase and energy circulates in a torus shape around the point of collapse in the beam due to self-focusing and propagates with the pulse.

RESULTS

- ▶ Two professional society awards. Two prestigious foundation fellowships. Four honorary degrees from prestigious foreign universities. Elections to the US National Academy of Science, German Academy of Science, American Philosophical Society, Royal Irish Academy.
- ▶ Pioneering research in understanding new optical / plasma phenomena.
- ▶ Three breakthrough discoveries of new physical phenomena with wide range of applications.
- ▶ Inspiration for two new MURI's.
- ▶ Strong laboratory collaboration with ARL-WMRD researchers.

Prof. Milchberg has also discovered for the first time that the optical beam collapse along the filament causes a spatial-temporal optical vortex in which the electromagnetic phase and energy circulate in a dynamic torus or “smoke ring” like structure around the propagating pulse (see figure below). This is fundamentally different than the much-studied Orbital Angular Momentum (OAM) vortex (e.g., a Laguerre-Gaussian beam). The STOV has a topological charge which protects the beam as it propagates from other propagating beams. He has shown theoretically that the STOV's are a general fundamental property of the collapse of non-linearly propagation of intense pulses in many other systems as well, for example, in the relativistic self-focusing and filamentation of accelerated electron beams. His work is the first ever discovery of this important topological feature of nature in non-linearly propagating beams.

Propagating the femto-second laser pulse through a high-pressure gas produces a laser filament in which the non-linear processes in the laser plasma support extremely high harmonic generation (HHG) of ultrashort pulses of extreme ultraviolet (EUV) radiation in a very bright, coherent, collinear, very broadband continuum. Support by Dr. Harvey and Dr. Hammond's ARO programs enabled the extension of the spectrum into the soft X-ray region up to several keV. ARO support resulted in the discovery that the HHG process was highly enhanced by using longer wavelength laser pulses and a high degree of phase matching between the driving laser field and the resulting X-ray field. Theory predicts that a 10 micron wavelength driving laser could extend the X-ray spectrum to 10 keV or more. ARO support also resulted in the discovery that an ultraviolet laser driving pulse provided highly enhanced conversion efficiency and a new phenomenon: the generation of well-separated narrowband peaks (~9 eV separation with linewidths of 70-700 meV). The discoveries in the HHG of coherent EUV and X-ray radiation open the way for table top sources with unique capabilities for the exploration of nanoscale magnetic, phononic, thermal, and phase-change phenomena in materials science. Although synchrotrons can produce coherent X-rays for materials science research, much of the range of phenomena are addressable with the much smaller and cheaper HHG sources, which can bring the capability within reach of every university, military, or industrial materials laboratory.

This research has over the years propelled Prof. Murnane to prominence in the Vannevar Bush Fellowship program, DARPA programs, and leadership of an AFOSR MURI. It has led to Prof. Milchberg being sought for the DARPA PULSE program. And has established Prof. Richardson and his collaborators as true pioneers of a new area of optical physics.

ARL-WMRD researchers are frequent collaborators in Prof. Milchberg's lab.

Way Ahead

These discoveries open the door to the development of new classes of electronic and structural materials with new properties. New insight into cellular biological processes will result from the ability to image living cells at the nanoscale in 3D. Military applications include controlled high voltage discharges for landmine/IED remediation, IR countermeasures, remote sensing of chemical and biological material, and directed

energy for counter missile, counter UAV, counter-battery. The prospect to remotely discharge and shut down a town's electrical generation system has been demonstrated. There is a potential for plasma antennas for selective radar and communications. In the future, with larger systems, the Army may have important new capabilities from the application of light filaments. These include knocking out airborne missiles as well as ground platforms at standoff distances. It may be possible to destroy all electronics, or just temporarily suspend their operation.

New Focus Area on the Potential for Electronics to Provide New Insight into Biological Cell Internal Functionality

Challenge

All biological processes in living organisms are ultimately initiated by the intracellular (inter- and intra-organelle) processes in the single cell or single cells acting together. These processes can be extremely sensitive and dramatically alter the physiology of the cell. Although the external effects of the intra-cellular signaling events occur at time scales of minutes to hours outside the cell, the events themselves within a cell occur at time scales between picoseconds to milliseconds. Moreover, organelles range from hundreds of nanometers to tens of micrometers and their biomolecules range from one to tens of nanometers. Traditional methods for investigating the intracellular processes lack either the temporal or spatial resolution and are very limited in their ability to manipulate the processes.

Action

In 2017, a Visioning Workshop was held by the ARO Electronics Division, bringing together a scientific panel from Duke University, Harvard University, MIT, and Notre Dame in addition to participants from the ARO Physics and Materials Science Divisions. With additional perspective and encouragement from the workshop to explore new areas of research, ARO program manager Dr. James Harvey reoriented the existing nano- and bio- electronics program to address areas of bioelectronics which had not already received major, focused government funding or attention, which had not been significantly explored, which represented very high-risk research, and which would push the envelope of scientific innovation.

"Signaling" is the process by which cells and cell components affect each other and initiate cellular and intra-cellular activity. Signaling within a cell is either a biochemical or mechanical process, with much of the biochemical signaling within a cell mediated by ion flow in ion channels. Furthermore, organelles, particularly mitochondria, generate small but measurable electrical signals during their internal processing of chemical energy in their "electron transport chain." A distribution of voltages in the cell and its components is caused by and drives these charge flows, is highly heterogeneous on a spatial nanoscale, and is highly dynamic temporally. Dr. Harvey recognized the key role of electrical processes in the single cell activity, and the opportunity to understand and manipulate the electrical (and mechanical and chemical) processes among the organelles using the unique capabilities of electronics. Dr. Harvey coined the term "Biotronics" to describe the new focus area and to distinguish it from the other very large number of efforts in bioelectronics.

Successful traditional methods for exploring single cell electrical processes are bio-chemical methods, optogenetics, and the patch clamp technique. Projects in the Biotronics program provide both highly innovative extensions of these techniques based on the unique capabilities of electronics and totally new, complementary methods, addressing the internal function and electrical processes within the cell with unprecedented spatial and temporal resolution and with minimal disruption of "normal"

This success supports these ARL Core Technical Competencies

Human Sciences



Protection Sciences



SUCCESS

ARO research is funding research into new instrumentation to explore the fundamental biological processes within the single cell which uniquely involve EM fields and currents or which are uniquely susceptible to EM control and modulation at the nano-scale.

If successful, entirely new understanding of the electrical processes in the cell will be gained and a new capability to control these processes will be achieved, with implications for disease prevention and treatment and protection from environmental hazards.

living cell function. The initial research efforts supported under this program have been active for little over a year, so significant accomplishments have not yet been produced, but the initial portfolio is characterized by aggressive science, major innovation, and risk. Dr. Harvey has identified researchers who were working outside the bioelectronics mainstream and has challenged other prominent bioelectronics researchers to moderate their research approaches to address the very difficult problem represented by the single cell processes. Some examples of the initial grants are described below.

Preliminary work supported by ARO has shown that the intracellular pathways related to the cell organelles respond to electrical charge patterns at the interface between a cell and a wide bandgap semiconductor. Here the charge distribution at the interface is written and controlled by an ultraviolet (UV) laser using the induced persistent photoconductivity (PPC) effect at the semiconductor surface. The interface charges induce activation or deactivation of metabolic pathways within the cell. The cell responds by the release of chemical signals which are analyzed to determine the intracellular processes quantitatively. The UV light does not directly illuminate the cell. The interrogation and analysis is entirely non-invasive and allows the cell function to be observed in its most natural state.

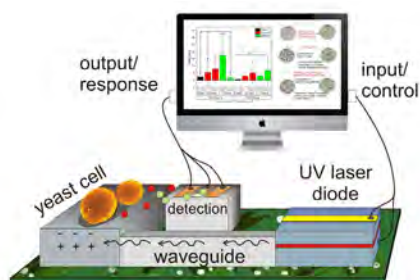


Figure 1. Biotronics platform for the manipulation of the intracellular processes of a single cell. The UV laser writes a charge distribution within the wide bandgap semiconductor. The resulting charge, chemical, mechanical properties of the surface induce changes in the metabolic pathways within the cell. The resulting chemical signals are detected and analyzed to reveal the intracellular processes.

In a second example, ARO supported researchers have demonstrated that, in addition to the well-studied biochemical and transcription pathways, single cells also use electrical and mechanical signals for processing intracellular information, which are manifested in rapid voltage changes across intracellular membranes and force generation within the cytoskeleton. This research investigates the bioelectric dynamics of individual organelles using nanoscale silicon-based electronic, optoelectronic, and thermal devices internalized with very high spatial resolution near single organelles and triggered optoelectronically to stimulate and read frequency domain bioelectric signatures. Mitochondria, cytoskeletal filaments, and the endoplasmic reticulum (ER) are being targeted.

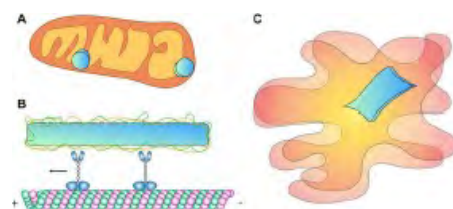


Figure 2. Bioelectric modulation at organelle / silicon interfaces.

- A. Silicon nanodisc / mitochondrial interface.
- B. Silicon nanorod / microtubule interface.
- C. Silicon nanomembrane / ER interface.

Additionally, ARO supported research is underway to develop a new scanning microscopy capability to non-invasively investigate the electrically active components of cells, such as mitochondria, and their role in intracellular pathways, such as cell death. The research will investigate the capacitance of single isolated organelles, capacitance of and between organelles in a single cell, fields and currents generated by organelles at audio to microwave frequencies, and the biological significance of the fields and currents. Preliminary results indicate that these fields and currents are important in the organelle to organelle signaling associated with apoptosis, wound healing, and several disease pathologies.

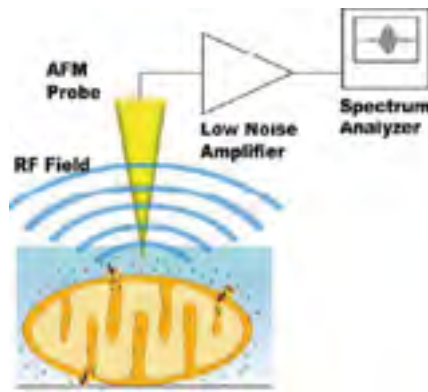


Figure 3. Passive imaging of the electromagnetic field spectrum vs frequency from a single mitochondria using a platinum RF probe.

Result

A suite of entirely new instrumentation concepts has been developed and is being implemented with unprecedented spatial and temporal resolution and minimal invasiveness to investigate intra-cellular processes in an entirely new domain. A nano-scale scanning microwave imaging system with the capability to non-invasively image the EM fields and inter / intra organelle capacitance at intra-organelle spatial scales has been developed. A capability to investigate inter-organelle electrical and mechanical signaling at the nano-scale using silicon nano-devices inserted in the cell structure has been pioneered. Additional research addresses other innovative electronic instrumentation concepts.

The research supported by Dr. Harvey is developing new understanding of fundamental cellular processes that will have a major impact on understanding and engineering Soldier performance, disease immunity, resistance to biological and chemical agents, and wound healing. The understanding can also drive new insights in synthetic biology and provide new approaches to interfacing electronic systems with human body.

Way Ahead

A workshop has been organized for the summer of 2019 to review the first year of effort and to define future direction of the program. It will also explore opportunities for collaboration between the researchers with unique new instrumentation to see if there are novel phenomena which will yield to combinations of the instruments or approaches. Bioelectronic engineers from ARL-WMRD have been engaged in developing the program and the project portfolio, and will be directly engaged in the workshop and its assessment. The next objectives of the program are to validate the new instrumentation and to start investigating unique intra-cellular measurements for new biological insights.

RESULTS

- ▶ Entirely new electronic based instrumentation concepts developed for unique characterization of the intra-cellular environment.

BIOTRONICS PROGRAM – CURRENT SCIENTIFIC OBJECTIVES

- ▶ Create new instrumentation and measurement approaches to elicit unique information about intra-cellular processes.
- ▶ Investigate intra-cellular processes in the single cell and/or immediate environment with unprecedented spatial and temporal precision and with minimal invasiveness.

SOLID-STATE ELECTRONICS AND ELECTROMAGNETICS PROGRAM



Dr. Joe Qiu

Program Manager, Solid-State Electronics and Electromagnetics
Electronics Division
ARO Engineering Sciences Directorate

Dr. Qiu completed his undergraduate studies at the State University of New York at Stony Brook, receiving his B.S. in Physics in 1991. He trained as a Physicist at the State University of New York at Stony Brook, receiving his Ph.D. in Physics in 1997.

He came to ARL in 2008 as an Electronics Engineer and then to ARO in 2013 as the Program Manager for Solid-State Electronics and Electromagnetics.



Dr. Marc Ulrich

Program Manager, Condensed Matter Physics
Division Chief, Physics
ARO Physical Sciences Directorate

Dr. Ulrich completed his undergraduate studies at Houghton College, receiving his B.S. in Physics in 1994. He trained as a physicist at Auburn University receiving his Ph.D. in Condensed Matter Physics in 2001.

He came to ARO in 2003 as the Program Manager for Condensed Matter Physics and was promoted to the additional role of Chief, Physics Division, in 2008.

Signature of Majorana Fermion in Topological Insulator-Superconductor Heterostructures

Scientific Challenge

Majorana fermions, which were predicted more than 80 years ago by Italian theoretical physicist Ettore Majorana, are particles that are their own anti-particles and carry zero electrical charge. They have been the focus of keen interest for quantum computing in large part because their neutral charge make them resistant to external interference and give them the ability to leverage and sustain a quantum property known as entanglement. Entanglement allows two physically separate particles to concurrently encode information, which could generate enormous computing power.

Although Majorana fermions were proposed as elementary particles, their analog can also be realized as quasiparticle quantum mechanical states in solid-state systems. There have been many attempts to experimentally confirm the existence of these quasiparticle states in the past decade, but all have produced inconclusive signals which could also be attributed to other effects, such as Kondo correlations, Andreev bound states, weak antilocalization, and reflectionless tunneling.

Action

In contrast to previous approaches, researchers at University of California, Los Angeles, led by Professor Kang Wang and funded by an ARO MURI award looked for 1D chiral Majorana edge modes in stacked layers of a superconductor thin film and a quantum anomalous Hall insulator (QAHI), i.e., a magnetic topological insulator (TI). The researchers were able to demonstrate quantized longitudinal Hall conductance occurred

This success supports these ARL Core Technical Competencies



Materials and
Manufacturing Sciences



Computational Sciences

during the transition between two integer quantum Hall states as predicted by theory. This quantized signature gives the first firm evidence of the presence Chiral Majorana fermions in the QAHI-superconductor system.

This accomplishment is also a direct result of ARO Solid-State Electronics and Electromagnetics program manager Joe Qiu's continuous strategic investments in magnetic heterostructures incorporating TIs and other dissimilar materials and understanding proximity phenomena at their interfaces. Professor Wang was initially funded by a Short-Term Innovative Research (STIR) award to investigate the origin of the spin-orbit torque (SOT) by using a uniformly doped magnetic TI sandwiched between two different dielectric materials. The use of two different dielectric films breaks the inversion symmetry of the structure and results in different SOT at the bottom and top surfaces. After the STIR award, the Professor Wang was awarded a single-investigator grant to continue his investigation of interface phenomena in topological-based magnetic heterostructure. Under that award, Professor Wang developed techniques to grow novel TI-based magnetic heterostructures interfacing TI to ferromagnetic insulator (FMI) and antiferromagnetic materials (AFM), and this resulted in successful demonstration of quantum anomalous Hall effect in a magnetically doped TI for the first time in the United States. These results ultimately led to a new understanding that sharp interfaces between TIs and other materials can be created so that TI can be used to effectively control the spin texture and dynamics of neighboring materials through strong spin-orbit coupling in TIs, and this could potentially enable a new type of energy-efficient terahertz-speed spintronic devices. Based on this understanding, a new MURI topic was developed collaboratively by ARO's Electronics, Materials Science and Physics Divisions. After a competitive selection process, a team led by Professor Wang, involving laboratories from University of California, Los Angeles (UCLA), California Institute of Technology, University of California, Irvine, University of Texas, Austin, North Carolina State University, and the University of Nebraska was awarded the MURI grant. Through the MURI award, Professor Wang continued his investigation of magnetic TI-based heterostructures which ultimately led to the discovery of chiral Majorana fermions.

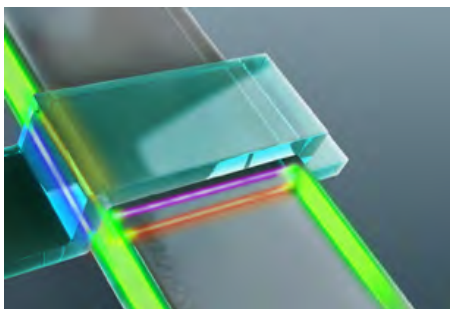


Figure 1. Rendering of the electronic device in which Majorana particles were observed. The device is made up of a superconductor (blue bar) and a magnetic topological insulator (gray strip). The Majorana particles result in transport channels (shown in red, pink, blue and yellow) in the electronic device.

Result

The discovery not only solves a long-standing problem in physics, but also opens up a potential avenue to control Majorana fermions for realizing robust topological quantum computing. The QAHI-superconductor system was realized as a prototype of the chiral TSC in two dimensions; more complex layouts could be engineered to host the bound states of Majorana fermions in solid state and enable their manipulation. The Majorana fermion modes are predicted to be topologically protected and thus may become a building block for robust topological quantum computing. The research leading to the discovery represents a close interdisciplinary collaboration between a team of researchers including electrical engineers, physicists and material scientists.

SUCCESS

The discovery of chiral Majorana fermions not only solves a long-standing problem in physics, but also opens up a potential avenue to control Majorana fermions for realizing robust topological quantum computing.

RESULTS

- ▶ Published in the prestigious journal *Science*
 - ▶ Featured in three invited talks presented by Professor Wang and his collaborators during the 2018 American Physical Society March Meeting
 - ▶ Professor Kanf Wang was awarded the 2018 Magnetism Award and Neel Medal for "the discovery of chiral Majorana fermions and outstanding contributions to topological spintronics."
-

This success supports these ARL Core Technical Competencies



Network and Information Sciences



Computational Sciences

SUCCESS

ARO supported research is the first to address physical layer security in terahertz data link and lays the foundation for continuous investment to enable communication networks with enhanced security and terabits/sec throughput.

The research, published in the prestigious journal *Science* in 2017, was featured in three invited talks presented by Professor Wang and his collaborators during the 2018 American Physical Society March Meeting. Professor Wang was also awarded the 2018 Magnetism Award and Neel Medal for “the discovery of chiral Majorana fermions and outstanding contributions to topological spintronics.”

Way Ahead

ARO has established a new collaboration between UCLA and an ARL-SEDD supported postdoctoral fellow who will be working at UCLA with Professor Kang Wang. UCLA and ARL will jointly develop techniques to synthesize and characterize heterostructures of topological insulators interfacing with other materials and create energy efficient and low power consumption electronic device concepts based on these heterostructures.

ARO-funded Scientists Expose Security Vulnerabilities in Terahertz Data Links

Scientific Challenge

The proliferation of radio and wireless technologies has created severe spectral congestion at RF and microwave parts of the electromagnetic spectrum, and is pushing DoD electronics systems in communications, radar and electronic warfare to operate at millimeter-wave (MMW) and even terahertz (THz) frequencies. Key advantages of these higher frequencies include the promise of virtually limitless bandwidth and the presumed covert nature of communication links, in comparison with conventional broadcasts at lower frequencies. However, despite many decades of research which has led to the impending roll-out of commercial 5G systems to include broadcast standard at MMW frequencies such as the 28 GHz band, no functional communication systems operating at 0.1-1 THz have been realized.

Action

Wireless communication systems are often described using an abstraction which distinguishes the hardware components (the physical layer) from the signal processing and algorithms which implement protocols for managing data flow, detecting and correcting transmission errors, and optimizing spectrum usage (the media access control (MAC) layer). It is natural, therefore, to separate the research tasks into these two categories. However, when the physics of the transmission channel changes very dramatically (as is the case in the transition from microwave to terahertz links), it becomes necessary to adopt a more holistic viewpoint. New physical-layer architectures, which are limited by material properties, atmospheric losses, or the physics of beam propagation, will have major implications for the design of new MAC layer protocols. These can present both new challenges and new opportunities for the implementation and optimization of network services. Therefore, although most of the research performed to date has focused primarily on the development of components or other hardware (and, to a lesser extent, on the development of new protocols), ARO Solid-State Electronics and Electromagnetics Program Manager Joe Qiu has strategically sought to merge these two sub-fields. Progress in device and sub-systems must be informed by the possibilities and limitations of signal processing and information theory; similarly, new approaches to implementing routing, discovery, and other network protocols must be aware of both current and future limits of source and detector technology. This situation demands a highly collaborative and multi-disciplinary approach to the problem. Expertise is needed in the physics of propagation and material properties at terahertz frequencies, network theory, circuit design, and packaging. Meaningful progress will require a coordinated research team including a diverse set of skills and expertise.

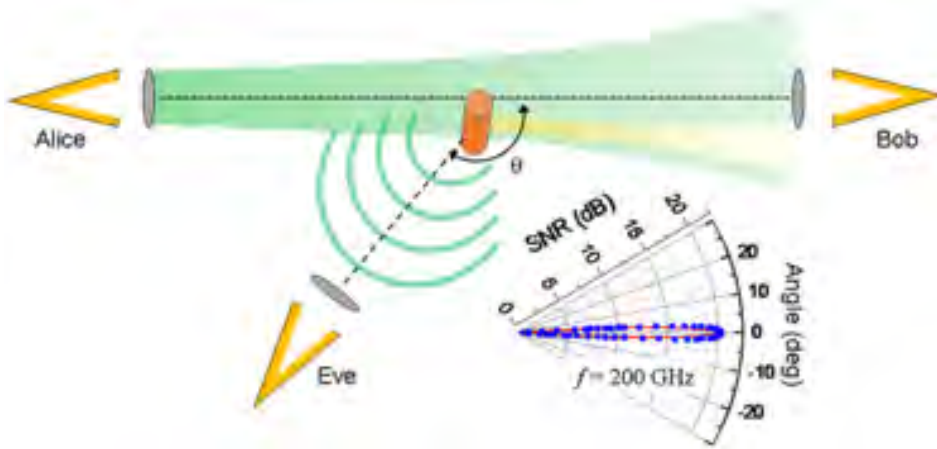


Figure 1. The schematic of the experiment shows a line-of-sight transmission channel between Alice (the transmitter) and Bob (the receiver). The inset shows the measured (blue) and computed (red) angular distribution of radiation emitted by the transmitter. The schematic also illustrates the eavesdropper's (Eve's) strategy: place a small (compared to the beam size) object (orange cylinder), which passively scatters radiation to a receiver located elsewhere, at an angle θ relative to the initial propagation axis of the beam.

Encouraged to pursue such a multi-disciplinary approach by Dr. Qiu, in 2018 ARO supported researcher Professor Daniel Mittleman of Brown University, together with colleagues from Rice University and the University at Buffalo, has experimentally demonstrated that THz data links aren't as immune to eavesdropping as many researchers have assumed. The research shows that it is possible for a clever eavesdropper to intercept a signal from a THz transmitter without the intrusion being detected at the receiver.

Result

Because of its higher frequency, THz radiation can carry up to 100 times more data than the microwaves used in wireless communications today, which makes THz an attractive option for use in future wireless networks. Along with enhanced bandwidth, it has also been generally assumed that the way in which high-frequency waves propagate would naturally enhance security. Unlike microwaves, which propagate in wide-angle broadcasts, THz waves travel in narrow, very directional beams. THz data links are therefore inherently immune to eavesdropping. The conventional wisdom in the terahertz community has been that it is virtually impossible to spy on a terahertz data link without the attack being noticed. This ARO supported research showed, for the first time, that undetected eavesdropping in the terahertz realm is easier than what has been assumed, and security will be an important issue for THz communication networks and must be carefully considered in implementing network architectures.

In the experiment, a line-of-sight configuration connecting a single transmitter and a single receiver (standard for a highly directional millimeter-wave or terahertz wireless link through the air) was used. In the scale model data link, objects are placed at various locations in the beam between the transmitter and the receiver. The signal strength and bit error rate detected by an eavesdropper at various receiver locations are evaluated. The eavesdropper's goal is to choose a scattering object, and its location, in such a way that the signal measured by the receiver is not attenuated too much and the signal that the eavesdropper measures is large enough for her to intercept the communication. This corresponds to a successful eavesdropping configuration. The experimental results show that the eavesdropper can always find a successful configuration that it is undetected, in the absence of any counter-measures. The research team also demonstrates one counter-measure for this eavesdropping technique, which involves characterizing the backscatter of the channel. This counter-measure can be used to

RESULTS

- ▶ Published in the prestigious journal Nature.
- ▶ This research shows that undetected eavesdropping in the terahertz realm is easier than what has been assumed, and security will be an important issue for THz communication networks and must be carefully considered in implementing network architectures.
- ▶ This study highlights the importance of physical-layer security in THz wireless networks and the need for transceiver designs that incorporate new counter-measures.

detect some, although not all, eavesdroppers. This study highlights the importance of physical-layer security in THz wireless networks and the need for transceiver designs that incorporate new counter-measures.

Way Ahead

To help develop a roadmap for basic research strategy in THz wireless communications, Dr. Qiu together with Dr. Henry Everitt from CCDC AvMc and Professor Mittleman organized an international workshop on the topic of terahertz wireless communications at Brown University in October 2018. This event involved many of the world's leaders in this research field, including experts in sources, detectors, signal processing components, channel characteristics, and network architectures. The goal of the workshop was to identify the key research challenges, which would ultimately enable the realization of terahertz wireless systems. This research directly supports Army CFTs in Network Command, Control, Communication, and Intelligence, and Future Vertical Lift.

SOLID-STATE ELECTRONICS AND ELECTROMAGNETICS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Discover and create unique electromagnetic phenomena in solid-state materials and structures that require theoretical formulations beyond well-established Maxwell's equations.
- ▶ Create novel device concepts with new functionality and unprecedented performance based on emerging phenomena in heterostructures and interfaces of engineered quantum materials.
- ▶ Develop novel electromagnetic structures to enable strong coupling with terahertz radiation (0.1-1 THz) and to achieve efficient generation, manipulation, and detection of the aforementioned spectral range.

MATERIALS SCIENCE DIVISION: FY18 SUCCESS STORIES

SYNTHESIS AND PROCESSING OF MATERIALS PROGRAM



Dr. Michael Bakas

Program Manager, Synthesis and Processing of Materials
Materials Sciences Division
ARO Engineering Sciences Directorate

Dr. Michael Bakas obtained his PhD in 2006 in Ceramic & Materials Science Engineering from Rutgers University.

He came to ARO in 2015 as a SETA Contractor to support the Synthesis and Processing of Materials Program, and was hired as the Program Manager in 2017.



Dr. David Stepp

Program Manager, Mechanical Behavior of Materials
Director of Engineering Science
ARO Engineering Sciences Directorate

Dr. Stepp completed his undergraduate studies at Harvey Mudd College, receiving his B.S. in Engineering in 1993. He trained as a materials scientist at Duke University, receiving his Ph.D. in Mechanical Engineering and Materials Science in 1998.

He came to ARO in 1999 as the Program Manager for Mechanical Behavior of Materials and was promoted to the Chief, Materials Science Division, in 2004, and to the Director, Engineering Sciences, in 2016.

Ultrasonic Manipulation for the Creation of Arrayed Reinforcement in Polymer Composites

Challenge

Many types of composite reinforcement, such as short fibers or nanotubes, can be very challenging to uniformly disperse. Clumping or agglomeration can occur, especially if a significant amount of reinforcement is used. In addition, it is very difficult to align or create specific patterns or arrangements of short fibers and nanoscale particles in the composite material. Addressing these challenges would improve the performance of composites that utilize these types of reinforcement, and open up a completely new tool for composite design by enabling the creation of ordered reinforcement arrays or structures.

Action

In 2014, ARO Synthesis and Processing of Materials Acting Program Manager David Stepp learned of a proposed method for creating particle patterns from Professor Raeymaekers at the University of Utah. Professor Raeymaekers believed that nanoparticles could be controllably dispersed into specific arrangements by using ultrasonic transducers. This would be done by calculating “acoustic trap” positions, locations where the acoustic forces acting on a particle would be zero. Particles subject to ultrasonic stimulation would naturally gravitate to the location of the acoustic traps. If all the relevant interactions could be properly calculated, it should be

This success supports these ARL Core Technical Competencies

Materials and
Manufacturing Sciences



SUCCESS

An initial STIR grant into a high-risk concept has resulted in a mature new tool for the flexible processing of advanced composites.

RESULTS

- ▶ Proof-of-concept obtained in STIR with simplified system
- ▶ Mathematical challenges for describing three-dimensional acoustic fields overcome.
- ▶ Three-dimensional patterns created with spherical and anisotropic reinforcement
- ▶ Dynamic patterns with reinforcements that shift repeatedly in response to acoustic stimulation created.

possible to incorporate them into a computer model capable of predicting the patterns that would occur for specific ultrasonic conditions. Those conditions would then be created using ultrasonic transducers, and the desired reinforcement pattern would be produced. The proposed process was polymer neutral, meaning it could be potentially employed to create any polymer matrix composite. If successful, this process could be a highly flexible tool for the fabrication of advanced composites. While innovative, the proposal was extremely high risk, so Dr. Stepp awarded in August of 2014 a Short Term Innovative Research (STIR) grant to obtain proof of concept.

By 2016, the STIR project was complete and showing promising results. Dr. Stepp and Dr. Bakas then encouraged a full proposal to be submitted on the topic. Dr. Bakas continued to monitor the resulting grant, keeping current on the project's progress and performing a site visit to Professor Raeymaeker's laboratory in 2018.

Result

The STIR effort was able to establish proof of concept by simplifying the problem using square reservoirs and spherical particles. While the patterns were limited to two dimensions, and there was considerable error, the University of Utah was nonetheless able to demonstrate the ability to rearrange carbon nanoparticles into simple patterns using ultrasonic transducers (Figure 1). The focus of the 2016 grant was to refine the computer model and understand the complex interactions governing the process to create more advanced and complex three dimensional patterns.

From 2016 on, the project has made considerable progress. A key breakthrough came in 2017 when the researchers determined how to approximate a three-dimensional pattern using equations that describe the acoustic waves as a two-dimensional field. The new approach was tested by creating some simple three-dimensional patterns. Pattern error was reduced as the model was refined. In 2018, the understanding of the interactions was sufficiently advanced enough that complex three-dimensional patterns were being created in polymer fluid. An octagonal reservoir was designed to enable further experimentation, and the researchers started exploring the creation of patterns with non-spherical particles that have more complex interactions (Figure 2).

Another key breakthrough was reached when it was determined how to create dynamic patterns, in which the position of the particles would repeatedly shift in controllable motions. This capability was first demonstrated by the controlled manipulation polystyrene spheres in air, but has also been used to create more complex dynamic

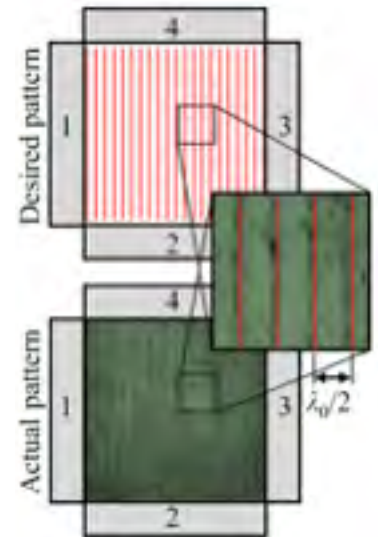


Figure 1. Nanoparticle pattern created during 2014 STIR project.

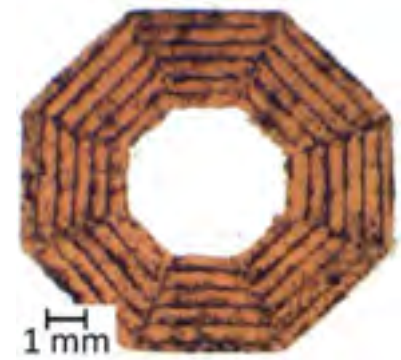


Figure 2. Carbon fibers dispersed into an octagonal pattern in 2018.

patterns in a fluid medium. As of 2019, the process has advanced from simple two-dimensional patterns of spherical particles to complex, three dimensional, dynamic patterns of fibers and other particles. The process is now sufficiently developed that Professor Raeymaekers is working to patent it and offer it as a processing platform to organizations in need of composite material development.

Way Ahead

With the model now established, and experimental results confirming that ultrasonic induced patterns are not only possible but repeatable and predictable, the next step is to attempt to employ the ultrasonic processing method to create practical composite materials. Dr. Bakas has communicated these results to researchers at ARL-WMRD and ARL-VTD who in advanced composite processing to explore opportunities to establish direct collaborations with Professor Raeymaekers developing these advanced composite materials.

Fifteen Years of Nanocrystalline Alloys Research Creates Mature and High Impact Field of Structural Materials Science

Challenge

The extremely small grain sizes inherent to a nanostructured material could theoretically lead to new alloys with unique properties for structural and protection applications. However, the strong thermodynamic driving force for grain growth makes these materials unstable under stresses and elevated temperatures, resulting in the loss of the nanostructure. In addition, the numerous grain boundaries inherent to nanostructured alloys can impair dislocation motion, causing brittleness. If nanostructured alloys are ever to be utilized in fielded equipment and infrastructure, knowledge of how to stabilize the structure and induce ductility is required.

Action

In 2003, ARO Mechanical Behavior of Materials program manager David Stepp supported a PECASE proposal submitted by Christopher Schuh of MIT to explore the mechanical differences between amorphous and nanocrystalline metals. Under this grant, Dr. Schuh discovered it was possible to create stable nanocrystalline materials by alloying with elements prone to segregation at the grain boundaries. This alloy segregation creates a thermodynamic driving force to retain nanocrystalline sized grains, as numerous grain boundaries are needed to accommodate the segregating element. Both Dr. Stepp, Dr. Schuh, and the ARO Synthesis and Processing of Materials program manager Suveen Mathaudhu recognized the potential of this discovery. While the original Ni-W alloy was created by electrodeposition, only suitable for films and coatings, if alternative processing methods could be developed, bulk nanostructured alloys could become possible.

Dr. Mathaudhu encouraged the submission of a new grant from Christopher Schuh to the Synthesis and Processing of Materials program, funding in 2009 an effort focused on identifying new binary alloy systems that exhibit the desired segregation and methods for creating powders of these alloys. This effort led to others, and over the period of 2009-2019 the Synthesis and Processing of Materials program; first under Dr. Mathaudhu, and later under Dr. Bakas; supported top extramural researchers to address both the challenges in fabricating these alloys and mitigating their brittle behavior.

Among the researchers supported was Professor Schuh's former student, Timothy Rupert, who began his own independent research career at University of California, Irvine. The Synthesis and Processing of Materials program supported a proposal in

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Materials and Manufacturing Sciences



SUCCESS

ARO PMs, through a decade of highly targeted investments, were able to establish the methods and methodologies for the fabrication of advanced nanostructured alloys, enabling ARL-WMRD researchers to demonstrate the creation of creep-resistant and high performance alloys.

2012 from Professor Rupert that focused on studying the role of the grain boundary phases, or "complexions" in determining brittle failure. In 2013, the program supported a grant with Professor Thompson at the University of Alabama to study the inherent stress states created by different alloying elements that occur in these alloys. In 2014, the Synthesis and Processing of Materials program supported a new effort from Professor Schuh to map all potential binary nanostructured alloys, with the intention of identifying systems that both exhibit the necessary alloy segregation and do not rely on inherently embrittling segregating elements.

In 2016, Dr. Rupert received a new grant from ARO to develop processing approaches to produce larger nanocrystalline alloy bodies. Professor Thompson reached out to Colorado School of Mines to submit a joint proposal with Professor Garritt Tucker in 2016. Thompson and Tucker proposed to perform a joint computational/experimental study to understand the influence of mechanical stress on the stability of these alloys. Professor Thompson would create and test nanostructured alloys under different stresses and at different temperatures, while Professor Tucker would explore the underlying mechanisms using Monte Carlo and Molecular Dynamic calculations. Dr. Bakas funded this joint effort in 2017 with Congressional funds provided to support new and innovative research directions.

RESULTS

- ▶ Binary alloy systems mapped, identifying all possible nanostructured alloy candidates.
- ▶ Ductility enhanced by controlling grain boundary phases and selective alloying.
- ▶ Students of supported PIs hired by ARL to continue work. WMRD created highly creep resistant alloy.
- ▶ Potential processing approaches for nanostructured powders and bodies established.
- ▶ Kinetic factors identified as key stabilization influence, work ongoing to quantify and understand these influences.

Result

The 2009 grant with Dr. Schuh revealed new potential binary alloys that exhibited the desired segregation and lack of second phase precipitation. Eventually, the grant was able to create W-Ti powders using high energy ball milling. The grain boundaries were stable at elevated temperatures, confirming the alloy segregation did stabilize the nanostructure. This work established the baseline features for a binary nanostructured alloy, and established at least one method for creating powders for such alloys. The 2014 grant with Dr. Schuh was also extremely successful, mapping out all potential binary alloy systems and narrowing down all possible compositions that could have the desired features. At the conclusion of the grant, Professor Schuh published a map identifying all viable binary alloy combinations that could potentially exhibit the desired segregation while avoiding embrittlement (Figure 1). Experimental verification is still needed to confirm specific systems, but the potential number of candidates to explore was greatly reduced.

Professor Rupert's work discovered that the cooling rate of the alloys had a significant impact on the nature of the grain boundaries. Rapid cooling rates would produce amorphous grain boundaries that exhibited much more ductility. Instead of the dislocations being pinned, resulting in brittle failure, essentially they are annihilated at these amorphous phases. As of 2018, Rupert's efforts have yielded a modified Cu-Zr alloy with Hf additions. These additions increased the thickness of the grain boundary phases (Figure 2a), and samples were successfully hot pressed to acceptable densities while still retaining the nanostructure (Figure 2b). He also found it was possible to use lasers to create desired phases on the grain boundaries. Work is still ongoing to improve the consolidation process, but thus far Professor Rupert's work has established potential solutions for the brittle behavior and processing challenges.

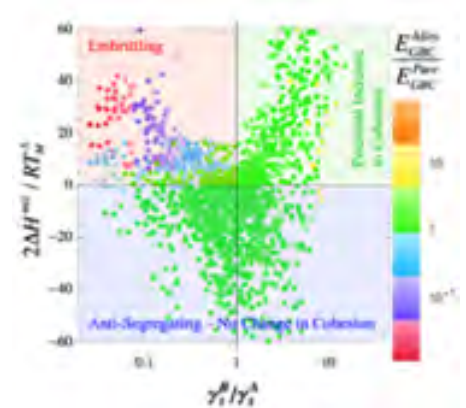


Figure 1. Map produced by Professor Schuh of MIT identifying potential nanostructured alloy compositions for binary alloys.

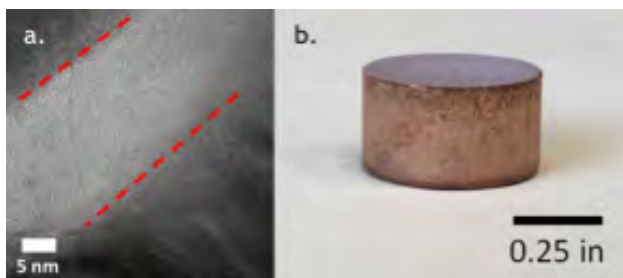


Figure 2. (a) Image of amorphous boundary phase in Cu-Zr-Hf alloy. (b) Sintered nanocrystalline alloy sample.

Professor Thompson demonstrated that certain alloying combinations, such as Fe-Cr, Cu-Ni and Al-Ag, could create tensile or compressive stresses in thin films of the alloys that would influence their mechanical properties. In 2018, by combining the experimental and modeling directly in a single effort, Professors Tucker and Thompson were actually able to quantifiably measure a real thermodynamic contribution to the stabilization of nanostructures in the Ni-P system. They have also defined the grain sizes in nanocrystalline materials in which the material would switch from Hall-Petch behavior to grain boundary governed deformation. While it was intuitively understood that there would be shifts in mechanical behavior at different grain sizes, this combined effort is actually quantifying these regimes and verifying the results experimentally.

Scientists ARL's Weapons and Materials Research Directorate (WMRD) have also made key contributions to this field. Former students from Professor Schuh's groups (Dr. Heather Murdoch), and Professor Thompson's group (Dr. Chad Hornbuckle) were hired and have continued to perform exceptional work in this area. In 2016, Dr. Kris Darling published in *Nature* results demonstrating extreme creep resistance in a Cu-Ta alloy. This work by Dr. Darling and other WMRD researchers provides a concrete example of the type of unique properties a nanostructured material can achieve. Dr. Darling has continued to make advances in this area, working closely with ARO supported researchers like Dr. Thompson and George Mason University's Professor Yuri Mishin. Professor Mishin's calculations, which were later experimentally confirmed, indicated that despite the emphasis on thermodynamics in stabilizing these alloys, Cu-Ta is stabilized by Ta clusters, more of a kinetic mechanism.

Way Ahead

In 2018, a group of researchers met at UC Irvine at a workshop supported by the Synthesis and Processing of Materials program, to discuss outstanding issues in this field. During the workshop, it emerged during discussion that other researchers had seen a strong kinetic influence on the stabilization of the alloys. This led to the conclusion that while the thermodynamic explanation for the stability of these alloys is an elegant one, it may not be the complete picture. Future grants in this area will be to focus on quantifying the role of kinetics in the stabilization of nanostructured materials. A joint PI project by Professors Martin Harmer and Jeffrey Rickman at Lehigh University was initiated in 2019 to plot Time-Temperature Transformation diagrams for the grain boundary phases, and Professor Mishin at George Mason University began a new effort to computationally explore the stabilization mechanisms of two alloy systems, Cu-Ta which is primarily stabilized primarily by kinetic pinning, and Cu-Bi which is stabilized primarily by thermodynamic mechanisms in theory. These efforts, along with other efforts occurring at WMRD, should help define the role of kinetics, and enable future bulk synthesis of these promising alloys. In addition, processing methods for the creation of the nanostructured alloys need to be further refined and advanced. The final direction to pursue is the exploration of stable nanostructures in ternary alloys, which offer a much greater range of potential compositions, but also much more complexity.

SYNTHESIS AND PROCESSING OF MATERIALS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Understand how processing methods and conditions influence the features and properties of structural materials, and how these influences can be leveraged for fabricating advanced structural materials. If successful, this will enable sophisticated synthesis of advanced structural materials that are stronger, lighter, and higher performance than the current state of the art.
- ▶ Develop new materials processing methods utilizing far-from-equilibrium and metastable conditions to create new phases and enable new synthesis strategies for creating advanced materials concepts. Successful development of advanced processing methods will make possible material concepts that are currently unrealizable, enabling synthesis of materials with unprecedented capabilities.
- ▶ Investigate the fundamental physical laws that occur during materials processing, with the goal of characterizing and defining previously ill-understood phenomena and behavior. Success in this area would mean more advanced and efficient materials fabrication processes as this knowledge is leveraged to create more sophisticated materials and eliminate undesirable influences that cause flawed or sub-standard materials.

MATERIALS DESIGN PROGRAM



Dr. John Prater (Retired)

Program Manager, Materials Design
Materials Science Division
ARO Engineering Sciences Directorate

Dr. Prater completed his undergraduate studies in Physics at Middlebury College in 1973. He trained as a materials scientist at The University of Pennsylvania receiving his Ph.D. in Metallurgy & Materials Science in 1978.

Dr. Prater joined the Materials Science Division at ARO in 1988.

Reconfigurable Materials

Challenge

The Army is increasingly interested in materials and systems that can directly respond or adapt to a diverse set of environments. These so-called reconfigurable or “smart” materials should be able to mimic the multifaceted behavior and complexity of living systems.

Considering that reconfigurable behavior in living systems has been honed over millions of years, longstanding engineering goal has been to design and fabricate reconfigurable materials with increasing complexity, adaptability, and (multi)functionality. Specific challenges include developing a fundamental understanding of microscopic forces governing self-assembly (e.g., entropy), fabricating complex hierarchical materials mimicking those found in biology (e.g., cell-fiber-muscle), and engineering robust pathways for reversible changes in material properties (e.g., structural changes for tunable optical properties). The Army Research Office began to confront these challenges in 2011.

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Materials and Manufacturing Sciences



Protection Sciences

Action

In 2011, ARO Materials Design Program Manager John Prater launched the new reconfigurable materials program. The program's goal was to develop reconfigurable materials capable of hosting the high levels of molecular recognition and self-organization that are employed by nature to construct systems with extraordinary levels of adaptability and complexity. In launching this new program, Dr. Prater used his extensive knowledge crossing many related fields to promote the program objectives and assembled a group of world-renowned experts together under the auspices of a Special Topics Workshop on Self Assembly (September 2011), organized through the Materials Research Society. The workshop established a new "bottom-up" paradigm for nanoscale synthesis of materials and clearly defined a path forward for the subfield. Years later, Dr. Prater co-organized the 2016 ARL Army Science Planning and Strategy Workshop on Microscale Adaptability, which surveyed emerging opportunities in the area of reconfigurable metamaterials and began to promote the concept of self-organizing materials at the Army Research Laboratory. These forward-looking activities by Dr. Prater have broadly positioned the Army's basic research program at the cutting edge of science.

Result

Professor Leila Deravi of Northeastern University was recently supported by ARO to investigate the molecular contribution to skin patterning and coloration in cephalopods (e.g., squid, octopus, and cuttlefish) and apply this knowledge to the design of synthetic materials capable of enhancing or otherwise manipulating the absorption and scattering of light. This work is important for closing the knowledge loop on how cephalopods undergo adaptive coloration in their natural habitats, as it is aimed at identifying the basic materials and fundamental material properties that modulate color. Professor Deravi, in collaboration with researchers at the University of New Hampshire and CCDC SC, hypothesized that dermal chromatophore organs in cephalopods are essential in regulating the optical feedback mechanism of the animals. Specifically, these researchers are seeking to demonstrate that nanostructured granules present within the organs are precisely engineered and arranged to participate in an ordered, cascading signal. This line of thinking is unique to the field; others have regarded the chromatophore as a simple color filter and a passive element of coloration.

In pursuing this goal, Professor Deravi has demonstrated a new method to extract, purify, and

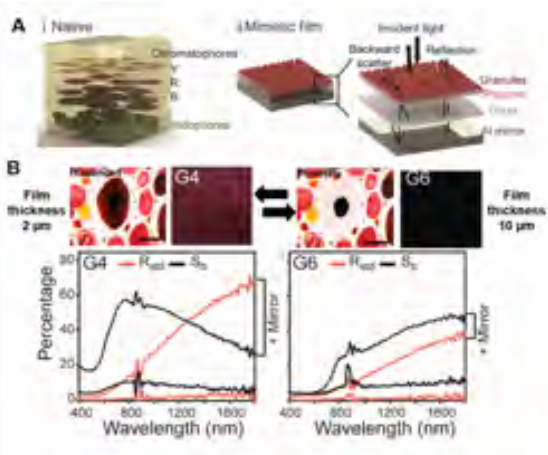


Figure 1. Effects of back-reflectors on color.

(A) Illustration of the bio-inspired design of experiments. (i) Squid dermal tissue with chromatophores (yellow, red, and brown) layered above the iridophore organs. (ii) An illustration of the film designed to mimic the squid dermal tissue with the granule material layered on top of the back-reflector (Al mirror). The exploded view represents how reflected and backward scattered light can potentially be amplified in the presence of the back-reflector.

(B) Forward scatter enhances visible color reflected from pigment granules in a multi-layer film, G4 and a saturated film, G6 measured with an Al- back-reflector. Here, the dashed lines represent the data with the Al-mirror (Labeled as + Mirror).

SUCCESS

Eight years of strategic investment in developing the scientific foundations required for designing self-assembling, reconfigurable materials with increasing complexity and (multi) functionality has led to new understanding of reconfigurable materials in nature, new methods for achieving positioning and short-range assembly, and strong Army-academic collaborations.

RESULTS

- ▶ Three MURI programs established in areas of reconfigurable colloids, DNA-organized matter, and hierarchical self-assembly
- ▶ New and sustained CCDC SC collaborations with Northeastern University, U. Penn.
- ▶ New fundamental knowledge generated about natural camouflage processes in squid.

identify the pigments confined within the chromatophore. Specifically, she isolated the phenoxazone-based pigments from the chromatophore and experimentally determined their complex refractive index. This refractive index is a powerful tool for predicting optical behavior: her team was able to calculate that the pigments assembled as discrete nanoparticles were more likely to scatter attenuated light than absorb it. Subsequently, they measured diffuse and specular scattering in films made from squid-extracted pigment granules and showed, for the first time, that films with as few as 2 granule layers (~1 μm thick) scatter over 20% of visible, near-, and short-wave infrared light. Finally, the intensity of scattered light across this broad spectrum increased when films containing the granule films were placed above a back-reflecting material, suggesting that tunable optical features can be controlled under different conditions (Figure 1). The major findings of this effort were published in four peer-reviewed publications.

Way Ahead

The team has nurtured a strong collaboration with scientists at CCDC SC. Together, they will continue to study cephalopod coloration mechanisms with ARO support. Their next efforts will focus on developing new, comprehensive understanding of how hierarchical assemblies of pigment granules (as opposed to individual granules) extract, dissipate, or otherwise manipulate light in cephalopod dermal tissue. To accomplish this, the PI's team, including CCDC SC scientists, will develop and synthesize artificial materials designed to mimic the optical behavior of chromatophore organs. Success here will enable a deep understanding of the mechanisms responsible for light sensing and manipulation in chromatophore organs, shedding light on the natural active camouflage processes of cephalopods. In turn, success in this research will facilitate the design of artificial reconfigurable optical materials, contributing to a long-range goal of developing synthetic pigment alternatives that can address future Army and DoD needs for environmentally benign coatings, conformable displays, and adaptive appliques for large-area Army textiles.

Magnetic Resonance Force Microscopy

Challenge

Nanoscale magnetic resonance imaging (nano-MRI) is a rapidly developing field with the potential to impact many areas of science and technology, including quantum information sciences and nanoscale imaging and characterization of novel materials and biological systems with unprecedented resolution. Magnetic Resonance Force Microscopy (MRFM), first proposed by J.A. Sidles in 1991, has more recently emerged as a leading nano-MRI technique. MRFM combines the nanoscale imaging capabilities of atomic force microscopy (AFM) with MRI to enable 3D, chemically selective, non-destructive imaging of electron and nuclear spins.

Despite the promise of this technique, however, it remains quite challenging to achieve the nm-scale resolutions required for MRFM to compete with other established imaging techniques like electron microscopy. This is because a large confluence of factors influence resolution, leading to multiple interdisciplinary challenges, including tip and cantilever design, tip-sample spacing limits, mechanical and electronic noise, radio frequency interference and signal processing, image reconstruction and signal processing algorithms, etc. For the past few decades, the ARO Materials Science Division has spearheaded the development of MRFM, with the goal of achieving single electron and single nuclear spin detection imaging. Success here would enable the development of single-spin MRI capability, which would permit revolutionary

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Materials and
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advances in materials and molecular characterization, including imaging subsurface defects in semiconductors or high-resolution imaging of the 3D structure and composition of single molecules and biological samples. 3D imaging of molecules with sub-nm spatial resolution will advance our understanding of biological processes leading to new intervention methods for injuries/disease and adaptation to man-made materials.

Action

Dr. Prater has supported MRFM research as an ARO PM for nearly 25 years. ARO support has included single investigator grants, Multidisciplinary University Research Initiatives, Small Business contracts, in addition to collaborative efforts with DARPA. Over this timeline, with a proactive and persistent focus on the long-term opportunities that could be enabled, Dr. Prater's ARO support produced a number of key advances in cantilever design. Furthermore, fabrication of nanoscale field gradient sources have led to more than a factor of 108 increase in detection sensitivity over conventional MRI, culminating in the detection of single electron spins in 2004 and the imaging of nuclear spins in single tobacco mosaic virus particles with sub-10-nm spatial resolution in 2009 by the Rugar group at IBM Almaden.

Result

Recently, Professor Raffi Budakian (Proposal: "Nanometer Scale Magnetic Resonance Imaging of Electron and Nuclear Spins"), supported by Dr. Prater's Materials Design program, has developed a new approach to MRFM that combines the high spin sensitivity of nanowire-based magnetic resonance detection with high-spectral-resolution nuclear magnetic resonance (NMR) spectroscopy. The most unique aspect of this approach is the ability to combine high-fidelity coherent spin control with ultra-sensitive MRFM detection. Using this method, his group demonstrated nuclear spin imaging in polystyrene with less than 2-nm resolution in one dimension. This is the highest resolution nuclear spin imaging demonstrated to date. Importantly, the 2-nm resolution is equal to the diameter of a DNA molecule (Figure 4), and marks an important time in MRFM development, when it is possible to image biologically-relevant molecular complexes.

Way Ahead

Future efforts will focus on further enhancing MRFM capabilities, with the goal of achieving atomic-level resolution and sensitivity, with the goal of being able to map the location, electromagnetic structure, and chemistry of every atom in biological, molecular,

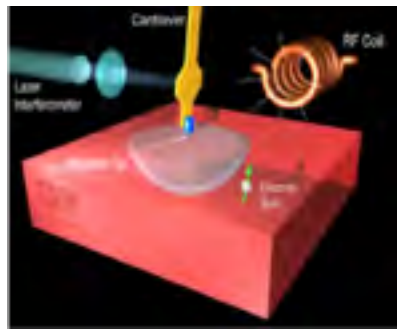


Figure 1. Detection of single electron spins using MRFM. Reference: D. Rugar, R. Budakian, H.J. Mamin and B.W. Chui, Single spin detection by magnetic resonance force microscopy, *Nature* 430, 329 (2004).

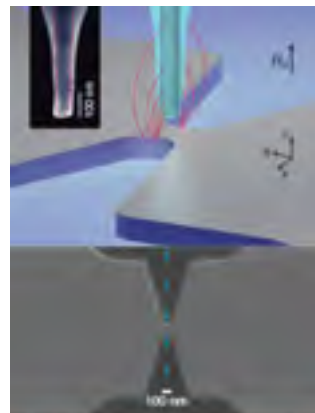


Figure 2. Top: schematic rendering of Prof. Budakian's nano-MRI experimental apparatus, incorporating a polystyrene-coated nanowire (blue) and a current-focusing field gradient source (CFFGS, shown in gray), which generates magnetic field lines (shown in red). Bottom: electron micrograph of the CFFGS. Reference: W. Rose, H. Haas, A. Q. Chen, N. Jeon, L. J. Lauhon, D. G. Cory and R. Budakian, *Phys. Rev. X*, 8, 011030 (2018).

SUCCESS

25 years of dedicated investment in nanoscale magnetic resonance imaging has resulted in 100 million-fold increase in detection sensitivity and resolution over conventional MRI, opening the door to directly probe and understand material defects and/or biological structures and processes at the nanometer scale, which will lead to new Army capabilities for treating injuries and creating smart materials.

RESULTS

- ▶ Detection of single electron spins ("Top Physics News Story" for 2004, AIP) and imaging of nuclear spins
- ▶ Nano-MRI imaging with 2 nm resolution (100 million times better than conventional MRI)
- ▶ Transition of hardware and techniques from ARO-funded MURI and SBIR programs to ARL-SEDD researchers

and electronic materials, assemblies, and devices. Additionally, efforts to directly apply MRFM to probing biological systems will be emphasized. Success here will result in better understanding of self-assembly processes and mechanisms employed by nature, resulting in new strategies for creating bio-mimetic reconfigurable or “smart” materials, with the ability to respond in real-time to internal or external stimuli. Enhanced MRFM capabilities and applications may also enable Army-relevant smart drug design and chemical/biological defense capabilities.

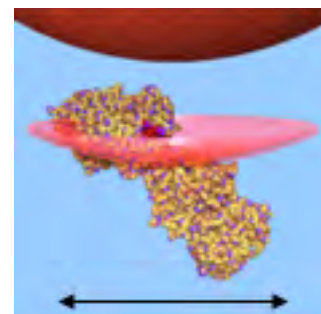


Figure 3. Schematic depiction of MRFM imaging of biological molecules (e.g., DNA) with 2-nm imaging resolution. Scale bar: 100 nm.

MATERIALS DESIGN PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Establish the scientific foundations needed to realize a new paradigm in materials synthesis: the ability to design and build materials from the bottom-up.
- ▶ Characterize, understand, and control local chemistry, physical interactions, structure, and ordering at hierarchical length scales.
- ▶ Engineer increasing complexity, functionality, adaptability, and reconfigurability into future materials systems to provide the Army with performance capabilities (e.g., adaptive camouflage) that go well beyond those achieved with conventional materials science and engineering.

MECHANICAL BEHAVIOR OF MATERIALS PROGRAM



Dr. David Stepp

Program Manager, Mechanical Behavior of Materials
 Director of Engineering Sciences
 ARO Engineering Sciences Directorate

Dr. Stepp completed his undergraduate studies at Harvey Mudd College, receiving his B.S. in Engineering in 1993. He trained as a materials scientist at Duke University, receiving his Ph.D. in Mechanical Engineering and Materials Science in 1998.

He came to ARO in 1999 as the Program Manager for Mechanical Behavior of Materials and was promoted to the Chief, Materials Science Division, in 2004 and to the Director, Engineering Sciences, in 2016.



Dr. Dawanne Poree

Program Manager, Polymer Chemistry
 Program Manager (Acting), Reactive Chemical Systems
 Chemical Sciences Division
 ARO Physical Sciences Directorate

Dr. Poree completed her undergraduate studies at Nicholls State University, receiving her B.S. in Chemistry in 2004. She trained as a polymer chemist at Tulane University, receiving her Ph.D. in Chemistry in 2010.

She came to ARO in 2011 as a SETA Contractor to support the Polymer Chemistry Program and was hired as the Program Manager in 2014. In addition, Dr. Poree has

served as the Program Manager (A) for Reactive Chemical Systems since 2014.

Mechanochemistry in Materials

Challenge

Structural materials are inherently susceptible to damage, and this damage is usually in the form of cracks that can occur deep within the structure where detection is difficult and repair is almost impossible.

The concept of a material that could repair or heal itself when subjected to force or damage has long captivated the chemistry and materials science research communities. Self-healing materials research blossomed under the National Nanotechnology Initiative and into the early 2000's. However, this work was based on classical composite designs and traditional manufacturing strategies, and was therefore limited to additive approaches that required a "payload" to drive self-healing. What disruptive opportunities might the frontiers of materials science or chemistry provide? Could a molecular-scale mechanism be discovered?

The Army Research Office began an initiative in 2006 that strategically pursued answers to these questions.

Action

Sensing an opportunity for a disruptive breakthrough, ARO Mechanical Behavior of Materials program manager David Stepp and Polymer Chemistry program manager Doug Kiserow organized a unique workshop in January 2006 to bring internationally renowned researchers in the areas of self-healing and self-repairing polymers and materials together with DoD scientists and engineers to establish emerging research opportunities. The workshop was organized for academic researchers to give tutorial presentations to highlight recent findings and approaches in their respective areas, Army and DoD attendees to describe potential applications in DoD for self-healing materials, and ARO program managers to actively moderate in-depth discussion by all attendees. This workshop identified a particular opportunity in the area of productive mechanochemistry where forces induced by mechanical stress could be harnessed and used to drive pre-defined, beneficial chemical reactions. More specifically, this opportunity was manifested in such research targets as: new compositions of matter; mechano-chemical transduction; molecular reconfiguration before failure; and advances in reversible chemistry.

Drs. Stepp and Kiserow devised the first ever multidisciplinary research opportunity at the forefront of materials and mechanochemistry, calling for "molecular dynamic and thermodynamic theory to be extended to describe mechanochemical transduction, to develop predictive computational methodologies, and to guide the rapid design and synthesis of novel mechanophores." This opportunity not only defines the etymology of "mechanophore" (a force-activated molecular unit), but captured the imagination

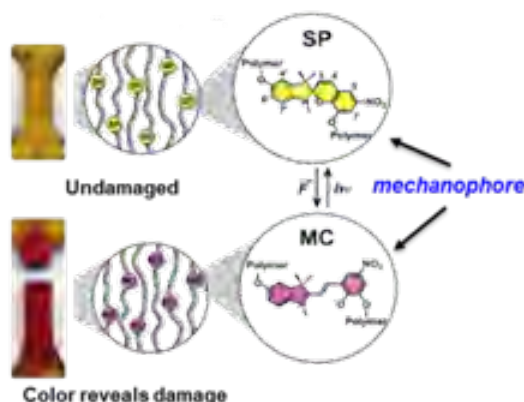


Figure 1. First demonstration of mechano-responsiveness in solid-state materials

This success supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Protection Sciences



SUCCESS

Initiating the first ever research effort to exploit mechanochemistry in materials led to new polymers that self-report damage and can be transformed from insulating to conducting with the application of force and are expected to enable new classes responsive polymers for self-healing structural materials, adaptive fabrics, and self-repairing electronics.

and attention of researchers internationally who envisioned the ability to embed these force-activated molecules into polymeric materials to realize a range of new materials with Army-relevant functional capabilities such as early-warning indicators for failure and the ability to remodel and strengthen in response to mechanical stress. ARO funded research soon produced the first-ever demonstration of mechano-responsive behavior in a solid-state material, when the spiropyran mechanophore was demonstrated to undergo a stress-induced conversion to merocyanin, resulting in an inherent and reversible color change in the region of damage (Figure 1). In recognition of this breakthrough, ARL-ARO was invited to organize and chair a Mechanochemical Transduction Convergence Workshop. This workshop served as a model study for scientific research forecasting, building upon the concept of research convergences in the advancement of science, and was published by the Center for Technology and National Security Policy at National Defense University.

Continued Army leadership and investment in this field by ARO program managers Dawanne Poree and David Stepp, integrating Polymer Chemistry and Mechanical Behavior of Materials respectively, has positioned the Army at the forefront of this research community. Symposia at major professional societies have begun to emerge (including Mechanochemistry in Materials Science at the Materials Research Society in Fall 2009 and Fundamental Studies of Mechanochemical and Tribochemical Processes at Interfaces at the American Chemical Society National Meeting in 2017). Furthermore, mechanochemistry has emerged as a powerful methodology in the search for sustainable alternatives to conventional solvent-based synthetic routes that has received broad support from federal and international funding agencies.

RESULTS

- ▶ Defined the new term “mechanophore” (a force-activated molecular unit) that captured the imagination and attention of researchers internationally.
- ▶ First-ever demonstration of a stress-induced molecular conversion that resulted in an inherent and reversible color change in the region of damage.
- ▶ First-ever demonstration of transforming a polymer from insulating to conducting with the application of force.
- ▶ Positioned the Army at the forefront of this research community.

Result

More recently, ARO extramural research investments have led to the development of new mechanophores with novel functional outputs including the ability to undergo a complete change in material properties by incorporating multiple mechanophore units in a single polymer chain. In particular, researchers at Stanford University have developed a unique polymechanophore system, termed polyadderane, which undergoes a force-induced rearrangement to polyacetylene. This effort received extraordinary acclaim when it successfully demonstrated transforming a polymer from insulating to conducting with the application of force. In 2018, this research team further showed that these responsive polyadderanes could be copolymerized with other commodity polymers which would impart stress-responsive capabilities to a diversity of materials that are not mechano-responsive on their own (Figure 2). The ability to extend this unique mechano-responsive behavior to more practically used polymers now enables new classes responsive polymers for use in a wide-range of applications, such as self-healing structural materials for Army vehicles or aircraft, breathable fabrics for uniforms that detect chemical agents and automatically close pores to protect the Soldier, and

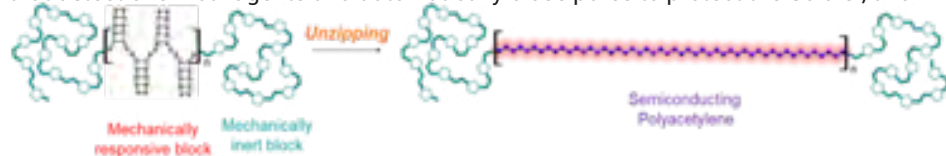


Figure 2. Mechanoactivation of polyadderane-containing copolymer

electronic components that self-repair or are programmed to deactivate if captured.

Way Ahead

The next objective in this effort is to target scale-up and integration of mechanochemistry into bulk materials more broadly. Collaborations with ARL-WMRD, CCDC Soldier Center, and DARPA are exploring new paradigms for detecting damage in composite structures and to revolutionize additive manufacturing and 3D printing with mechanochemistry and mechanophores. Additional collaborations with ONR are exploring opportunities to amplify the effects and sensitivity of force activation in bulk

materials.

Tunable Shear Jamming at the Forefront

Challenge

Dense suspensions of solid particles in liquid can display unusual mechanical behavior when subjected to shear stress; the viscosity of the suspension can rise dramatically when a certain shear rate threshold has been reached. Shear jamming (SJ) is the extreme case that occurs when the flow is completely arrested and the suspension becomes solid-like, which could provide a powerful tool for researchers to design materials with reversible fluid/solid behavior.

While shear jamming had long posed a considerable challenge for industrial processes, especially for slurries and suspension-based processes, the vast majority of previous research about the phenomena had been focused on how to prevent its manifestation. What if shear jamming could be exploited? Could it be controlled, engineered, or even used to provide unprecedented materials that could transform between fluid and solid states? The Army Research Office and the Weapons and Materials Research Directorate, cooperating as part of the Army Research Laboratory, launched a unique initiative in 2004 that strategically pursued answers to these questions.

Action

In 2004, ARO Mechanical Behavior of Materials Program Manager David Stepp, in coordination with ARL-WMRD scientist Dr. Eric Wetzel identified a new opportunity to incorporate SJ phenomena into composite materials for a novel form of extremity protection. Based on the scientific advances made under the resulting ARL-ARO funded effort, Dr. Stepp was invited in 2007 to serve as a technical advisor to the contracting officer's representative on the DARPA Chemical Robots Program, which sought to develop a robotic system that could be structurally rigid but, on command, "dissolve" into a state that is highly malleable or flows like a slurry. This collaboration between DARPA and ARL-ARO developed the first universal robotic gripper based on jamming. These efforts also spurred conversations between Dr Stepp and researchers funded under the DARPA program about emerging scientific opportunities of a much more fundamental nature.

By 2011, significant interest in shear jamming was being exhibited by the soft condensed matter community. The Soft Condensed Matter Gordon Research Conference focused on the topic of soft matter far from equilibrium and was specifically interested in the SJ phenomenon. Concurrently, Dr. Stepp and ARO Complex Dynamics and Systems program manager Sam Stanton worked with leading experts to establish a novel research effort exploring the jamming / unjamming dynamics in granular materials as a multidisciplinary effort between mechanical behavior of materials and

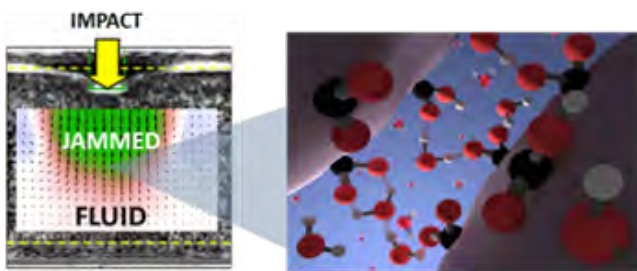


Figure 1. (Left) 3D ultrasound slice with overlaid particle image velocimetry that shows shear jamming in dense suspensions within an aqueous solvent. (Right) Jamming behavior in the suspension controlled through tunable frictional forces between particles.

This success supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Protection Sciences



SUCCESS

Over a decade of strategic investments and intentional discussions with international experts to elucidate the shear jamming phenomenon led to a robust and highly tunable system to characterize and engineer shear jamming in dense suspensions for stress-adaptive structures and impact-mitigating applications.

RESULTS

- ▶ In collaboration with DARPA, demonstrated first universal robotic gripper based on shear jamming.
- ▶ Initiated, supported, and hosted unique workshops to bring together international experts across multiple disciplines and drive research to extend the state-of-the-art in shear jamming.
- ▶ First-ever demonstration of the link between nanoscale particle surface chemistry and bulk rheological shear jamming.
- ▶ New ARL-Central collaboration initiated with U. Chicago.

structural dynamics. This research effort dramatically advanced the understanding of the SJ phenomenon by demonstrating robust control of the jamming / unjamming transition in particle-based systems under stress loading, in addition to the governing nonlinear dynamic system responses for these systems. However, little was known about the particle characteristics or dynamic driving conditions that could be used to exploit SJ. Dr. Stepp leveraged this opportunity to co-host a workshop with AFOSR in 2015, and brought together a small group of renowned international experts to discuss the dynamics of heterogeneous materials and how these might be engineered and exploited to manifest desired bulk responses.

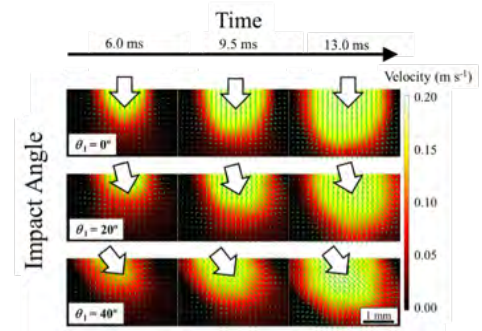


Figure 2. Shear jamming front evolution as a function of impact angle and time.

Result

In 2018, ARO funded researchers at the University of Chicago, working under the direction of Professor Heinrich Jaeger, discovered that SJ in dense suspensions within aqueous solvents may be controlled through tuning hydrogen bonding between the particles (see Figure 1). Particle surfaces were functionalized with hydroxyl end groups to enable hydrogen bond bridging and to provide exquisite control over the frictional forces within the suspension. The group also introduced an ultrasound technique to obtain high speed imaging of the three-dimensional flow fields and to quantify the porosity and compressibility of the particles in the dense suspensions (see Figure 2). In response to Dr. Stepp's persistent interest in determining maximal responses and properties, and to exploit recent breakthroughs in the theory and simulation of complex particles, the researchers also developed a model that relates the SJ front speed and the packing fraction of the jammed particles. These results are the first demonstration of a link between particle surface chemistry, which operates at the nanoscale, and SJ, which is a macroscale rheological phenomenon.

Way Ahead

It is anticipated that this fundamental understanding of tunable SJ could enable materials for a variety of stress-adaptive and impact-mitigating applications. With the support of Dr. Dan Cole, an ARL-WMRD scientist working as an ARO Tech Advisor with Dr. Stepp, a new collaboration was initiated between the University of Chicago researchers and Army scientists at ARL-Central to exploit SJ and develop novel materials for low-velocity impact protection. It is expected that the engineering and design of tunable SJ could constitute the next paradigm for a wide range of protective

MECHANICAL BEHAVIOR OF MATERIALS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Create, design, and optimize a broad range of robust mechanochemically adaptive materials, based on exquisite control of force-activated molecules and force-activated reactions that if successful could lead to self-reporting structural components and adaptive symbiotic fabrics.
- ▶ Tailor the deformation and failure mechanisms in materials to mitigate the propagation of intense stress-waves and control energy dissipation that if successful may lead to blast reflecting materials and novel therapeutics for blast battlefield exposure.
- ▶ Establish and optimize new atomic-scale strengthening mechanisms governing bulk mechanical behavior that if successful is anticipated to lead to new lightweight protective fabrics and equipment.



PHYSICAL PROPERTIES OF MATERIALS PROGRAM

Dr. Chakrapani (Pani) Varanasi

Program Manager, Physical Properties of Materials

Division Chief, Materials Science

ARO Engineering Sciences Directorate

Dr. Varanasi completed his M.S. in Materials Science and Engineering at the Indian Institute of Technology, Kanpur, India in 1990. He trained as a Materials Scientist at the University of Notre Dame, IN, receiving his Ph.D. in Materials Science & Engineering in 1994.

He came to ARO in 2009 as the Manager for the Physical Properties of Program and was promoted to Chief, Materials Science Division in 2017.

Near-Field Transport of Energy Using Nanostructured Materials

Scientific Challenge

Although several decades old theoretical predictions on near-field radiative heat transfer dramatically exceeding the far field blackbody limit (by several orders of magnitude) between planar surfaces were available, robust experimental validation had not been achieved. Could recent developments in nanotechnology and thermal property characterization techniques, make such validation possible for the first time? Could near field radiative heat transfer be adequately explored and exploited for new Army capabilities? In 2012, the Army Research Office began a unique effort that strategically pursued answers to these questions.

Action

ARO Program Physical Properties of Materials program manager Pani Varanasi identified a new scientific opportunity to experimentally explore near-field radiative heat transfer between nanostructured materials in 2012. Supporting basic research in this area was identified to be critical because successful elucidation of near-field heat transfer phenomena could have a broad impact on developing various future Army relevant applications in thermal management, thermal to electrical energy conversion and solid-state refrigeration. For nearly six years Dr. Varanasi supported novel single investigator research proposals and instrumentation grants and collaborated with ARL-SEDD (Dr. Mike Waits) to made strategic investments to exploit this opportunity. Based on the success of these investments, and after realizing a major opportunity to tailor the spectral output with advanced materials, a 2019 MURI program is initiated in collaboration with ARO Condensed Matter Physics program manager Dr. Marc Ulrich and Dr. Mike Waits. This MURI is scheduled to start in FY19 to address some of these basic research issues. Dr. Varanasi also collaborated with ONR and AFOSR program managers to develop this program and to leverage investments/expertise.

Result

These efforts led to a number of significant results including the development of unique metrology tools and elucidating important new phenomena, namely: the first demonstration of heat transfer rates that exceed the blackbody limit by ~800 times; demonstration of a 100 fold enhancement in far-field heat transfer rates via nano-

This success supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Propulsion Sciences



SUCCESS

Strategic and bold investments in instrumentation development and experimentation has resulted in first ever experimental confirmation of decades old theories of near field radiative heat transfer and enabled other novel phenomena to be discovered that could impact future DoD capabilities in power and energy and electronics as these knowledge products could enable more efficient electric power generation from heat and thermal management of high power electronics

RESULTS

- ▶ A new MURI program was initiated in collaboration with ARL-SEDD in FY19 to explore the influence of material composition/ structures on near field radiative heat transfer and energy conversion.
- ▶ Heat transfer rates that exceed the blackbody limit by ~800 times
- ▶ 100 fold enhancement in far-field heat transfer rates via nano-structuring
- ▶ Forty-fold enhancement in power output near-field-based thermos-photovoltaic energy conversion compared to the far-field

structuring; and demonstration of near-field-based thermophotovoltaic energy conversion where a forty-fold enhancement in power output was achieved compared to the far-field.

Early ARO support to Professors Meyhofer and Reddy at the University of Michigan enabled development of a novel instrumentation platform that made possible for the first time direct studies of near-field radiative heat transfer between plane parallel surfaces. Using this platform this team demonstrated breakthrough results where they showed that when the gap size between planar surfaces is reduced to the nanoscale (~60 nm) it is possible to enhance radiative heat fluxes by a hundred fold compared to those predicted by the established Blackbody limit. Upon further improvement of their instrumentation, they were able to achieve even smaller gap sizes (approaching 25 nm) and showed an almost 800 fold enhancement compared to the blackbody limit. These studies provided first experimental evidence of the dramatic effects and enhancements that arise in near-field radiative heat transfer and energized the research community.

Professors Meyhofer and Reddy also explored a second challenging problem that is to experimentally address the question of whether the blackbody limit can be overcome by nano-structuring. By employing nanofabricated calorimeters they achieved detailed experimental evidence, which demonstrates that heat transfer rates between sub-wavelength structures can surpass the blackbody limit by 100 times. These results disproved longstanding dogma in thermal radiation and provided a new perspective on the impact of nano-structuring on radiative heat transfer.

One of the technological areas that near-field radiative heat transfer could have a strong impact on is thermophotovoltaics (TPV). Traditional photovoltaic cells use photons (light) from the sun, which are converted to electrical energy. In contrast, in a thermophotovoltaic device, light from a hot object heated by any source (e.g., industrial waste heat, burning a fuel, by concentrating solar energy onto the object etc.) can be converted into electricity directly. Unlike traditional photovoltaic technologies, thermophotovoltaic devices do not rely on sunlight for generating power. They can use any source of heat and thus can be especially useful to Soldiers in the field. Further, TPVs are particularly well-suited for generating power at night or indoors, and they can even be made portable for generation in remote locations. A recent breakthrough result demonstrated a 40-fold enhancement in the power output in comparison to a traditional TPV device by employing new physical phenomena such as photon tunneling that arise in the near-field. To elaborate, these enhancements occur because photons that usually cannot be transferred from the emitter to the receiver can now be readily transferred due to a process akin to tunneling that is observed in quantum mechanical devices (see Figure 1). Devices built using this approach can work far more effectively for remote power generation as well as in waste heat recovery.

Way Ahead

These recent advances in near-field heat transfer, bring us little closer to realizing novel TPV devices and near-field based solid-state refrigeration devices, which can offer

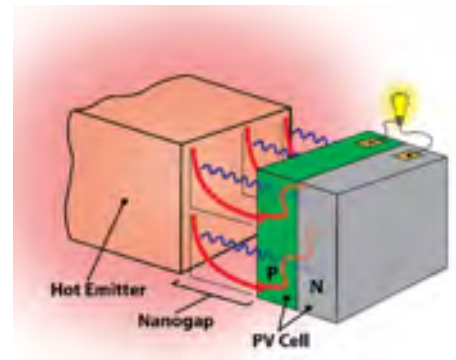


Figure 1. Thermal radiation from a hot emitter is directly converted to electricity in the PV cell. Experimental work from the UM team reveals that the power output is enhanced ~40-fold due to contributions by tunneling of photons (red) in nanoscale gaps (also called the near-field), in addition to the far-field propagating wave contribution (blue) from the emitter to the PV cell.

superior performance with higher efficiency than the current technologies. However, before such devices can be demonstrated, several other fundamental basic science questions need to be addressed such as understanding how the tunneling rates and processes can be controlled via suitable material composition/ structures. The new MURI team will be looking at these issues. In addition, this team will also be looking at other new phenomena such as extreme- near field radiative heat transfer etc. to shed light on new mechanisms of heat transfer in these conditions. The MURI team is planning to collaborate with ARL-SEDD team (POC: Dr. Mike Waits) to identify and enable possible tech-transfer opportunities as the program progresses.

Two Dimensional Materials Beyond Graphene

Challenge

Early research efforts in the functional nanomaterials research community were mainly focused in the area of graphene, a two dimensional (2D) single atomic thick carbon material that was discovered in 2004. Graphene has unique properties such as extraordinary mechanical strength, electron mobility, and very high thermal conductivity; however graphene doesn't have an essential semiconducting property (a bandgap). What if other two dimensional semiconducting materials could be discovered with bandgaps and unique complementary properties to transform Army relevant electronic applications? Could they be fabricated with scalable methods such as chemical vapor deposition and standard lithography techniques to enable robust device manufacturing? In 2010, the Army Research Office began a unique effort that strategically pursued answers to these questions.

Action

In 2010, ARO Program Physical Properties of Materials program manager Pani Varanasi initiated a new focus area titled, "2D materials beyond graphene" by encouraging academic researchers to propose high risk ideas to explore synthesis and characterization of other layered materials (oxides, nitrides, transition metal dichalcogenides like h-BN and MoS₂) to create 2D semiconducting materials. ARO is the first federal agency to take such a bold step towards exploring other 2D materials. Several single investigator grants were awarded to different researchers (including Professors Rod Ruoff, Deji Akinwande, Shriram Ramanathan, and Yong Zhang) to explore different 2D material systems. Based on the success of the initial results, a Multidisciplinary University Research Initiative (MURI) was proposed and funded in 2011 exploring atomic layers of nitrides, oxides, and sulfides under the leadership of Professor Pulickel Ajayan at Rice University. A first workshop in the area of 2D materials beyond graphene was supported by ARO and organized by Professor Josh Goldberger of OSU in 2012 to bring together researchers from academia and scientists from government agencies to discuss the opportunities and prioritize the research directions in this area. Several other similar workshops have been since periodically supported by ARO over the past several years to monitor and prioritize the research investments. A short summary of the effort titled "Beyond Graphene - Novel Nano-sheets of 2D Crystalline Materials with Revolutionary Properties" was written by Dr. Varanasi and appeared on the Materials Research Society website in 2011 highlighting the opportunities of 2D materials research. Based on the demonstrated success of these research efforts, other funding agencies followed suit and a large number of research programs on 2D materials were supported shortly thereafter.

Over the past several years, in addition to single investigator grants and MURIs, several other funding vehicles were strategically utilized by Dr. Varanasi to address several different aspects of synthesis, processing and characterization of these novel 2D

This success supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Computational Sciences



Network and Information Sciences



SUCCESS

ARO program manager's vision coupled with bold, strategic, timely, investments in two dimensional (2D) materials beyond graphene has resulted in the discovery of hundreds of novel 2D materials with extraordinary properties creating opportunities for DoD to positively impact future capabilities in electronics, photonics, energy storage, and quantum technologies.

functional materials. Initial investments in the 2D materials beyond graphene area has also created an opportunity over the several years since 2010 to launch several other new multidisciplinary efforts, including: multiscale modeling of 2D material hetero-structures with the ARO Computational Mathematics program manager Joe Myers; 2D organic polymers with ARO Polymer Chemistry program manager Dawanne Poree; and novel defect/host materials (platforms) based on 2D materials for quantum technologies with ARO Quantum Information Science program manager Sara Gamble. These new efforts are expected to have impact on several different future Army applications that were not initially envisioned when the first 2D materials beyond graphene program was started.

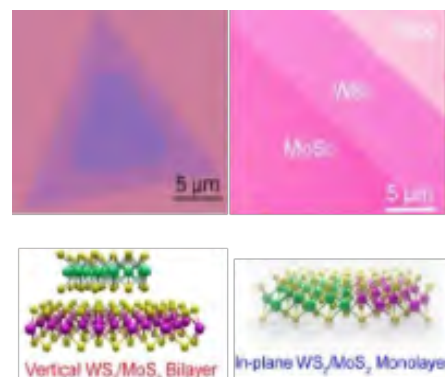


Figure 1. Large area novel two dimensional materials (WS₂, MoS₂) and their hetero-structures synthesized in a laboratory for the first time with ARO support

RESULTS

- ▶ Hundreds of peer-reviewed publications, dozens of patents, and follow-on funding from almost all federal funding agencies
- ▶ Initiated in-house research programs at ARL-SEDD, ARL-WMRD, and the CCDC Armaments Center due to interactions with ARO funded researchers.
- ▶ ARO-supported graduate student was hired at ARL-SEDD as a permanent employee
- ▶ Four new MURI programs have started based on two-dimensional materials
- ▶ ARO-supported research has led to a new start-up company to commercialize these novel two-dimensional materials

Result

The first ever MURI project on 2D materials beyond graphene supported by ARO focused on the development of 2D materials from oxides, sulfides and nitrides, expanding the envelope of possible compositions, electronic structure and bandgaps into a major field over the next several years. The MURI program made very important fundamental scientific contributions to the field of “2D Materials beyond graphene.” Some of the seminal contributions of this MURI program on 2D materials are: chemical vapor deposition synthesis of dichalcogenide lateral/vertical heterostructures; large scale synthesis of 2D B-C-N layers and their low dimensional structures such as CN quantum dots; theory driven development of descriptors for monolayer TMD catalysts and their

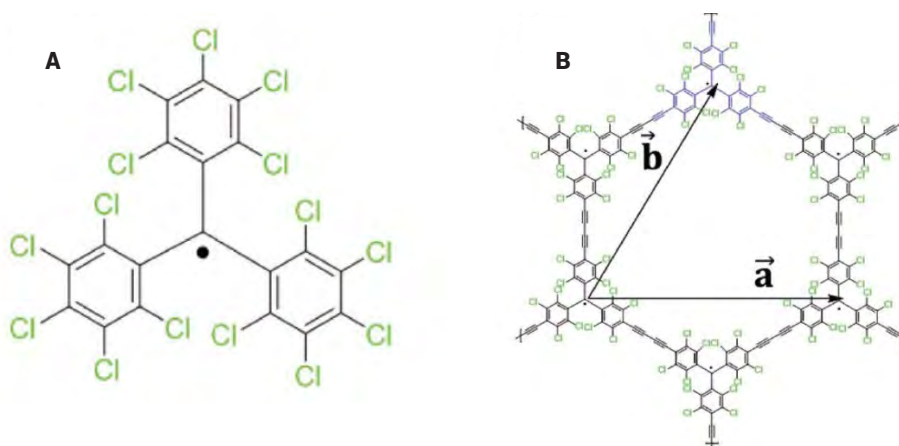


Figure 2. (A) Chemical structures of the perchlorotriphenylmethyl radical (PTM) (B) Illustration of the 2D radical-carrying COFs based on the PTM cores connected via diacetylenic linkers

experimental verification; and development of intercalation and exfoliation chemistry of layered materials to 2D nano-sheets.

ARO funded researchers from various grants collaborated with Army researchers that resulted in numerous in-house programs. These collaborations have resulted in several high impact journal papers from the Army labs, patents, student hires as permanent Army scientists, and technology transfers from academia to the labs. A new area of research “twistronics” has even emerged that has shown extraordinary properties such as

superconducting properties when the subsequent layers of 2D materials are positioned at a “magic” angle.

In addition to the initial target of discovering 2D materials for flexible electronics, the investments in 2D materials have resulted in the discovery of several hundreds of other new 2D materials that could also impact other areas such as photonics, spintronics, fundamental physics and quantum technologies and structural applications. New journals in 2D materials have started recently to document the results of increased research activity in the 2D materials research area. ARO funded research has even produced a start-up company to commercialize the newly discovered 2D semiconductor materials. ARO has played a significant role in creating all these new opportunities/developments.

In 2018, ARO funded researchers (Professors Will Dichtel at Northwestern University and Jean-Luc Bredas at Georgia Tech) showed the first theoretical evidence of the realization of an antiferromagnetic Mott insulating phase in 2D π -conjugated covalent organic frame works (COFs). This work paves the way to strategies to design π -conjugated 2D COFs that could span the electronic-structure phase diagram from antiferromagnet to spin liquid and to semimetal.

Way Ahead

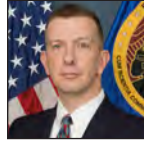
As new 2D materials with unique properties are continuously being discovered, the anticipated future applications based on these materials is expanding every day. ARO funded researchers continue to collaborate closely with S&Es at ARL- SEDD, ARL-WMRD, and Armaments Center to transfer technology in various areas such as in neuromorphic computing, ultra-low power flexible electronics, quantum technologies,

PHYSICAL PROPERTIES OF MATERIALS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Create materials of novel compositions and structures with unique physical properties through developing fundamental understanding of nucleation/growth mechanisms that if successful is anticipated to lead to low power electronics and unique sensors.
- ▶ Invent unique characterization techniques and discover novel functional properties (electronic, photonic, magnetic and thermal) of materials through establishing composition/structure- property correlations that could enable new paradigms for communication, sensing, and lightweight power.

MECHANICAL SCIENCES DIVISION: FY18 SUCCESS STORIES

PROPULSION AND ENERGETICS PROGRAM



Dr. Ralph Anthenien

Program Manager, Propulsion and Energetics
Division Chief, Mechanical Sciences
ARO Engineering Sciences Directorate

Dr. Anthenien completed his undergraduate studies at the University of California, Berkeley, receiving his B.S. in Mechanical Engineering in 1993. He received his Ph.D in 1998 in Mechanical Engineering from the University of California, Berkeley.

He came to ARO in 2006 as the Manager for the Propulsion and Energetics Program and was promoted to Chief, Mechanical Sciences Division, in 2013.

Fundamental Mechanisms of Impact Initiation of Reactive Materials

Scientific Challenge

Understanding detonation phenomena in reactive and energetic materials is key to the development of future Army and DoD systems involving munitions, explosives, and propellants. Experimental work to investigate detonation typically requires large quantities of material to characterize the transition from a sub-detonative reaction to a full detonation. The ability to investigate detonative behavior and the associated chemistry with small or minute quantities of materials will open the door to rapid evaluation of novel materials and the development of more predictive models from the increased understanding afforded from additional data across a wider range of materials.

Action

ARO Propulsion and Energetics Program Manager Ralph Anthenien developed a strategic focus in 2006 to support experimental methods to enable the investigation of reactions in energetic materials under extreme conditions using only minute quantities of material (i.e., milligrams). This represents a multiple order of magnitude decrease in material required for typical characterization tests. In 2009, Dr. Anthenien supported an add-on request from a multidisciplinary university research initiative focused on the investigation of the behavior of nano-engineered energetic materials. Part of this add-on was a novel approach to use laser-launched flyer plates to investigate impact initiation of materials. This technique was initially only able to achieve launch speeds up to ~5km/s, but Dr. Anthenien encouraged the Professor Dana Dlott of the University of Illinois at Urbana Champaign to continue the work. Since that time, ARO has supported the further development of this technique, resulting in a unique “detonation on a tabletop” facility that enables robust study of detonation propagation using only milligram samples of material.

This success supports these ARL Core Technical Competencies



Propulsion Sciences



Ballistics Sciences

SUCCESS

ARO drove development of experimental methodology to study detonations in energetic materials with minute (milligram) quantities.

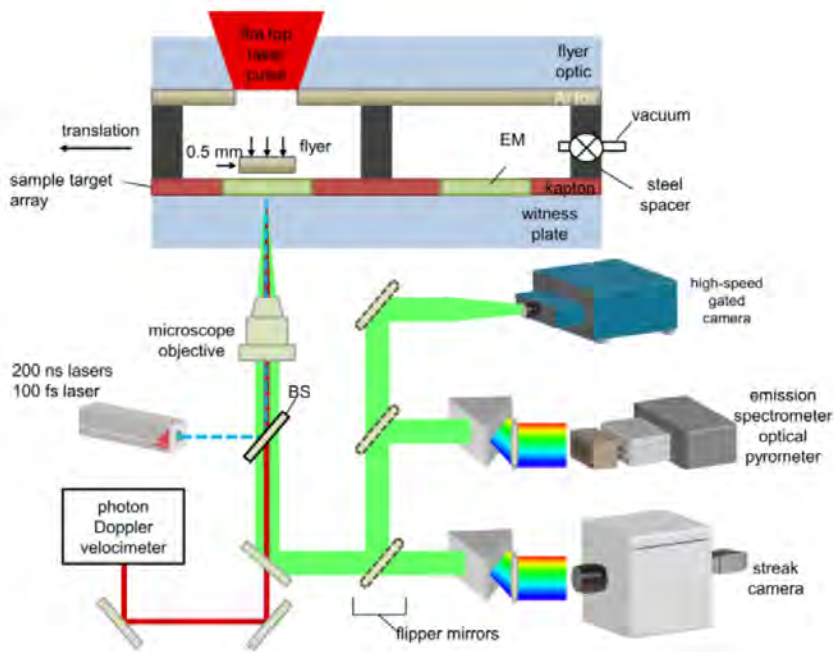


Figure 1. Schematic of the shock microscope and a multi-element shock target array. The instrument can measure the pressure, density, temperature, composition and microstructure of a shocked energetic material.

Result

Professor Dlott has developed diagnostic techniques that now enable novel energetic materials to be completed in a single day. This allows study of shock in a material with unprecedented detail and under a wide variety of conditions. Shocks can be generated in materials as small as 0.5mm in diameter, and lasting only 20us. Professor Dlott's group has developed what they call a "shock compression microscope," as shown in Figure 1. The facility can launch flyer plates at velocities up to 5 km/s and uses a photon Doppler velocimeter (PDV) to measure velocities. The system is also instrumented to measure pressure, density and an optical multi-channel pyrometer to measure temperature profiles. A high-speed camera is interfaced to the microscope to produce diffraction-limited nanosecond imaging of shocked microstructures. A separate mid-IR reflection-absorption microscope is also available to study molecular composition. The facility has the ability to test liquid as well as solid explosive materials.

Using the facility, the origin of hot spots in PBX was determined. This was accomplished with a "homemade" mix of 80% PETN and 20% PDMS binder made in two microstructural forms. The first is "as cast" which contains micropores; the second is pressed to homogenize the PBX resulting in a nanoporous composite. Both structures were subjected to shock initiation in the facility, also varying the gas composition in the pores. Results show that the high temperature hot spots are created by gas compression.

Way Ahead

The work has received the attention of CCDC Armaments Center because of the ability to rapidly and cheaply screen minute quantities of novel energetic materials. Further, it can generate statistical amounts of data compared to previous "one-shot" tests. Novel energetics can now be quickly tested significantly reducing risk of scale-up. ARO is coordinating with CCDC Armaments Center to transition the technology.

RESULTS

- ▶ Novel technique developed for studying detonation in energetic materials with only milligram quantities
- ▶ Laser flyer plate can impact at velocities up to 5 km/s
- ▶ Emission spectra obtained from each impact to determine probe temperature of sample
- ▶ Origin of hot spots determined for PBX. Thermites and reactive materials also studied

This success supports these ARL Core Technical Competencies



Propulsion Sciences

SUCCESS

ARO leadership and funding led to development of High-Pressure Experimental Combustion Facility to allow investigation of autoignition behavior of heavy hydrocarbon fuels at high pressure and low temperature.

RESULTS

- ▶ Unique high-pressure experimental combustion facility developed for studying auto-ignition and extinction of gaseous and heavy hydrocarbon fuels up to 60atm
- ▶ Determined current models did not correctly predict “flip” in relative extinction sensitivity of progressively heavier fuels at high pressures

High Pressure Auto-Ignition of Hydrocarbon Fuels

Scientific Challenge

Most Army ground propulsion systems operate on a diesel cycle which relies on consistent and predictable ignition of heavy hydrocarbon fuel at high pressure (over 60 atm) and relatively low temperatures (approximately 800K). While these engines were designed to run on diesel fuel, the DoD has mandated the use of aviation fuel as a single fuel for all land-based operations. While close in physical and thermodynamic properties, the chemical makeup of jet fuel is different from diesel and consequently has different ignition characteristics. Developing understanding of the ignition chemical kinetics and behavior of these heavy fuels is key to enabling predictive modeling capability to design future resilient and fuel flexible engines for the Army and DoD.

Action

ARO Propulsion and Energetics program manager Ralph Anthenien proactively encouraged the hydrocarbon combustion research community to probe reactions and flames at high pressures to address a significant lack of understanding of transport effects (both heat and mass). Historically, data beyond shock-tube “0-D flame” was at atmospheric pressures. In 2008, he convinced Professor Kal Seshadri at the University of California San Diego to attempt to install a flat flame burner (a “1-D” flame setup) into a high-pressure chamber. As this had not been attempted previously, a facility was designed for moderate pressures of up to 25atm, built with ARO support, and used for experiments on both gaseous and condensed fuels in an opposed flow flat flame beginning in 2010. The initial moderate pressure work was completed in 2015, and the experimental data revealed that there were kinetics and transport occurring at higher pressures that were not understood. Dr. Anthenien then encouraged Professor Seshadri to design and build a pressure chamber that could attain pressures of up to 60atm. The upgraded system was completed early in 2018 under ARO support, allows opposed flow flat flame experiments with preheated air, enables variation of oxygen concentration, and provides optical access for characterization of the flame and flow field.

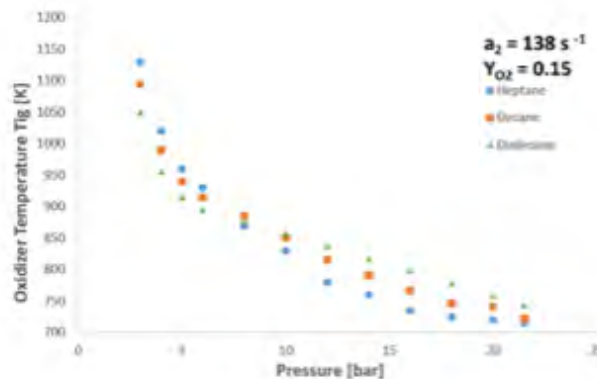


Figure 1. Autoignition temperature as a function of pressure for fixed strain rate and oxidizer concentration at increasing pressures. Notable: the lighter fuels ignite at lower temperature at high pressure whereas the heavier fuels ignite a lower temperature at lower pressure.

Result

The work in this unique high-pressure combustion experimental facility has only begun and has already allowed models to be refined to better predict behavior. Tests have been conducted on Jet-A, JP-8, and JP-5 as well as several surrogate fuels of each of these. Preliminary data shows that previous models did not accurately predict extinction behavior at high pressure. Experiments at pressures up to 22atm (approximately 22 bar) indicate a reversal of ease of ignition trend (see Figure 1). At low pressure, heavier

fuels were found to ignite a lower temperature than lighter fuels. This trend was shown to reverse at higher pressures. Current simulations with detailed chemistry have not predicted this trend. The data is also being used in support of the National Jet Fuel Combustion Program, an interagency effort (with FAA, DoD, and DoE), to develop predictive models for jet turbine combustor design.

Way Ahead

This is a work in progress with experiments continuing. The experimental data will continue to be used to improve chemical kinetic models and transport models. The experimental work will be taken up to 60 atm. This final push to Army relevant pressure was enabled by a recent ARO Research Instrumentation grant which upgraded the gas handling system allowing significantly higher rate of experimentation.

PROPULSION & ENERGETICS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Establish well-quantified mechanisms to predict ignition and initiation of energetic materials, especially undergoing thermal and physical insult.
- ▶ Establish and quantify the key rate controlling processes (e.g., oxygen diffusion) in energetic materials.
- ▶ Develop novel methodologies and approaches (beyond detailed chemical kinetics) to combustion modeling of heavy hydrocarbon fuels that will enable fully predictive large-scale modeling.
- ▶ Develop understanding of the reaction kinetics, chemistry and transport processes of combustion phenomena in heavy hydrocarbon fuels to enable predictive models at high pressures, especially for low-temperature ignition.

FLUID DYNAMICS PROGRAM



Dr. Matthew Munson

Program Manager, Fluid Dynamics
Mechanical Sciences Division
ARO Engineering Sciences Directorate

Dr. Munson completed his undergraduate studies at Illinois Institute of Technology, receiving his B.S. in Aerospace Engineering in 2002, as well as a M.S. in Mechanical and Aerospace Engineering in 2003. He received his Ph.D. in Aeronautics from the California Institute of Technology in 2012.

He came to ARL-VTD in 2012 as an Aerospace Engineer and then to ARO in 2014 as the Program Manager for Fluid Dynamics.

Building Extramural Research Partnerships to Advance Army Rotorcraft

Challenge

During years of operating in Iraq and Afghanistan, the U.S. Army experienced the challenge of operating rotorcraft in “high-hot” conditions. In conditions of elevated temperature and/or elevated altitude, the ambient density decreases to a point where engine performance and rotor performance are degraded. In order to expand the

This success supports these ARL Core Technical Competencies

Propulsion Sciences



operational envelope of U.S. Army rotorcraft, engine and rotor upgrade programs are underway. One such program is the Block II upgrade for the CH-47F "Chinook" heavy-lift helicopter, which aims to increase the hover payload performance at 4,000 feet and 95°F. One of the enabling technologies is the Advanced Chinook Rotor Blade (ACRB), which has achieved remarkable improvements in hover performance, but at high forward flight speeds the rotor exhibits a vibrational response that can lead to premature fatigue failure.

Engineers at the Aviation Development Directorate (ADD) of the Combat Capabilities Development Command-Aviation and Missile Center (CCDC-AVMC) realized that fundamental aerodynamic data was missing that could help them validate their numerical results and overcome this design limitation.

The design of the ACRB consists of a spanwise blending of the VR-7 and VR-12 airfoil sections, both commonly used shaped for rotorcraft blades. One of the potential root causes identified by the ADD team was that the VR-12 airfoil was experiencing an aerodynamic regime much slower than the conditions it had originally been designed for. As the ADD engineers attempted to gain confidence in the results of their computations, they found that aerodynamic performance data for the VR-12 at these speeds simply did not exist in the open literature. Furthermore, while ADD had access to many testing facilities, they did not have the specific capability to perform this test.

Action

In January 2018, MAJ Shawn Naigle (APM Block II, Cargo Helicopters PMO, PEO Aviation) contacted ARO Fluid Dynamics program manager Matthew Munson for assistance with identifying a university resource that could help to verify the root cause of this vibration. There are currently only a handful of wind tunnels across the United States university system capable of running experiments to provide the required aerodynamic data. During discussions with MAJ Naigle, it was determined that the Ohio State University (OSU) likely possessed the required capability, both in terms of physical facilities as well as well-qualified scientific investigators. An in-person meeting was conducted in late February 2018 at OSU with Dr. Jim Gregory and Dr. Jeffrey Bons and the PM Cargo team (led by Mr. Terry Hice, Modernization Tech Chief for Cargo Helicopters PMO) to discuss capabilities and requirements.

SUCCESS

ARO PM provided a fast response to close a scientific knowledge gap that had immediate implications on enhancing U.S. Army rotorcraft performance.

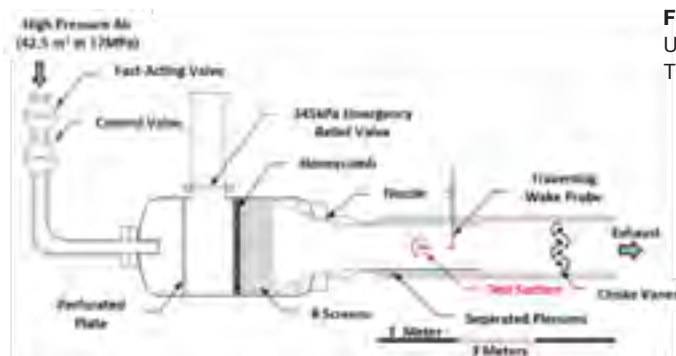


Figure 1. The Ohio State University Unsteady Transonic Wind Tunnel

Result

The resulting OSU research effort involved three airfoil sections, the previously mentioned VR-7 and VR-12, along with the Eppler E-387. Coefficients of lift, drag, and pitching moment were measured from surface pressure measurements at both static and dynamic angle of attack conditions. A range of Reynolds numbers and reduced frequencies were tested; the main dynamic condition (governed by mean and fluctuating angle of attack) would be considered "light" dynamic stall.

At the end of October 2018, the team reconvened at OSU to get a preliminary report on the scientific findings, as the test matrix had been completed. Mr. Hice and MAJ Green (APM Block II, Cargo Helicopters PMO, PEO Aviation and MAJ Naigle's replacement) were very pleased with the quality and scope of the effort, as well as the careful attention to uncertainty management and measurement techniques. Dr. Preston Martin (CCDC-AvMC ADD) was also present via telecon and was very excited about the results. OSU is currently preparing a technical report summarizing their results and detailing their findings. Dr. Martin is currently running additional simulation cases incorporating the new knowledge and assessing its potential impact to the ACRB effort.

Way Ahead

This is a work in progress and the eventual impact of this aerodynamic performance characterization on the Block II upgrade is still being determined. Conversations in late FY19 with Cargo Helicopters PMO, ADD and OSU will determine whether additional test cases are required to gain greater insight into the specific flow physics responsible for the most troublesome configurations.

Leading the Field of Aerospace

Challenge

Effective communication of breakthrough scientific results is critical to the initiation of new technology. Facilitating such communications between scientific researchers and technology developers is critical for transition of knowledge products into spaces where innovation can occur. Professional societies have long been a part of bringing communities together in order to share new results, challenge pre-conceived notions, and identify opportunities to form relationships that lead to effective collaborations. Given the finite bandwidth of individual researchers and research communities, it can be a challenge to focus attention on the most pressing problems the U.S. Army faces. In order to initiate the future technological superiority of our Soldiers, Army and Nation, ARO Program Managers proactively seek out opportunities to focus the scientific and engineering communities on those problems with the greatest opportunity to shape the future of the Army.

Action

One professional society devoted to the advancement of aerospace science, technology, and capabilities is the American Institute of Aeronautics and Astronautics (AIAA). Established in 1963, it has become one of the premier international organizations for the aerospace field, with more than 30,000 members from more than 80 countries. Of the many events supported and enabled by AIAA throughout the year, the SciTech Forum (held every January) and the Aviation Forum (held every June) are the two primary events where the Fluid Dynamics and Applied Aerodynamics communities gather to present their latest findings, identify opportunities for collaboration and hear from industry leaders about the current state-of-the-art, as well as cast and debate visions for the future. These events are well attended by members from academia, industry, and government, from the U.S. and the international community.

Nearly all of the technical direction and organization of AIAA is provided by its membership. The society's foundational structure for this activity are Technical Committees, which are typically comprised of no more than 50 representatives selected competitively from among the community. These committees are responsible for the technical execution of their respective conferences: evaluating conference papers for awards, identifying worthy recipients of various society awards, and leading working groups that drive the direction of the field.

RESULTS

- ▶ Fundamental aerodynamic performance data measured for reference geometry and rotorcraft relevant geometries.
- ▶ Static and dynamic data were obtained at a range of speeds and pitching frequencies.
- ▶ Aerodynamic database provided to CCDC-AvMC and Cargo Helicopters PMO for incorporation into ACRB design analysis.

This success supports these ARL Core Technical Competencies

Propulsion Sciences



Ballistics Sciences



SUCCESS

ARO Program Managers demonstrate proactive personal attention to shape science for the future of the Army through leading scientific communities.

In early 2015, ARO Fluid Dynamics Program Manager Matthew Munson was approached by the Chair of the Fluid Dynamics Technical Committee (FDTC) and specifically encouraged to apply for membership to the committee. Dr. Munson's background, technical knowledge and basic research portfolio management responsibilities made him a prime candidate to be directly engaged with the activity of the FDTC. Dr. Munson was installed in May of that year and assigned to the "Fundamentals of Flow Phenomena" subcommittee. He quickly engaged, serving as an assistant organizer for the Aviation 2016 Fluid Dynamics Conference and the SciTech 2017 Aerospace Sciences Meeting. In this role, he was responsible for overseeing the review process for 30-40 extended abstracts, assigning experts to review the author submissions and making technical judgments on which abstracts would be invited to submit a full paper for each conference. His recognized objective judgement, coupled with the timely and efficient implementation of these duties, contributed directly to the ultimate overall quality of these two conference events.

Dr. Munson was also selected by FDTC leadership to serve on the Standing Committee for Awards. Among other duties, this committee selects the AIAA Fluid Dynamics Award each year. This award is one of the top prizes in the field and is presented for outstanding contributions to the understanding of the behavior of liquids and gases in motion as related to need in aeronautics and astronautics. Winners of this award are considered leaders in the field; the opportunity to highlight their contributions to the field of flow physics emphasizes to the community areas that are of most significance to the future.

Result

As a result of his proficiency as an assistant organizer and his proactive personal attention within the FDTC community, Dr. Munson was named the Technical Discipline Chair for Fluid Dynamics for the SciTech 2018 Aerospace Sciences Meeting. In this role, he had significant responsibility for the planning and execution for the conference. To begin, he substantially revised the call for papers in order to drive the scientific direction of the conference toward more basic research in fluid dynamics. This was done in coordination with the Applied Aerodynamics Technical Committee; this revision and coordination led to a better engagement for the communities at large, since authors had a clearer indication of where their paper contributions would best fit within the overall conference. Leading a team of seven assistant organizers, Dr. Munson oversaw the review of 394 abstract submissions, from which 292 conference papers were selected. Dr. Munson organized the talks into 55 conference sessions, carefully coordinating with other Technical Committees to ensure conflicts were minimized and overlapping interests were accommodated. The Fluid Dynamics conference represented 12% of all accepted papers for the forum and was the largest single effort among the other fields participating in the forum. While conducted domestically, the forum was attended by more than 4,000 participants from 39 countries, making it a significant international event.

The resulting conference was a tremendous success and featured special sessions and topics that included hypersonic boundary layer transition prediction, massively separated flows, and Reynolds-Averaged Navier-Stokes solutions for benchmark configurations.

Way Ahead

As a result of the success of the conference, Dr. Munson was selected by the FDTC Chair to serve as the Chair of the Fundamentals of Flow Phenomena Subcommittee. In this role, Dr. Munson provides support to a number of active discussion groups on topics such as: boundary layer transition, high-speed fluid/structure interaction,

RESULTS

- ▶ Provided scientific direction to a major professional society conference event
 - ▶ Oversaw review process for ~400 abstracts; selected ~300 papers for inclusion.
 - ▶ Coordinated special sessions to disseminate highly relevant findings to the community
-

theoretical fluid mechanics and reduced complexity flow modeling and analysis. These groups are comprised of active researchers in the field and provide a forum for discussing the latest research results and planning for the future. In addition, the subcommittee has the responsibility for execution of the 2020 Theoretical Fluid Mechanics Conference, which occurs triennially in the summer. Similar to the SciTech 2018 event, Dr. Munson will be responsible for the scientific direction and execution of the event, providing leadership to the theoretical fluids community and shaping the modern definition of “theoretical.” He will also be proactively looking for opportunities to leverage the best ideas presented at the conference to address the many challenging problems facing the U.S. Army.

FLUID DYNAMICS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Identify critical parameters governing boundary layer separation in unsteady flows and manipulate separation dynamics to control flow evolution. If successful, U.S. Army vehicle and weapons systems will experience substantial increase in performance metrics, such as speed, range, endurance, and maneuverability.
- ▶ Determine underlying frameworks for turbulent flows that leverage the existence of coherent structures. If such frameworks can lead to predictive models requiring substantially reduced computational loads over current capabilities, control of U.S. Army vehicle platforms, weapons systems, and precision air drop systems will be significantly improved.
- ▶ Identify, describe, and control flow phenomena via exploitation of the non-linearities inherent in the Navier-Stokes equations. Novel flow phenomena are likely to be discovered as the crutch of linearity is discarded, or if promising operator methods can recast the equations to allow linearity to be exploited without traditional linearization.

COMPLEX DYNAMICS AND SYSTEMS PROGRAM



Dr. Samuel Stanton

Program Manager, Complex Dynamics and Systems
 Mechanical Sciences Division
 ARO Engineering Sciences Directorate

Dr. Stanton completed his undergraduate studies at the U.S. Naval Academy, receiving his B.S. in Aerospace and Astronautical Engineering in 2004. He completed his graduate training at Duke University, receiving his Ph.D. in Mechanical Engineering in 2011.



He came to ARL in 2011 as the manager for the Complex Dynamics and Systems Program.

Operator-Theoretic Approaches to High Dimensional Dynamical Systems

Challenge

The principal analytical techniques of nonlinear system dynamics rely upon a century-old and physically intuitive geometric framework. Extending such geometric insight beyond a small number of dimensions (typically three or less) has been a longstanding barrier. Unfortunately, many problems facing modern science and engineering are

This success supports these ARL Core Technical Competencies

- Computational Sciences 
- Propulsion Sciences 
- Network and Information Sciences 

necessarily high-dimensional or present problems characterized by unstructured high-dimensional data. A variety of methods in reduced order modeling have been developed to address high-dimensional nonlinear systems, yet these methods are typically not robust to parameter variations and often require many degrees of freedom (e.g., upwards of 106 in coupled fluid-structure interaction problems to 1020 in the case of geophysical flows). Modern computational capabilities also fail to provide accurate and expedient solutions to fully general problems in complex flows.

Action

In view of the shortcomings of existing analytical frameworks as well as computational considerations, ARO Complex Dynamics and Systems program manager Samuel Stanton realized that new approaches would be necessary. Accordingly, Dr. Stanton began to look more closely at new findings being presented at applied mathematics meetings, such as those of Professor Igor Mezic at the University of California at Santa Barabra. Professor Mezic was focused on a nearly forgotten set of results from the early 1930s concerning an operator-theoretic formalism for classical mechanics that mirrored many of the mathematical methods and techniques used in quantum mechanics. This approach, known as the Koopman-von-Neumann (KvN) theory, established a common mathematical framework for dynamics spanning from quantum mechanical to classical statistical regimes. KvN theory examines spectral properties of operators associated with dynamical system evolution that could transform the analysis of strongly nonlinear systems into an infinite-dimensional and, even more importantly, linear and global domain of observables.

Result

Dr. Stanton recruited a proposal from Professor Mezic to develop the mathematical framework for the analysis of large-scale interconnected systems through a combination of operator-theory, geometric dynamical systems theory, graph-theory, and probabilistic measure theory. This research program resulted in seminal review papers in the Annual Review of Fluid Mechanics as well as the journal Chaos. Shortly thereafter, the data science and fluid dynamics communities began to demonstrate the utility of the Koopman operator approach to extracting global nonlinear features of data and dynamical systems. Operator-theoretic approaches are now impacting a broad range of research areas such as coherence in nonlinear fluid and neurophysiological dynamics, instabilities in networks, and information processing in complex systems. Moreover, spectral analytic approaches have shown remarkable potential to overcome longstanding challenges facing high-dimensional data such as sensitivity to parameter variations, dynamically evolving sources of instability, and continued need to retain many degrees of freedom (upwards of 106 in fluid-structure interaction and 1020 for geophysical flows).

RESULTS

- ▶ A new and rigorous approach to complex systems has been developed.
 - ▶ New approaches led to ARL Director's Research Initiatives and DARPA programs.
 - ▶ New expertise hired by VTD.
-

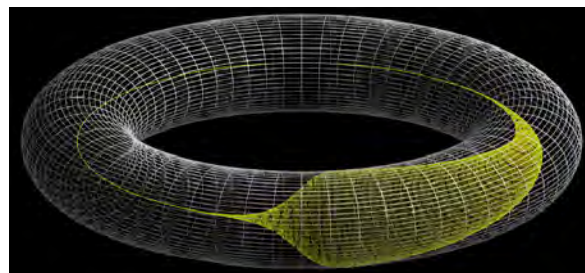


Figure 1. An ARL-UCSB collaboration orchestrated by ARO PM led to the discovery of a new type of dynamic behavior called quasi-periodic intermittency.

In 2013, Dr. Stanton brought these breakthroughs to ARL-VTD scientist Dr. Bryan Glaz, who saw the opportunity to apply these methods and advance the theory into new domains by considering rotorcraft dynamic stall. This required examining new aspects of the spectrum of the Koopman operator as well as accounting for the influence of control. Dr. Glaz carefully selected the problem of vortex shedding from an oscillating cylinder as a canonical system for challenging the theoretical state-of-the-art. Soon thereafter, Prof Mezic and Dr. Glaz began collaborating and discovered a type of behavior they named “quasi-periodic intermittency” that may give rise to fundamental understanding and control of complex physical and engineered systems.

Furthermore, motivated by the ARO supported research results, in 2015 DARPA began a program on Enabling Quantification of Uncertainty in Physical Systems (EQUiPS), which invested in the theory, numerical analysis, and data structures for extending uncertainty quantification methods to high-dimensions using Prof. Mezic’s Koopman operator formalism.

Way Ahead

Despite the rapid success and adoption of Prof Mezic’s methods, scientific progress continued to mostly focus upon asymptotic properties of particular operators associated with deterministic systems. Recognizing this shortcoming, the Army Research Office proposed a 2017 Multidisciplinary University Research Initiative (MURI) to target spectral decomposition algorithms, competing path integral approaches, and control formalisms for time-varying, nonequilibrium dynamical systems of DoD interest (i.e., systems where transients, hysteresis, dissipation, or broadband frequency content can strongly modulate global behavior).

Today, a multidisciplinary team supported by ARO is taking these next steps. Future research has significant potential to establish a new set of rigorous mathematical formalism and data-driven tools to tackle the DoD’s toughest challenges from interdependent networks to vortex interactions.

New Science of Terradynamics

Challenge

Granular systems are often far-from-equilibrium, characterized by non-smooth dynamics, and exhibit a wide range of counter-intuitive and emergent behaviors. These problems are nearly impossible to describe with a set of elegant constitutive relations. Most equations leveraging plasticity theory and continuum mechanics for granular materials are typically ill-posed and lack uniqueness.

Fundamental understanding of these types of complex rheological materials remains a prescient need due to the variety of DoD applications immersed in such substrates, such as shear-mediated materials for body armor, projectile penetration in varying granular earth materials, and all-terrain mobility and agility.

This success supports these ARL Core Technical Competencies

Propulsion Sciences



Materials and Manufacturing Sciences



Protection Sciences



SUCCESS

ARO PM was able to develop new approaches leading to first-principles based predictive understanding of movement in complex media.

Action

In 2011, ARO Complex Dynamics and Systems program manager Samuel Stanton developed new program directions to address these scientific challenges, inspired by a wide range of biological organisms operating with remarkable agility in complex rheological environments. Dr. Stanton recruited a proposal from Professor Dan Goldman at the Georgia Institute of Technology to investigate the mechanics of organisms filling ecological domains dominated by loose granular terrain or at the interface of water and land.

Professor Goldman also began to explore the novel use of robots as active experimental probes capable of generating controlled and repeatable experimental data. Robots in Professor Goldman's labs were designed to function as the simplest possible surrogates for the organisms under study. Carefully focused experiments on specific physical effects, such as the role of leg stiffness or foot flexibility in granular interactions, could be conducted.

To the surprise of both Dr. Stanton and Professor Goldman, the data emerging from the robotic experiments not only very closely replicated the behavior of the organisms, but was also displaying consistent and repeatable interaction patterns. This suggested an opportunity for theoretical characterization that had heretofore eluded researchers. In particular, the experimental data indicated that locomotion within and upon granular media at low speeds emulated the classical Resistive Force Theory (RFT) for viscous fluid mechanics. These results were highly unexpected and counter-intuitive; RFT is a linear simplification of the highly nonlinear Navier-Stokes equations for bodies immersed in fluids, but dynamics of granular media were difficult to describe with formal constitutive equations. Nonetheless, the agreement between the theoretical approximation and the experimental data was precise. Professor Goldman's group demonstrated the first theory of terradynamics, earning publication in the journal *Science*.

These peculiar yet undeniable patterns in the data still lacked rigorous theoretical foundation built upon first principles. Accordingly, Dr. Stanton encouraged Professor Ken Kamrin, an applied mathematician at MIT to develop a Short-Term-Innovative-Research proposal to re-examine the hierarchy of models for granular media to possibly elucidate the reason that RFT worked so well. Surprisingly, this initial foray was inordinately successful. Professor Kamrin was able to establish scaling relations from first principles that not only explained why RFT behavior was emerging, but also described the types of intruder geometries and speeds were amenable to simple RFT models. Moreover, theoretical results also indicated that such simple models would also govern cohesive granular media such as suspensions, gels, and mud—the latter being especially relevant to Army mobility.

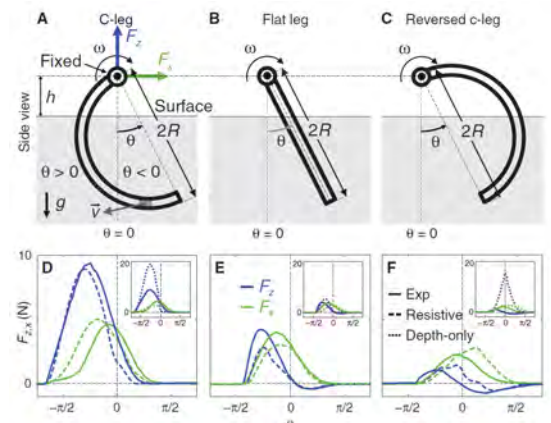


Figure 1. Experimental results from Li, et al (*Science*, 2013) showing that resistive force models predict forces on various morphologies moving in granular media.

Result

Today, Professors Goldman and Kamrin are collaborating to test the speed limits of RFT. They are hoping to discover and describe how fast an object can move within and upon granular media while still obeying the RFT relations. They also hope to extend the RFT formulation to permit high-speed interactions. This research holds promise to elucidate fundamental understanding of new and predictive constitutive relations which could lead to rules for designing novel and shape-adaptive granular intrusion and propulsion devices.

Way Ahead

All of the students trained in the Goldman and Kamrin labs in terradynamics have accepted faculty positions in top tier research institutions. ARL-VTD has hired research scientists who have trained under the scientists behind these advances, bringing this expertise to Army in-house laboratories. This allows for predictive design of new propulsors to achieve agile locomotion across length scales in robotic vehicles. Greater Army impact will be achieved by research that is underway to push the approach to higher inertial and speed regimes.

COMPLEX DYNAMICS AND SYSTEMS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Discover general principles governing the dynamics and control of moderately high-dimensional and strongly coupled interacting systems. If successful, this research could lead to a massive change in DoD tools to perform design, pursue inference from data, and control for a class of systems possessing a very broad set of nonlinear features.
- ▶ Control and exploit underlying geometry, information flow, and energy in nonequilibrium dynamical systems. If successful, fundamental understanding will lay the foundations for developing nano-scale systems capable of coordinating molecular assembly of materials and systems with novel properties. This research could also yield a generation of denser, faster, cheaper, and more energy efficient computing devices capable of manipulating large-scale, complex data structures, as well as self-organizing nanoscale motors capable collectively interfacing with the physical world with maximum power and efficiency.
- ▶ Discover and shape hierarchical interactions leading to emergent phenomena in programmable active matter and complex collectives. If successful, this will enable new understanding of the mechanics of naturally occurring active soft matter that could be translated to synthetic systems and materials with active microstructures of Army and DoD relevance. Such systems and materials include modular robotics, reconfigurable assemblages of autonomous swarms, confined space robotic locomotion and soft robotics, soft armor, and adaptive, reconfigurable materials.
- ▶ Control and exploit multi-stable energy landscapes to engineer novel adaptive nonlinear meta-structures. If successful, this may lead to complex material and structures for actuation, vibration protection, and shock mitigation in ground and air vehicle technologies.

RESULTS

- ▶ First principles-based foundations for a theory of terradynamics for ground movement as powerful as hydrodynamics and aerodynamics.
 - ▶ Major publications in Science, Nature Materials, and Physical Review Letters.
 - ▶ New expertise hired by VTD.
-

EARTH SCIENCES DIVISION: FY18 SUCCESS STORIES

EARTH MATERIALS AND PROCESSES PROGRAM



Dr. Julia Barzyk

Program Manager, Earth Materials and Processes
Earth Sciences Division
ARO Engineering Sciences Directorate

Dr. Barzyk completed her undergraduate studies at the University of Rochester, receiving her B.A. in Geology in 1998; she received a M.S. in Geological Sciences from the University of Florida in 2000 and a M.S. in Environmental Science & Public Policy from the University of Chicago in 2002. She received her Ph.D. in Geophysical Sciences from the University of Chicago in 2007.

She came to ARO in 2012 as a SETA Contractor to support the Earth Materials and Processes Program, and was hired as the Program Manager in 2015.

New Foundational Science for Urban Operations

Challenge

Continued global urbanization will have profound implications for society. With the majority of the global population living in cities by 2050 and the continued growth of megacities, Army operations in the urban environment are expected to increase. In order to sense environmental conditions, communicate, and maneuver within this environment, detailed knowledge of the physical properties of the built environment and how the built environment interacts with its surroundings is required. Although many disciplines have been involved in constructing cities, including civil and environmental engineering and urban planning, historically there has been very little inquiry into the physical science of the built environment. Furthermore, what has been considered has typically been of insufficient resolution to be of use to the Army, such as climate models that consider the impact of a city as a whole on a regional climate system. Fine-scale predictions of weather and environmental conditions with this type of terrain, which is complex in both its topography in its material composition, are lacking.

Action

In 2013 Dr. Julia Barzyk, in coordination with the ARO Earth Materials and Processes program manager, conducted an intentional proactive outreach to the academic community to communicate ARO's interest in advancing basic science for urban operations. After extensive discussions to foster the development of novel scientific opportunities, Dr. Barzyk recruited a proposal from Professor Elie Bou-Zeid of Princeton University to study the thermal effects of rainfall on the built environment (Figure 1). Additionally, she invited Professor Enrique Vivoni from Arizona State University to propose a study of land-atmosphere interaction in desert urban environments.

Result

In 2018, after sustained proactive outreach to university researchers, Dr. Barzyk was able to support four new research grants to early-career scientists that are expected to provide the foundational knowledge critical to ensuring operational success in urban

This success supports
these ARL Core Technical
Competencies



Computational Sciences

SUCCESS

ARO PM developed an investment strategy to address a scientific knowledge gap that has resulted in research currently underway to support operations in the Dense Urban Environment.



Figure 3. Heavy artificial rain generated over the impervious concrete surface

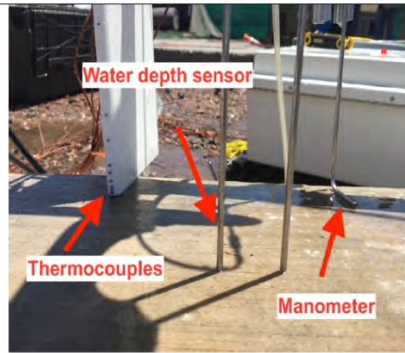


Figure 4. Thermocouples, Pitot tube, and water depth sensor

Figure 1. The Princeton – Arizona State University experimental arrangement

environments. This program area growth coincides with the completion of the ARL Atmospheric Science Center Meteorological Sensor Array (MSA), and with the initiation of coordination with USMA urban geographers. Professor Dan Li from Boston University is exploring the interaction of heat wave and urban heat island phenomena. Professor Prathap Ramamurthy from the City College of New York began work is developing a new method to use remote sensing to quantify heat storage by urban surfaces. Professor Hernan Moreno from the University of Oklahoma is attempting to relate soil temperature profiles to water and energy exchange at the ground surface. Additionally, Professor Inanc Senocak from the University of Pittsburgh is investigating the controls on wind speed at the 10-meter scale in complex terrain.

Way Ahead

While diverse in topic area and approach, these ARO supported research efforts are addressing fundamental challenges where basic research by the academic community has been lacking. Building a community of university researchers studying how air, particles, water, and energy move throughout the built environment is critical to effective Army operations in the future. For this reason, the ARL Atmospheric Science Center has recently prioritized study of the ‘dense urban environment,’ and these ARO-funded researchers are poised to increase the impact of the MSA through ARL’s Open Campus initiative and to support the design of an instrumented field-scale mock urban cluster of buildings in the future. This test environment will be used to validate microscale models (10 meter grid) and to develop tactical decision aids including UAV routing. ARO supported researcher visits to the MSA, additional coordination with USMA researchers, and participation in a DOE-led urban modeling workshop are planned for FY19. Also for FY19, a joint ARL- City College of New York field measurement campaign will be conducted with Professor Ramamurthy to collect the high resolution ground-truth data required to enable modeling and prediction in the built environment.

Advancing Ground Mobility

Challenge

Erosion of earth materials by shear flow is very common in nature and is responsible for shaping landscapes; controlling and mitigating erosion are critical to land management and the maintenance of infrastructure. However, erosion of earth materials is a very complex process, and therefore descriptions of erosional processes put forth by geoscientists have often been simplified and largely based on field observations. Another complex process involving surface materials is that of vehicle-terrain

RESULTS

- ▶ Network of academic partners developed to support ARL- Atmospheric Science Center’s on-going and future Dense Urban Environment research
- ▶ ARL-CISD and City College of New York joint field campaign to collect high-resolution environmental data in New York City
- ▶ Coordination between USMA physical geographers and Princeton University civil and environmental engineers

This success supports these ARL Core Technical Competencies

Computational Sciences



Propulsion Sciences



SUCCESS

ARO PM cultivated basic research efforts from two initial universities, and findings resulting from those efforts are now under further development at four universities including Naval Postgraduate School, with efforts targeted to ground vehicle applications.

RESULTS

- ▶ Improved approach to erosion management in development
 - ▶ New models of ground surface materials properties in development
 - ▶ ARO-supported postdoctoral fellow appointed to faculty position at Naval Postgraduate School
-

interaction, which are also predicted from empirical models. To move from the use of empirical models in both the study of earth surface processes and in terramechanics, fundamental knowledge must be developed.

Action

In 2013, the ARO Earth Materials and Processes program manager, advised by Dr. Julia Barzyk, recruited a unique proposal that attempted to use approaches from the granular materials community to investigate erosional processes in granular beds. To investigate erosional processes from a granular materials perspective rather than the traditional empirical one, Professors Corey O'Hern and Nick Ouellette from Yale University combined experiments and numerical simulations to explore what factors are most important in controlling the onset and cessation of motion for particles in a granular bed (Figure 1). This work involved experiments performed in an annular flume, and a closely integrated numerical modeling effort. Looking to such an idealized system involved risk that the results would not be applicable to natural systems with their complexity in terms of particle sizes, shapes, size distribution, and the non-uniform flow conditions to which they are exposed. Nevertheless, Dr. Barzyk encouraged development of the research with the potential to provide a physical justification for observed relationships between fluid shear stress and flow properties.

During the course of the effort, Professor Ouellette moved to Stanford University, and was supported, with Professor O'Hern, by ARO in 2017 to begin a new project focused on geometric strengthening and armoring (segregation) processes. The 2013 effort was considered successful in terms of achieving results of theoretical and practical significance, and the decision to begin a new effort in 2017 was made to capitalize on this investment and develop ways to design granular beds in which strength can be controlled.

Beginning in 2014 and concurrent with the above efforts, Dr. Barzyk pursued a novel research proposal from Professor Emily Brodsky from the University of California at Sana Cruz to investigate differences in behavior observed in laboratory experiments on spherical glass beads and angular natural sands. This work determined that acoustic noise generated by the sand grains moving against each other was responsible for grain compaction at an intermediate shear rate that did not occur with the glass spheres (Figure 2). This research team elucidated the role of this phenomenon, termed auto-acoustic compaction, in grain compaction through a series of experiments involving sands of different mineral types.

Result

During the course of these ARO supported research efforts, Dr. Barzyk encouraged communication between Professor Brodsky and Professor Abram Clark, who had served as a postdoctoral researcher on the original proposal by Professors O'Hern and Ouellette, and was now at the Naval Postgraduate School. It became clear that Professor Clark's expertise in numerical simulation and perspective from the physics and granular flow community would be invaluable in the further study of compaction in natural sediments. Furthermore, Professor Clark and Professor Brodsky are now co-advising a postdoctoral researcher on the use of novel numerical simulations to study a range of conditions beyond what can be studied in laboratory experiments.

Way Ahead

Currently, CCDC Ground Vehicle Systems Center is leading efforts away from simple terramechanics, which involves making measurements on ground materials to determine their properties and trafficability, to complex terramechanics, which takes a physical modeling approach to vehicle interaction with the ground surface. Such terrain characterization and modeling of vehicle-terrain interactions are critical to mobility, supporting the Next Generation Combat Vehicle Army Modernization Priority. For FY19, an on-site visit to CCDC-GVSC is planned to coordinate ARO supported research efforts under the Earth Materials and Processes program to inform and enhance the CCDC-GVSC mobility model.

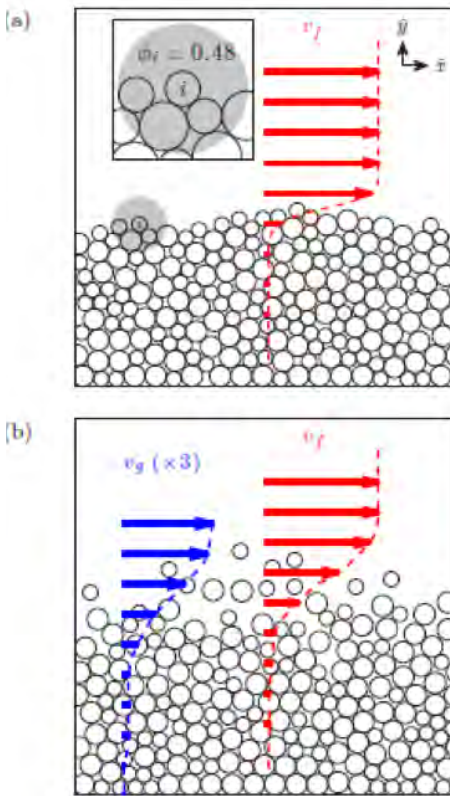


Figure 1. Investigating the onset and cessation of motion for particles in a granular bed (O’Hern and Ouellette)

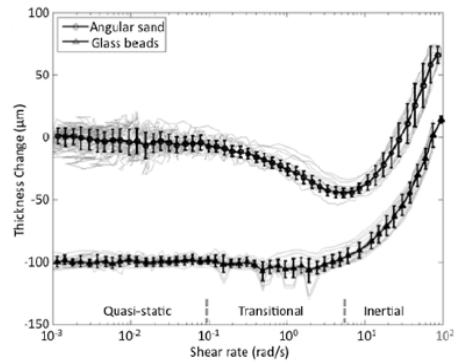


Figure 2. Acoustically generated compaction of natural beach sands (Brodsky)

EARTH MATERIALS AND PROCESSES PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Determine how grain-scale features influence bulk properties in unconsolidated earth materials.
- ▶ Enable prediction of earth surface interaction with air and water at Warfighter-relevant spatio-temporal scales (microns to 100s of kilometers).
- ▶ Develop methods to remotely determine earth surface properties.

COMPUTING SCIENCE DIVISION: FY18 SUCCESS STORIES

COMPUTATIONAL ARCHITECTURE AND VISUALIZATION PROGRAM



Dr. Mike Coyle

Program Manager, Computational Architectures and Visualization
Computing Sciences Division
Information Sciences Directorate

Dr. Coyle completed his undergraduate studies at Boston College, receiving his B.A. in mathematics in 1976. He trained as an applied mathematician at Rensselaer Polytechnic Institute, receiving his Ph.D. in mathematics in 1990. He began working for the Army as a mathematician in 1984 and came to ARO in 1999 as the Manager for what was then called the Discrete Mathematics and Computer Science Program

Interactive Computational Algorithms for Acoustic Simulation in Complex Environment and Real-World Scenes

This success supports these ARL Core Technical Competencies



Computational Sciences



Materials and Manufacturing Sciences

SUCCESS

Interactions with Army acoustic scientists and researchers led to the design and implementation of a novel technique that for the first time can automatically generate high fidelity acoustic simulation models from real-world indoor environments. These models can be directly used in augmented/virtual reality systems to enhance Soldier training and mission rehearsal.

Scientific Challenge

Recent advances in computer vision have made it possible to generate accurate 3D models of indoor and outdoor scenes from a sequence of images and videos. The resulting models are frequently used for visual rendering, physics-based simulation, or robot navigation. In many applications including computer-aided design, teleconferencing, and augmented reality, it is also important to augment such scenes with synthetic or realistic sound effects. It has been shown that good sound rendering leads to an improved sense of presence in virtual and augmented reality (VR and AR) environments. The simplest methods for generating acoustic effects in AR/VR are based on artificial reverberation filters which use simple parametric decay models. However, the specification of these parameters is time consuming and these techniques cannot simulate many effects, such as diffraction or direction-dependent reverberation. Most accurate methods for acoustic simulation are based on directly solving the acoustic wave equation. Many numerical algorithms have been proposed based on finite differences, finite elements, or boundary elements. Due to the underlying complexity, these techniques have been limited to small spaces (e.g., less than 1,000 cubic meters) and low frequencies (e.g. less than 1KHz), and are currently not regarded as practical for large spaces. For AR/VR to be a truly effective tool, the challenge is to develop methods that are accurate and can produce simulations at an interactive rate for large complex environments.

Action

In response to the above scientific challenge and the Army's interest in enhanced sound rendering and simulation for applications such as virtual reality training and battlefield acoustic sensor placement, and after discussions with some of the Army's top acoustic scientists and a computer scientist from ARL-SLAD highly interested in interactive wave propagation in urban environments, ARO awarded a single investigator grant to Professors Dinesh Manocha and Ming Lin of the University of North Carolina – Chapel Hill, world renowned researchers and experts in modeling and simulation and virtual reality to investigate new interactive algorithms for acoustic simulation for

analyzing wave propagation in complex environments as well as new methods that can be used to perform acoustic simulation and rendering in reconstructed real-world models generated by modern scanning and sensing techniques. Such research could offer fundamental scientific capabilities for solving wave/sound propagation problems in highly complex, vast domains for not only the Army but civilian applications such as seismology, geophysics, meteorology, geomagnetism, urban planning, and gaming.

Result

In FY18, these researchers have designed and implemented a novel technique that for the first time can automatically generate high fidelity acoustic simulation models from real-world indoor environments that can be directly used in augmented/virtual reality systems to enhance Soldier training and mission rehearsal. In comparison to current methods this technique is superior in that it can handle diffuse reflections, diffraction, is robust to measurement noise, and it's simple, practical, and relatively fast. The method first applies a convolutional neural network to generate a coarse simulation model from data obtained using a simple microphone and speaker setup, and then iteratively optimizes the model until the virtual acoustic simulation converges to the measured acoustic response. The research team has applied their algorithm to several reconstructed real-world indoor scenes and evaluated its fidelity for augmented reality applications. The results show the simulated acoustic environment is indistinguishable from the measured data.

RESULTS

- ▶ Acoustic material classification research resulted in two peer reviewed conference proceeding articles.
- ▶ Software has been made available as open source software which has been downloaded by hundreds of researchers and developers.

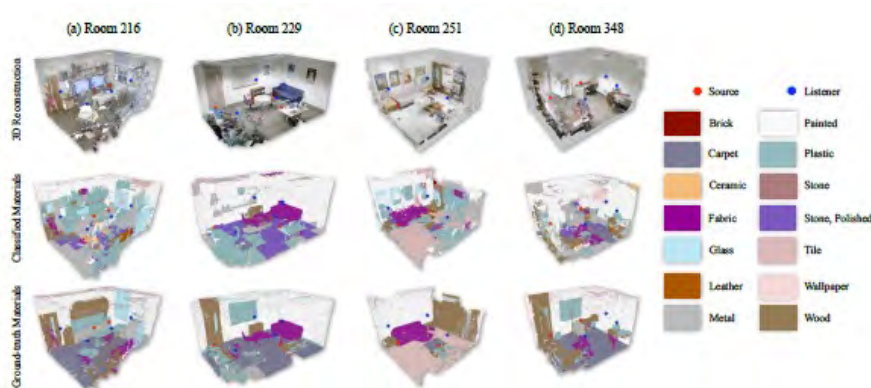


Figure 1. The results of material classification algorithm for four benchmark scenes. Colors indicate the material category that has been assigned to each triangle of the reconstructed model. The middle row shows the results of the material classification, and the bottom row shows the manually-generated ground-truth classification that are used for validation. The source and listener positions for the acoustic measurements within the real room are shown as red and blue circles, respectively. These are used to optimize the acoustic materials present in the scenes.

Way Ahead

The research team will continue to enhance this technique with a focus on extending it to larger indoor and outdoor scenes, making it applicable to a greater number of Army training and mission rehearsal scenarios. Once the research has reached the appropriate maturity level, we will begin discussions with the Army's Simulation and Training Technology Center (STTC) for possible transition. Past interactions with this research team and STTC resulted in significant enhancements to the Army's OneSAF combat simulation system.

This success supports these ARL Core Technical Competencies



Computational Sciences



Network and Information Sciences

SUCCESS

Interactions with Army terrain scientists and researchers at Duke University led to the design and implementation of a novel high-speed algorithm to perform flood risk analysis on a high-resolution large-scale terrain model. The new algorithm which is exponentially faster than existing techniques can determine the flooding probability of a region on a terrain surface caused by rainfall and flowing water filling up depressions in that terrain to the point of overflowing. The new technique will be incorporated into Army terrain analysis systems for mission planning, as well as for civilian projects.

Scalable Techniques for Modeling and Analyzing Big Spatial Data

Scientific Challenge

Terrain analysis is an integral part of the military intelligence preparation of the battlefield, commonly used to support both defensive and offensive operations. It consists of interpreting natural and manmade terrain features, together with the influences of weather, to determine their effects on military operations. The main challenges to terrain analysis are due to the size of the data sets: 1) it is impossible to compute exact solutions for most of the problems; 2) it is too expensive even to perform a constant number of passes over the data set; and 3) when data is arriving in form of a stream, one cannot afford to store the entire data set in many cases. In addition, the time spent in transferring data between main memory and disk becomes the bottleneck (commonly known as the I/O-bottleneck) while performing computations on such massive data sets, which do not fit in main memory. Consequently, the performance of many CPU-efficient algorithms deteriorates significantly. Other challenges are related to uncertainty and noise and the dynamic nature of the data. In order to provide effective terrain modeling and analysis capabilities, the challenge is to develop methods that are accurate, robust, efficient, and scalable when dealing with such massive, dynamic, and noisy data.

Action

In response to the above scientific challenge and the Army's interest in scalable terrain analysis, and after discussions with Army scientists from the Army's Topological Engineering Center and ARO's Environmental Science Program manager, ARO PM, Dr. Coyle, recruited Professor Pankaj Agarwal of Duke University, a world-renowned researcher and expert in computational geometry, BigData, and external memory techniques. This researcher was asked to provide enhanced terrain modeling and analysis capabilities by developing sophisticated algorithms that function with massive non-standard datasets, such as point clouds, and that produce a confidence level for the results. Such research could not only significantly reduce the computational effort associated with military applications of terrain analysis but also for a wide range of critical civil and environmental engineering tasks in natural disaster management (e.g., flood predictions, landslide risk analysis), natural resource management (water quality analysis, soil conservation, ecological forecasting), transportation (mobility related planning), and several other civilian areas.

Result

In recent years, the potential of terrain information systems is greatly enhanced by new terrain mapping technologies such as Light Detection and Ranging (LIDAR), ground based laser scanning and Real Time Kinematic GPS (RTK-GPS) that are capable of acquiring millions of geo-referenced points within short periods of time (minutes to hours). However, while acquiring and geo-referencing the data has become extremely efficient, transforming the resulting massive heterogeneous data sets to useful information for different types of users and applications is lagging behind because of scarcity of robust, efficient algorithms that are scalable. Researchers at Duke University investigated scalable Big Data methods and created a novel high-speed algorithm to perform flood risk analysis on a high-resolution large-scale terrain model, namely water flows across a terrain which produce floods by filling up depressions. The model could be incorporated into Army terrain analysis systems for mission planning, as well as civilian projects. In FY18, this researcher and his students developed high-speed algorithms to perform flood risk analysis on a high-resolution large-scale terrain for both multi-direction flow (MDF) and single direction flow (SDF) models, namely water flows across a terrain which produce floods by filling up depressions. In particular, given a rain

distribution over a region on the terrain and a point on the terrain, their MDF algorithm can quickly determine how much rain has to fall so that the point is flooded, or which portions of the terrain are flooded for a given volume of rain over a specified region. By preprocessing the terrain data into a novel data structure, the flood-risk queries can be answered very rapidly through local computations. This is the first MDF algorithm that can answer flood-risk queries by performing local computations. For the SDF model, they developed and employ a logarithmic rather than the traditional linear technique to determine the amount of rainfall necessary to produce flooding. The worst-case performance of their algorithm is exponentially faster than the previously best-known algorithm.

Way Ahead

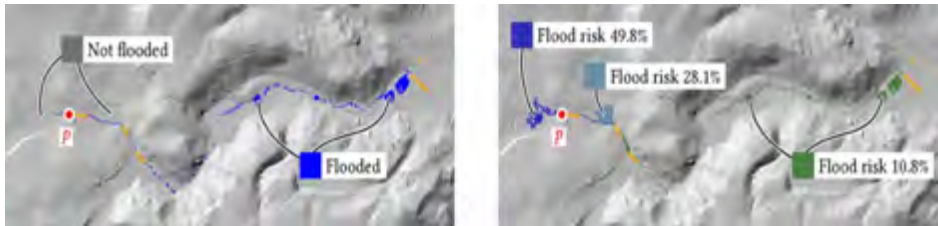


Figure 1. (Left) Deterministic model for analyzing flood risk for a given amount of rain at point p; (Right) Duke stochastic model for flood risk in presence of uncertainty in data.

This researcher and his students will continue to improve the system's performance by expanding and refining its data quality and increasing the feature set dimensionality. Once the research has reached the appropriate maturity level, we will begin discussions with the U.S. Army's Topological Engineering Center (TEC) for possible transition. Past interactions with this research team and TEC resulted in significant reductions in memory requirements and processing time for TEC projects.

INFORMATION FUSION AND PROCESSING PROGRAM



Dr. Liyi Dai (Retired)

Program Manager, Information Fusion and Processing
Computing Sciences Division
Information Sciences Directorate

Dr. Dai received his Ph.D. in Engineering Science from Harvard in 1993.

He came to ARO in 2005 as the Manager for the Information Fusion and Processing Program

Compressive Sensing MRI

Scientific Challenge:

The challenge of increasingly larger and higher-dimensional data sets has led sensing and imaging systems to an endless pursuit of ever faster capture, sampling, and processing rates; ever lower power consumption; ever smaller form factors; and ever more novel sensing modalities. However, the speed of data acquisition is physically limited by the response time of the sensors capture of a signal which, in turn, is quite often governed by the physics and the engineering design of sensors.

RESULTS

- ▶ Flood risk analysis effort resulted in two peer reviewed conference proceeding articles including a best paper award.
- ▶ Flood risk analysis techniques being evaluated by a small company, Scalable Algorithmics, for incorporation into their hydrology software.
- ▶ Flood risk analysis techniques being incorporated by hydrologists at Duke University into their models.

This success supports these ARL Core Technical Competencies

Computational Sciences



Network and Information Sciences



SUCCESS

ARO investment in compressive sensing has led to great technology transfer and is making a great impact to real world applications. Recently, compressive sensing technology developed by Prof. Richard Baraniuk of Rice University has been granted six U.S. patents. The technology has been licensed by Siemens Healthcare to radically speed up their magnetic resonance imaging (MRI) data acquisition. The company has reported speed-ups on the order of 10-15x over conventional imaging techniques. Particular MRI applications that are being improved by Siemens using compressive sensing technology include:

- ▶ Cardiac MRI. Rather than taking nearly six minutes with multiple breath-holds, a cardiac scan can now be performed in 25 seconds with free-breathing.
- ▶ Musculoskeletal MRI.
- ▶ Whole body imaging.

RESULTS

- ▶ Compressive sensing MRI technology has reduced MRI scan time from up to 45 minutes to as low as under one minute.
 - ▶ Compressive sensing MRI technology transitioned from Rice U. research to Siemens has obtained FDA approval for use.
 - ▶ Compressive Sensing algorithms also adopted by Conoco-Phillips Inc. to perform seismic sensing data analysis for oil exploration.
 - ▶ Prof. Richard Baraniuk was elected as Vannevar Bush Faculty Fellow and Fellow of American Academy of Arts and Sciences.
-

Action

Motivated by the physical constraints of data acquisition speed, the idea of creating new computational sensing systems that replace certain physical system elements (e.g., sensors, lenses) with computer algorithms was proposed. The ARO PM of Information Processing and Fusion, Dr. Dai, saw the opportunity of creating a brand-new concept of exploiting the sparsity of a signal that allows the reconstruction of a signal using fewer samples than the sampling theorem would require. He spear-headed the basic research investment by way of a new MURI topic on opportunistic sensing, and successfully launched the new MURI project led by Prof. Richard Baraniuk, Rice University.

Result

The MURI team explored the novel idea of compressive sensing and advanced the field by demonstrating the signal recovery as a solution to an underdetermined linear system using far fewer samples than a normal signal processing system would conventionally require. Compressive sensing has stimulated a re-thinking of sensor and signal processing system design. In compressive sensing, analog signals are digitized and processed not via uniform sampling but via measurements using more general, even random, sampling functions. In contrast to conventional wisdom, the new theory asserts that one can combine "sub-Nyquist-rate sampling" with large-scale optimization for efficient and accurate signal acquisition when the signal has a sparse structure. They developed theory and principles that integrate feature selection, signal collection, and data exploitation to provide methodologies and algorithms. These have demonstrated a superior performance that is robust to missing data and is adaptive to variations in dynamic conditions. The Rice team has applied the newly created compressive sensing framework to MRI data processing. Current MRI scans can take up to 45 minutes and would normally require patients to stay still, which in turn could be very challenging for many patients. Compressive sensing for MRI system now reduces MRI scan time to as low as 25 seconds, a significant reduction in patient scan time.

Way Ahead

Rice University has been a leader in compressive sensing theory, algorithm, and hardware development for the past 15 years and has transferred numerous technologies to DoD labs and defense/security companies.

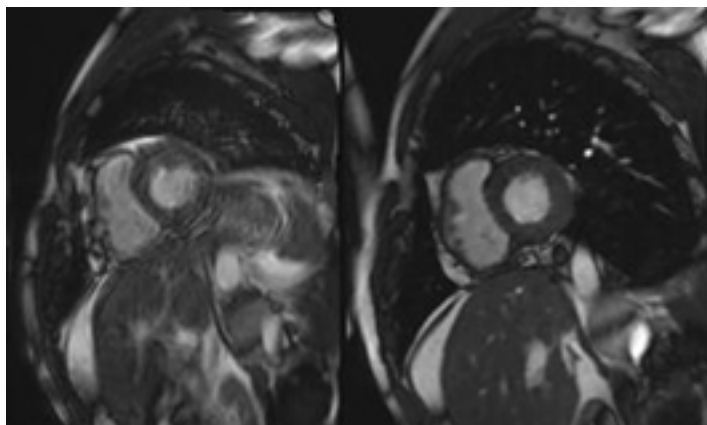


Figure 1. (Left) Conventional MRI time-lapse imaging of the beating heart must be averaged over multiple heart beats (eight in this case), which causes significant blurring and other artifacts due to patient breathing and dynamic changes in the heart. (Right) Compressive sensing MRI time-lapse imaging of the beating heart requires only a single heart beat and thus achieves high resolution in both space and time. [Images from <https://www.siemens.com/press/IM2016110154HCEN>]

A Novel Machine Learning Algorithm for Unknown Domains

Scientific Challenge

Deep learning is a very successful machine learning technology for recognizing objects in an image, a success that has been fueled by huge amounts of labeled training data. While significant efforts have been made by the research community to annotate large datasets for various machine learning tasks, it is unreasonable to expect that these datasets represent all possible variations encountered in the real world. Unfortunately, deep learning systems are known to be sensitive to such variations in data distributions. Hence, the performance of these systems drops when tested on novel data variations not seen during training. Thus, one key challenge to deep learning is how to train such learning scheme so that it can still provide correct answers when dealing with data variations or data unseen before.

Action

The ARO Information Processing and Fusion PM has been investing in novel concepts in image processing and machine learning for the past several decades. Seeing the opportunity in applying deep neural network for imaging analysis and classification, the ARO PM has focused on meeting the challenge of improving robustness and resiliency of machine learning algorithms for more accurate classification and recognition tasks in changing conditions. In 2016, the ARO PM proposed the MURI topic of building novel frameworks for characterizing semantic information content in multimodal data. The MURI project was launched in 2017 and led by Prof. Rene Vidal of Johns Hopkins University. The MURI team has been working on enhancing machine learning performance through many aspects of learning, including the approach of using multimodal data for better comprehension.

Results

To make machine learning more robust and resilient to unknown or uncertain conditions, one of the MURI team member Prof. Chellappa of U. of Maryland addressed the challenge of developing generalizable machine learning algorithms that perform effectively on unseen test conditions. As one example, one may consider the task of sentiment classification of product reviews on the “Amazon” website. Given a user review for each consumer product, the goal is to tag the review as representing “positive” or “negative” sentiment. The reviews of each product category (also called a “domain”) vary in text description, and the neural networks are sensitive to these variations. Hence, a sentiment classifier trained on the reviews of “kitchen appliances” performs poorly when tested on the reviews of “jewelry.” Also, collecting data for every domain is unreasonable as some domains have very few reviews, and new products are constantly added. Hence, developing machine learning algorithms that generalize to unseen domains is crucial.

MetaReg, a recent breakthrough developed by Prof. Chellappa and his team at the University of Maryland, addresses these issues in the context of neural networks. The MetaReg pipeline takes n source domains as inputs, each one portraying one type of variation in the input data distribution, and trains a neural network that generalizes to unseen domains. The pipeline is a two-stage approach: In the first stage, a regularization function that explicitly models the notion of “domain generalization” is trained. In the second stage, a neural network is learnt on the input data using the learnt regularization function. MetaReg was empirically validated on two machine learning tasks: (1) sentiment classification on “Amazon” reviews, and (2) object recognition on photos, art, cartoon and sketch domains were shown to improve generalization in novel

This success supports these ARL Core Technical Competencies

Computational Sciences



Network and Information Sciences



SUCCESS

The Maryland research team has successfully created a new way to perform domain generalization in deep learning. This novel approach opens doors for much more robust neural networks training that leads to improved performance with regards to an increase in classification accuracy and a reduction in misclassification rate. The powerful concept of domain generalization may lead to new generalization techniques in machine learning that can provide much better, robust and resilient learning, classification, and cognition.

RESULTS

- ▶ High-Impact keynote speech at 2018 British Machine Vision Conference and keynote speech at 2019 Conference on Computer Vision and Pattern Recognition.
 - ▶ Created a novel way of learning to recognize new entities without knowing the entities too well.
 - ▶ The new learning regime enables the establishment of perception in unknown environments.
-

This success supports these ARL Core Technical Competencies



Computational Sciences



Network and Information Sciences

SUCCESS

Collaboration between ARL and academic researchers created a highly effective detection algorithm based on machine learning of software usage patterns that can detect highly sophisticated Android Banking Trojans that use deception to steal user credentials to compromise mobile systems and are quite often missed by regular virus scanners due to its stealth nature.

test domains. This new paradigm opens doors to a wide range of algorithms for training neural networks with improved performance and may lead to new generalization techniques in machine learning that can provide much better, robust and resilient learning and cognition.

Way Ahead

The Army impact of this research is the use of this new machine learning technique in potentially helping the Army to build future AI/ML systems that can cope with unexpected battlefield conditions due to situation change or to unseen/unknown events. The ARO PM will introduce the research results to key CCDC ARL in house researchers and establish collaborative research going forward.

INFORMATION ASSURANCE PROGRAM



Dr. Cliff Wang

Program Manager, Information Assurance
Division Chief, Computing Sciences
ARO Information Sciences Directorate

Dr. Wang received his BS degree in Electrical Engineering in 1987, and MS degree in Biomedical Engineering in 1992, and his PhD in Computer Engineering in 1995 at North Carolina State University.

He came to ARO in 2003 as the Manager for the Information Assurance Program and was promoted to Chief, Computing Sciences Division in 2007.

Machine Learning Algorithm Discovers New Android Malware

Scientific Challenge

Although malware detection tools have been developed for many years, they are mostly reactive in nature, meaning they are only effective against known malware. The real danger lies in the fact that these malware detection tools are not effective in stopping unknown malwares. The key challenge is we need to build comprehensive software behavior models that can not only identify known malicious acts but also reliably classify benign usage patterns in order to detect future malware. But this is not an easy task since every device/gadget has different hardware/software, of different versions, and with different configuration, causing a significant challenge in both data dimension and scale. A good model for capture key characteristics and usage behavior that can share across different systems with different settings are the key to successfully identify malware.

Action

The ARO PM of Information Assurance, Dr. Wang, engaged with academic communities to address the challenges in zero-day malware defense for mobile platforms. He foresees the opportunity of using machine learning techniques to build software usage and system behavior patterns for cyber defense and has been working with several PIs to advance the state in malware detection and mitigation. Several single investigator grants were awarded in this space and concurrently a Small Business Technology Transfer (STTR) project has been launched to transfer research results from university research into prototypes for field testing.

Results

Prof. V.S. Subrahmanian and his collaborators at Dartmouth College developed algorithms for the prediction of Android Banking Trojans (or ABTs). ABTs are malware that use deception to steal banking credentials from a user and then use those stolen credentials to access and siphon off money from the victims' bank accounts. The team developed several new innovations: first, they proposed the notion of a package call graph based on static analysis of Android APKs. Second, they proposed the highly novel concept of a triadic suspicion graph or TSG which choose randomly sampled ABTs and goodware and builds a graph consisting of three kinds of nodes: ABTs, goodware, and package calls.

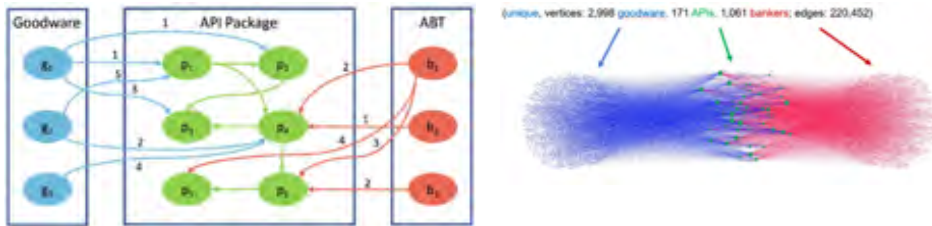


Figure 1. Algorithms for the prediction of Android Banking Trojans. A small sample is shown below on the left, and a visualization of the entire goodware vs. malware dataset is shown on the right.

Third, they developed families of suspicion ranks and suspicion scores to attack package calls and developed novel ways of harmonizing minor differences in these scores. They defined a set of features based on these new ideas and used traditional machine learning models to predict whether a piece of code was goodware or malware. They were able to discover a new code sample that was not labeled as malware by any of the 63 anti-virus engines on VirusTotal, a site that most major anti-virus members use to share samples and to share results. Google's anti-virus team confirmed the correctness of the algorithm's discovery. The predictive accuracy (measured by the well-known Area under ROC curve metric) of the new algorithm in distinguishing ABTs from goodware is over 99% with a false positive rate of just 0.3%. The algorithm is also capable of distinguishing ABTs from other forms of malware – in this case, the accuracy is over 95% with a false positive rate of 2.7%.

Way Ahead

The Army impact of this research will potentially help Army to build resilient mobile devices that will be critical components of future battlefields applications. The initial research results will be shared with key CCDC ARL researchers to foster collaborative research.

DeepRadio: Deep Learning for Wireless Communications and Security

Scientific Challenge:

Although brute force jamming attacks have been known for a long time, the new crop of stealthy wireless attacks such as carrier-sensing attacks, signal emulation, and radio interference are posing more severe challenges. These new types of attacks could be as effective as brute force jamming. But with a much smaller footprint, they can be easily blended in without being detected. Low signal to noise ratio (SNR) of these attacks and the fast, transient nature (as short as micro-second or below) makes it extremely hard for the defenders to detect and defend. The net consequence of undetected stealthy

RESULTS

- ▶ New AI/ML based malware detection system that provides 99% detection accuracy.
- ▶ The new detection algorithm is highly successful in finding stealth malwares that are often missed by commercial malware scanners.
- ▶ First highly accurate tool that can automatically check whether an Android Application Package contains banking Trojan virus or not.

This success supports these ARL Core Technical Competencies

Computational Sciences



Network and Information Sciences



Protection Sciences



SUCCESS

The IAI team working with its academic partner in a close collaboration with CERDEC has successfully created an AI/ML learning-based radio wave analysis and classification algorithm that can be used to learn and build radio wave models so that both normal and irregular transmission patterns can be easily identified. The algorithm has been implemented into tactical radios and been successfully field tested.

RESULTS

- ▶ New AI enabled radio wave learning, analysis and classification algorithms.
 - ▶ Successful commercialization by the creation of a prototype on tactical radios called DeepRadio .
 - ▶ DeepRadio field tested in 2018 U.S. Army CyberBliz exercise at Ft. Dix, demonstrating over 85% accuracy in predicting the onset of jamming.
 - ▶ Potential licensing opportunity of the technology to major defense vendors.
 - ▶ Active R&D partnership with U.S. Army CERDEC (Now CCDC C5ISR) on developing resilient and trusted Soldier battlefield communication systems.
-

attacks is that our wireless systems are seemingly working fine from network setup and operation perspective, but users/systems experience delays and information loss, leading to degraded mission execution capability.

Action:

Since 2013, ARO has been investing in basic research on how to make wireless communication more robust and resilient against new generations of stealthy attacks. Unlike broadband jamming types of attacks, this new crop of “smart” attacks leaves small, but fast changing foot prints, making traditional attack detection methods less useful. Dr. Wang discussed the challenges with lead researchers who suggested using AI/ML to identify these attacks. He started a new STTR project that aims to create new detection methods based on dynamic radio wave profiling through machine learning. The Phase II project was awarded to IAI Inc. in 2017.

Results

To counter the threat from the new generation of stealthy attacks, Intelligent Automation, Inc. (IAI) developed the DeepRadio technology to provide reconfigurable embedded implementation of deep neural networks as a stand-alone radio platform for characterizing the RF spectrum environment in real time and adapting to spectrum dynamics. DeepRadio uses deep learning to detect and classify RF signals (tactical and commercial waveforms as well as cognitive jammers),

identify spectrum opportunities, and reconfigure the software-define radio (SDR) transceiver. Each DeepRadio device is an integrated unit consisting of a SDR front-end, an embedded processor, and a field-programmable gate array (FPGA). Deep neural network architecture is reconfigurable and supports adaptation to spectrum dynamics, including topology, channel, interference, and traffic effects. The outcome is real-time and accurate characterization of the RF spectrum, spectrum efficiency improvement, and support signal co-existence on busy spectrum bands. Ft. Dix field test of DeepRadio with tactical and commercial radios demonstrated the effectiveness of DeepRadio in detecting RF interfering sources and mitigating their effects on wireless communications. In the field test, DeepRadio successfully learned the behavior of a dynamic jammer (that does not transmit continuously and is hard to detect) using a deep neural network model. Consequently, DeepRadio predicted with high accuracy (>85%) when the jammer intends to jam the spectrum. Using this information, DeepRadio suspends traffic flow transmission until it predicts the spectrum is reliable, reducing packet loss rate over jammed channels and boosting reliability of tactical communications.

Way Ahead

US Army CERDEC has been a key technology collaboration partner and transition partner. CERDEC researchers and engineers are adopting DeepRadio technology in its own R&D efforts. With the full support of ARL senior leadership, ARL key stakeholders are engaged with IAI to explore further collaborations.

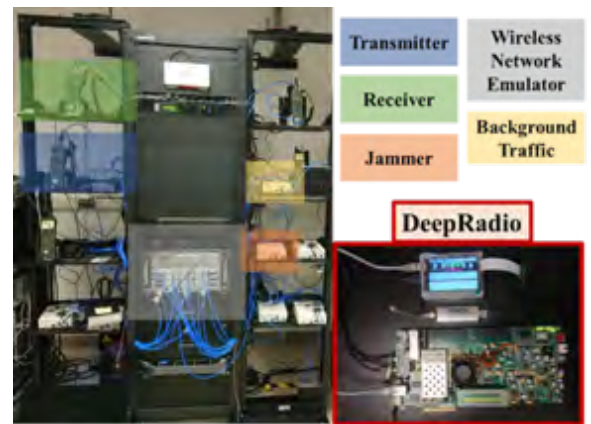


Figure 1. Deep radio to provide protection against silent jammer.

MATHEMATICAL SCIENCES DIVISION: FY18 SUCCESS STORIES

COMPUTATIONAL MATHEMATICS PROGRAM



Dr. Joseph Myers

Program Manager, Computational Mathematics
Program Manager (Acting), Modeling of Complex Systems
Division Chief, Mathematical Sciences
Information Sciences Directorate

Dr. Myers has served as a logistician from platoon to brigade combat team level, has served as a Combat Developments Officer, and served on the Mathematics faculty at West Point. He holds a doctorate in Applied Mathematics from Harvard, four Master's degrees from various academic institutions, including the Industrial College of the Armed Forces, and a PE license from Indiana.

After retirement from active duty, he joined ARO in 2008.

Reliable Simulation of the Complex Physics of Internal Multiphase Processes

Scientific Challenge

The physics of gun (viz., howitzer) tube performance and wear is a longstanding area of interest to both the artillerists who wear and break them and to the Ordnance Corps maintainers who strive to keep them online. Computational modeling is key to the successful design of future robust advanced armament systems, yet remains difficult due to the complexities in modeling multiphase reacting processes, incomplete combustion, grain dynamics, thermal expansion and tube wear, balloting, lining/relining, muzzle break design, rust, and others.

Action

In early 2014, Dr. Myers began a conversation with Dr. Laurie Florio (ARDEC Picatinny Arsenal) on the computational challenges involved in the reliable simulation of the complex physics associated with multiphase processes in armaments. He had been impressed with the performance of a computational group at RPI led by Mark Shephard in a previous investigation in multiscale energetic modeling and thought that some of their capabilities and insights might be pertinent, he helped start discussions between RPI and ARDEC, and soon received a related proposal from RPI on the reliable simulation of the complex physics associated with multiphase processes of combusting internal flows, such as occur in gun tubes, that he was happy to be able to support. This resulted in a five-year \$1M Single Investigator (actually double the size of a Single Investigator grant and longer in term, with two principal researchers in computational physics and in numerical analysis), and enhanced with a \$200K DURIP award for additional computational capability. Based on successes in the first few years, Dr. Myers coauthored with ARDEC (Laurie Florio again) STTR Phase 1 and Phase 2 topics to develop and market computational tools pertinent to these types of computational models; these were performed by a joint team led by Simmetrix Inc. and partnered with RPI.

This success supports these ARL Core Technical Competencies

Ballistics Sciences



Materials and Manufacturing Sciences



SUCCESS

Academia and small business have teamed to develop modern mathematical methods for the multiphase/multiscale modeling of internal gun tube processes, resulting in new predictive and design capabilities that are now being marketed in engineering design tools available to the defense industry, and that will enable high fidelity design in Army applications including howitzer design, but also related areas such as parachute design.

RESULTS

- ▶ 30 peer-reviewed publications
 - ▶ Benet Labs (ARDEC) employee earned Ph.D. with part of this topic as his thesis and helped transition code to Benet
 - ▶ Beginning transitions to AMRDEC CREATE rotocraft modeling program, and to ERDC flood management code for evolving geometry components
-

Result

This project is addressing the above challenges through the development of: (a) consistent models for mass, momentum, and energy flux across phase boundaries; (b) a sequential atomistic-to-continuum multiscale strategy for modeling three-phase problems; and (c) efficient modeling strategies in the stochastic space based on compressive sampling and adaptive sampling approaches, and (d) adaptive control of models, meshes and scales. The methods being developed are being used to address the significant multiphase issues involved in phase changes driven by chemistry and three interacting phases (solid, liquid and gas), with evolving grain and metallic contact boundaries. This work adds new capability for modeling propellant burn in small arms, modeling the motion of a projectile through a barrel, and modeling the molten phase of copper along internal surfaces during firing. The issues addressed are chosen and addressed as most relevant to the issues seen in Army applications through discussions and feedback with scientists at ARDEC and Benet Labs. These developments are being implemented through new algorithms that take full advantage of massively parallel computers and are being made widely available through the Army STTR program.

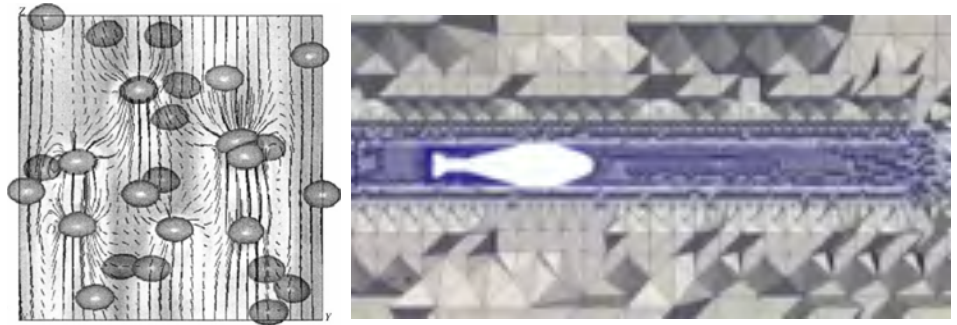


Figure 1. Modeling spans scales from grain boundary to projectile.

Way Ahead

The research team and small business are meeting periodically with ARDEC scientists, principally from Benet Labs, on use cases and parameter ranges of particular interest to future design. CREATE developers at AMRDEC are aware of the new capabilities and are interested in the new adaptive meshing capabilities. The new geometry and meshing capabilities are being integrated into marketed Simmetrix components, making them available to DoD and industrial users of CAE and to research simulation tools that employ Simmetrix geometry and meshing packages, now used by 30+ software vendors, labs and universities with on the order of 20,000 seats of users in industry, DoD, DoE, and universities. These will enable defined transition path activities for Precision fire simulations with U.S. Army ARDEC RDAR-DSM & WSB and Vertical lift simulations with ARL-VTD and Sikorsky.

Multiscale Mathematical Modeling for the Design Realization of Novel 2D Functional Materials

Scientific Challenge

The Mathematical Sciences Division sees one of its roles as identifying difficulties in other disciplines that may be made more tractable if we better-understood some of the related fundamental mathematical concepts, especially within the context of the application area. In the years leading up to 2012, we were seeing a lot of efforts in Material Science doing multiscale modeling with homogenization approaches,

This success supports these ARL Core Technical Competencies



Materials and
Manufacturing Sciences

using specialized fine scale models with local environmental/material parameters to successively populate the parameters of higher scale models. In commonly-used weakly linked multiscale models, a macroscale exerts at most a homogeneous influence on a greatly separated finer scale and lacks constitutive properties, which are supplied by reaching down to the smaller scale to compute, average, and report back. Such weak multiscale dilutes or eliminates nonlinearities and the resulting models misrepresent the observed macroscale behavior. Variabilities in microfunctional parameters not only generate uncertainty within a scale, but also propagate uncertainties between scales, both up and down, resulting in a potentially significant spread in macroscopic properties. In 2D heterostructures, the incommensurability makes it impossible to apply the standard tools of solid state physics, which are based on perfect crystalline order (involving reciprocal space, Brillouin zones, band structure, Fourier transform, etc.).

Action

In response, we teamed with the Material Division with its deep interests in 2-D materials and proposed a MURI topic that went very counter to the above approaches, seeking a strongly-coupled multiscale approach for 2-D materials that developed rigorous mathematical models at a variety of scales and geometries that would preserve high fidelity and enable for the first time true predictive capability that could be used to explain known phenomena and predict and engineer designer properties to enable new applications. This joint focus resulted in a novel and successful MURI effort between universities of Minnesota, Harvard, and Delaware to collaboratively develop theory, computation, and experiment for 2D van der Waals heterostructures. More general and powerful methods have been made possible by the team's development construction of a library of tight-binding Hamiltonians for graphene, molybdenum disulfide, etc. that for the first time includes strain terms and accurate interlayer interactions. These new Hamiltonians have been utilized within their novel configuration-based approach to compute electronic structure and transport in incommensurate 2D heterostructures. The new approach parametrizes the degrees of freedom by the compact local configuration space rather than real space, bypassing the need for the standard supercell approximation and making possible the investigation of true incommensurate structures. The team's modeling and computational methods can accurately account for strain, buckling, electromagnetic fields, vacancies, and twisting in incommensurate 2D heterostructures of sizes up to 100s of nm (millions of atoms). They now have a number of methods now available for computing density of states, conductivity, and selective optical activity. Depending on the system size and periodicity, they are able to choose the best tool for the job.

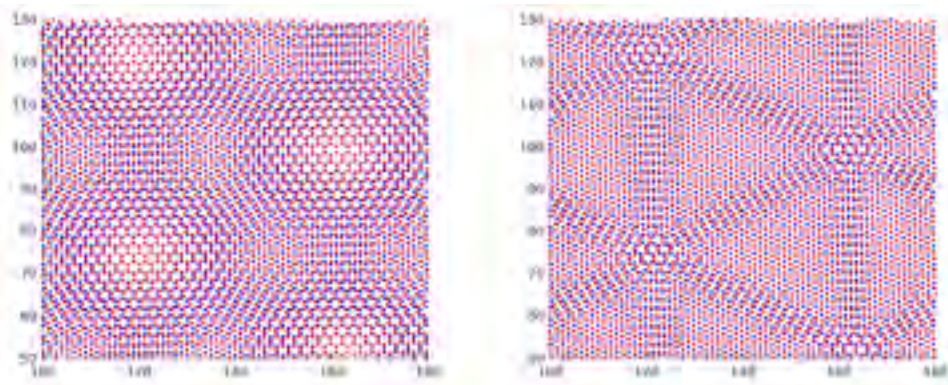


Figure 1. Relaxed vs unrelaxed states of 2D material

SUCCESS

PMs from Mathematics and Material Science have teamed to develop modern mathematical methods for the modeling of 2D materials, resulting in new predictive capabilities that are now being used to investigate new superconductive phenomena, and that will enable the design of novel Army capabilities in energy generation, storage, and transmission.

RESULTS

- ▶ First high fidelity twistrionic models for 2D functional materials
 - ▶ 85 peer-reviewed publications
 - ▶ 11 papers in Science/Nature, 2017-18
 - ▶ Two Postdocs placed in DoE labs.
 - ▶ Will be used to design QIS materials in the DoE QPress program
-

Result

The team's new theory, fast numerical methods, and codes for the electronic structure, transport, mechanical relaxation, and diffraction of incommensurate 2D heterostructures are now capable of exploring previously inaccessible physical regimes (e.g., small twist angle, low temperature). Some of the key results include determining the density of states of 2D material stacks with different twist angles, and the effects of external stimuli on the transport properties of these 2D heterostructures. This is now helping explain unique hydrodynamic and 'twistrionic' behaviors that have been recently observed in these heterostructures, providing a new foundation for ultra-low power, terahertz applications of semiconductor devices.

Way Ahead

These theoretical and computational methods are now enabling experimental investigations of controlled doping by lithium intercalation and atomic reconstruction at van der Waals interfaces between 2D materials. Fortuitously, very recent experimental results at MIT have demonstrated superconductivity in 2D materials, setting off intense interest within the community. As a result of our foresight in jointly developing this topic five years ago, our supported team is now the only team in the world with the computational tools to model, explain, predict, and help engineer within these materials and the MIT team has brought them in as partners to help them do this. Some of the team's mathematicians have been selected for support under the DoE QPress program, to automatically catalog, retrieve, and assemble bits of 2D materials to build optimal 2D layered structures for QIS applications such as computing, encryption, sensing, and communications.

COMPUTATIONAL MATHEMATICS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Develop the mathematics for models and computational methods for common themes in anomalous physics: anomalous transport, exponentially accelerated fronts, non-Markovian behavior and long-range interactions, self-similarity and scaling, singular behavior, interfaces, and finite-domain decorrelation effects that if successful is anticipated to lead to more efficient/longer-lived turbine/rotor and related systems.
- ▶ Create models and computational methods for material-related issues in layered and 2D geometries, energetic crystals, and porous media that if successful is anticipated to enable post-silicon electronics for new sensing/processing capabilities.

MODELING OF COMPLEX SYSTEMS PROGRAM



Dr. Joseph Myers

Program Manager, Computational Mathematics
Program Manager (Acting), Modeling of Complex Systems
Division Chief, Mathematical Sciences
Information Sciences Directorate

Dr. Myers has served as a logistician from platoon to brigade combat team level, has served as a Combat Developments Officer, and served on the Mathematics faculty at West Point. He holds a doctorate in Applied Mathematics from Harvard, four Master's degrees from various academic institutions, including the Industrial College of the Armed Forces, and a PE license from Indiana.

After retirement from active duty, he joined ARO in 2008.

Inferring Social and Psychological Meaning in Social Media

Scientific Challenge

The rapid ascent and adoption of social media as the dominant form of communication has led to significant analysis challenges. In particular, there is a gap in theoretically informed methods to analyze data mined and collected from social media. One primary cause of this gap is the lack of fusing structural sources of information (e.g., social network topology) with non-structural sources (message content, demographics). As a result, significant social patterns and meaning that should be detected often are not.

Action

In 2012, ARO initiated a sequence of projects under the STTR program to address this apparent opportunity, and selected a team led by Securboratorion Inc. and including Dr. Carlos Guestrin from Carnegie Mellon University and Mr. Thomas Morello from a leading commercial marketing company to address this gap. The overall objective is to develop analytical tools that improve the theoretical relevance, meaning, reliability and validity of data mined and extracted from social media sources. To this end, the team has developed methods for ingesting social media data streams, reducing noise within those streams, performing topological characterization, including motif discovery, performing content analysis and meaning inference, performing linkage discovery that spans entities and motifs, and promoting the resulting Social Understanding and Reasoning Framework -- SURF -- for rapid commercial and Army transition. SURF provides improved algorithms and tools for mining social media that spans domains from marketing to military intelligence. Motif detection is generally structural, based on graph theory algorithms (e.g., Edge Sampling Algorithm- ESA, Randomized Enumeration) to identify network motifs, or recurring significant patterns or sub-graphs of interconnections within a large network, and then complements with non-structural exploration such as the semantic content analysis, demographic classification, and meme tracking to provide motifs that are based not only on structure, but also content and demographics.

Result

The work (culminating in the marketed package "SURF": Social-media Understanding and Reasoning Framework) is a service-based suite of analytical tools that uses proprietary algorithms based on the above on structured and non-structured social media information to identify significant topologies, motifs, embedded online

This success supports these ARL Core Technical Competencies

Human Sciences



Network and Information Sciences



SUCCESS

Small business and academia have partnered to develop an intelligence tool that is agnostic to language and content, resulting in a state-of-the-art advancement over current content-based social media scanning algorithms and which is now providing significant increases in accuracy and decreases in time and effort required by intelligence gatherers.

RESULTS

- ▶ Tests on worldwide data yields impressive performance vs trained analysts (e.g., 0.8 F-measure, where F-measure is harmonic mean of precision and recall).
- ▶ Demonstrations and installations at Ft Bragg 1st SOCOM, Army G2-OSINT, DIA, others.
- ▶ Currently used by Joint Inter Agency Task Force South (JIATF-S Truman Annex in Key West, FL) to assist in drug interdiction. Other similar deployments are ongoing.



Figure 1. SURF Concept of Operations

communities, and individual characteristics. SURF leverages social media research on reciprocity, degrees of separation, and quantitative comparisons; and extends it based on noise reduction and link analysis research performed by Dr. Guestrin and on semantic content analysis techniques pioneered by Securborator. As one example, demonstrations to USASOC at Ft Bragg has led to referrals to the the Army G2 OSINT Directorate and DIA, leading to their participation in ongoing operational tests by USASOC and their plans to arrange for complementary deployment with other threat scanning and analysis tools.

Way Ahead

The small business will expand its marketing of this new technology to Army and defense intelligence communities for use in dark web applications, similar to the current successes described above.

Network-based Hard-Soft Fusion

Scientific Challenge

Prior to 2009, networks almost universally meant signal networks, while analysis to combine signal data with human-based data was practically nonexistent. The paradigm was that SIGINT would capture, process, and optimally present signal data, human analysts would collect and analyze HUMINT, and then human analysts would merge the two through judgment, experience, and understanding of mission priorities.

Action

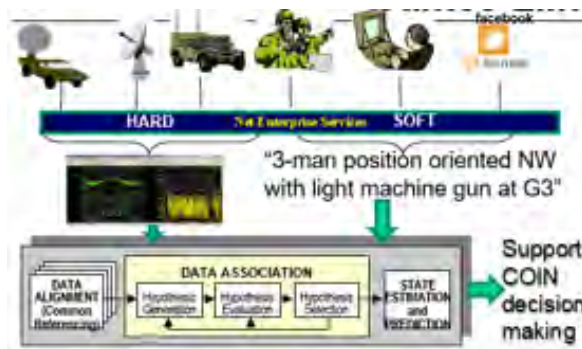
In 2009, the ARO PM recognized the need to not just combine information from physics-based sensors ("hard data") with information from human sources ("soft data") in order to achieve a more complete situational picture, but to do this in such a way as to adapt the analysis to the distributed communication/sensor structure prevalent in operations. This focus on fitting the synthesis to the network structures (both communications and human) marked this effort as unique among the few but growing number of efforts being contemplated for hard/soft fusion, and held promise for enhancing situational awareness in Army operations, especially in asymmetric operations. This was selected

This success supports these ARL Core Technical Competencies



Network and Information Sciences

as a MURI topic and awarded to a research team from the University of Illinois at Urbana-Champaign, University at Buffalo, Penn State University, Tennessee State University, and Iona College. The team made significant advances in new graph association methods for fusing information from different modalities, such as text, video, and acoustics. The team is investigating the problem of merging many graphs that collectively describe a set of possibly repeated entities and relationships into a single graph that contains unique entities and relationships, is working on combining “highly orthogonal” hard and soft information, and is developing a relaxation approach that quickly iterates to a near-optimal synthesis of the data. Other related advances include reduced order Natural Language Processing methods for SITREP-structured data, methods for removing bias from human observations, and low-dimensional bases for video and acoustic information that fit well with graph association methods. The team has implemented these fundamental advances into software that can help support commanders’ Priority Intelligence Requirements (PIRs).



Result

The team has developed a “Synthetic Counter-Insurgency” (SYNCOIN) data set for testing and evaluation of hard/soft fusion algorithms along with newly developed software for text processing that is robust against the ambiguities of natural language. It has transitioned this to the ARL/CISD Tactical Information Fusion Branch for further research in the area of hard/soft information fusion, and has also transitioned the work to CERDEC-I2WD’s A2SF program. Recently, ARL and DIA initiated a collaboration that will leverage these developments from ARO-funded academic institutions to drive new capabilities in artificial intelligence and machine learning. The collaboration has developed systems to identify, extract, and analyze data from multiple sources, such as human observers and physics-based sensors. This advance may be combined with artificial intelligence and human-machine collaborative decision making to provide the warfighter with enhanced situational awareness to rapidly apply new capabilities against an adversary’s specific vulnerabilities.

Way Ahead

The ARO and DIA collaboration will develop situational understanding and support analytics from multiple data sources within DoD that, if successful, will help to address DoD’s 3rd Offset for integrating autonomous learning systems, human-machine collaborative decision making, assisted human operations, and machine-to-machine information flows.

SUCCESS

Researchers from University of Illinois, University of Buffalo, and others have developed a fused situational understanding system for understanding the world sensed by both human observers (soft) and physics-based sensors (hard), generating concepts used by both ERDC for autonomous systems and DIA for intelligence uses, and with the potential to help enable the next generation of autonomous systems.

RESULTS

- ▶ 145 peer-reviewed publications
- ▶ Datasets now used by DIA
- ▶ System being explored by ERDC for use on autonomous engineer vehicles.

MODELING OF COMPLEX SYSTEMS PROGRAM –CURRENT SCIENTIFIC OBJECTIVES

- ▶ Design geometric and topological data modeling techniques for both coarse, sparse data and large, noisy data that are amenable to tractable computation, efficient and robust feature extraction, and practical statistical analysis.
- ▶ Exploit deeper topological frameworks (e.g., homological, categorical) and geometric modeling techniques to develop accurate, explanatory, and/or causal mathematical models of social group structure and dynamics.

PROBABILITY AND STATISTICS PROGRAM



Dr. Michael Lavine

Program Manager, Probability and Statistics
Mathematical Sciences Division
ARO Information Science Directorate

Dr. Lavine completed his undergraduate degree in Mathematics at Beloit College in 1974, his MS in Mathematics at Dartmouth College in 1977, and his PhD in Statistics at the University of Minnesota in 1987. Highlights of his 30-year academic career include 20 years as a faculty member at Duke University, 10 years as a faculty member at University of Massachusetts, Department Head of Mathematics and Statistics at UMass, and Fellow of the American Statistical Association.

Dr. Lavine joined ARO in 2018 as Program Manager for Probability and Statistics.

Modeling Rare Events: Multivariate Heavy Tail Phenomena

Scientific Challenge

How high should we build a dyke to ensure, say, a 99% chance of protecting the land behind it from flooding over the next 50 years? How strong should we make ceramic armor to ensure, say, a 99.99% chance of withstanding a burst of automatic weapons fire? Such questions lie at the heart of extreme value theory and heavy tailed phenomena. Most observations of high water or automatic weapons fire are less extreme than those we are trying to protect against. The scientific challenge is to use the common but less extreme events to help predict the size of extreme events.

The mathematical study of such questions is a delicate blend of probability and statistics. Figure 1 shows a hypothetical sample of 10 flood measurements that illustrates some of the issues. The 10 tick marks at the bottom of the figure represent the sample and the two curves represent two possible probability models for them: the Normal, in black, and the Cauchy, in red. Both probability models represent the data reasonably well and it seems not to matter very much which model we use. However, as Figure 2 shows, the two models make very different forecasts of extreme flooding. The Normal model says 99% of floods will be below 2.3 units high (in the adjusted scale of Figure 1) while the Cauchy model says 99% of floods will be below 31.8 units high (read the percentile on the x-axis and the size of flood on the y-axis of Figure 2). In the language of probability and statistics we say the Cauchy model has heavy tails while the Normal model does not. We would build the dyke to very different heights depending on whether we think extreme floods are better described by the Normal, the Cauchy, or some other probability model.

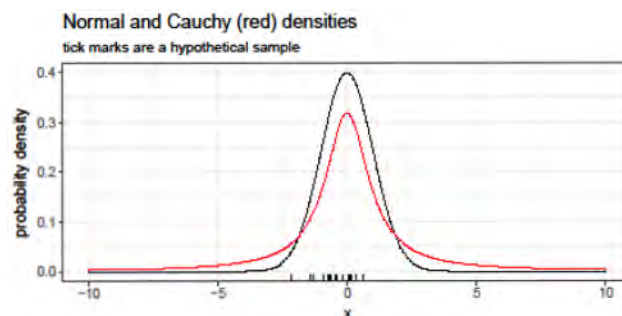


Figure 1. 10 hypothetical measurements of flood height. Tick marks: the hypothetical sample, adjusted to be centered at 0 and have standard deviation of 1. Black curve: the standard Normal density. Red curve: the standard Cauchy density.

This success supports these ARL Core Technical Competencies



Network and Information Sciences



Computational Sciences

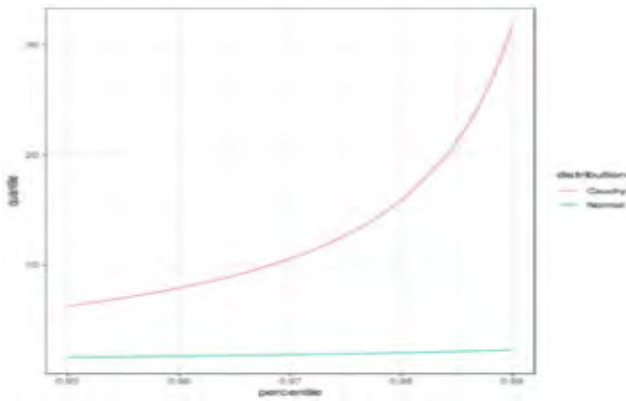


Figure 2. Upper percentiles of the Normal and Cauchy distributions.

In real-world applications, we often have to model several phenomena together, such as wind speed, rain fall, flood height, and temperature. Models for several phenomena together are called multivariate. ARO's aim in funding research on multivariate heavy tailed models was to develop reliable diagnostic, inferential, and model validation tools for heavy tailed multivariate data; to generate new classes of multivariate heavy tailed models that highlight the implications of dependence and tail weight; and to apply these statistical and mathematical developments to the key application areas of network design and control, social network analysis, and signal processing.

Action

In 2012, ARO Program Managers recognized the lack of and need for multivariate Extreme Value theory, and so proposed a multidisciplinary effort in this area because "virtually all known results about heavy-tailed distributions are for univariate distributions. While there have been attempts to define and characterize multivariate heavy-tailed distributions, basic forms and principles are still poorly known. This research seeks to create basic knowledge about multivariate heavy-tailed distributions and to discover how to use that knowledge to create system models."

Result

The resulting research efforts have generated useful results in a number of Army-relevant areas of application:

- ▶ Communication networks can be dominated by a small number of very large files or messages. Therefore, communication times depend on extreme values.
- ▶ Social networks can be heavily influenced by a small number of users who have many more social ties than the typical user. Therefore, social influence can depend on extreme values of social connectivity.
- ▶ The value of compressive sampling can depend on the extreme values of the quantity being sampled.
- ▶ The performance of a networked computer system can depend on how long the biggest jobs take to run. Therefore, the possibility of extremely long jobs should be taken into account when scheduling jobs on computer networks.

This advance is also applicable to civilian applications, including models for financial time series and urban transit systems.

SUCCESS

The topic resulted in award of the grant Multivariate Heavy Tail Phenomena: Modeling and Diagnostics by Sidney Resnick of Cornell University. The grant is a collaboration among mathematicians, statisticians, computer scientists, and others that would not have occurred had the PMs not recognized the need for research in multivariate extreme values and heavy tails.

The grant spurred additional research on multivariate extreme values and heavy tailed models, some of which was funded by ARO. It also led to a patent application and prompted the CCDC SC Multiple Hit (armor performance) STTR.

RESULTS

- ▶ 254 peer-reviewed publications; approximately one publication every week
 - ▶ CCDC C5ISR evaluating use of results in frequency-hopping applications
 - ▶ Inspired CCDC SC STTR to predict/design for closely-spaced bullet impacts in body armor.
-

This success supports these ARL Core Technical Competencies



Network and Information Sciences



Computational Sciences

SUCCESS

The PM's initiative resulted in joint research by Shu and Rozovsky, with the first year results establishing the solution to any linear SDE. During the second year the PIs extended their work to non-linear SDEs. Reducing an SDE to a system of non-stochastic DEs is a major step because it provides a path for constructing a solution to the SDE. Such solutions can be used in the Army-relevant applications mentioned here.

RESULTS

- ▶ Representation of the solution to any linear SDE as a special system of non-stochastic DEs

Way Ahead

Mathematical theory from this topic is now being used by the Natick Soldier Systems Center to model the performance of armor against multiple hits. The Multiple Hit STTR is now in Phase II, so the way ahead includes introducing more mathematical extreme value theory into the STTR and bringing those problems to the attention of mathematicians for further research.

Deterministic Approach to Solving Stochastic Partial Differential Equations

Scientific Challenge

A differential equation (DE) is a mathematical model for a real-world physical system that describes how the system changes in response to its current state. For example, if one part of an object is hot and another is cold, the rate at which heat flows from the hot part to the cold part is described by a DE. Many physical systems are well described by DEs but others are too complex or beyond our current state of knowledge. Some such systems can be described by adding a stochastic term to the DE, creating a Stochastic Differential Equation (SDE). Early SDEs included simple stochastic terms, typically following Gaussian or Poisson probability laws. But simple stochastic terms are insufficient for describing some physical phenomena so scientists need SDEs with other types of stochastic terms.

A solution to a DE is an evolutionary path of all the variables the DE describes. Some DEs have closed-form solutions, but many do not. For those that do not, it is necessary to approximate the solutions via computer algorithms. Finding solutions to SDEs is more difficult than finding solutions to deterministic DEs, and finding solutions to SDEs with complex probability laws is even more difficult. The scientific challenge is to improve our ability to find solutions to complex SDEs.

Action

In 2015, the ARO Program Manager recognized that further progress in the area would likely require collaboration between experts in SDE solutions and experts in devising SDEs for specific physical problems and identified and contacted the current PIs and began discussions about the parameters of a possible new joint research project.

Result

The SDEs solved by this research have wide ranging applications including the following that are Army relevant:

- ▶ Modeling weather at a fine scale across a battlefield, accounting for local conditions such as mountains and lakes;
- ▶ Modeling how stress and cracks propagate through a piece of armor hit by a projectile;
- ▶ Modeling how air flows around a helicopter rotor;
- ▶ Modeling how electrical signals travel through the brain of a soldier under stress; and
- ▶ Modeling how an infectious disease spreads through soldiers in a compound.

Way Ahead

ARO will continue to support research in efficient methods for SDEs. We plan to investigate stochastic hybrid systems that have important applications in synthetic biology; this will have Army-pertinent applications not just in synthetic biology but also in communication networks, network control systems, neuronal dynamics, air traffic control, projectiles subject to environment noise, and modeling of energy grids and smart buildings. We will investigate uncertainty quantification in statistical models in dynamic environments, with Army applications in the fracture of brittle materials such as ceramic body armor. Success will depend on gaining understanding of new classes of SDEs devised for specific physical problems.

PROBABILITY & STATISTICS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Develop novel and robust filtering methods and techniques.
- ▶ Develop novel and robust inference methods for data sets of extreme size (big-data, small-data) or distribution (heavy-tailed).

BIOMATHEMATICS PROGRAM



Dr. Virginia Pasour

Program Manager, Biomathematics
Mathematical Sciences Division
ARO Information Sciences Directorate

Dr. Pasour completed her M.S. in Biostatistics at UNC – Chapel Hill in 1995. She trained as an Applied Mathematician at Cornell University, receiving her Ph.D. in Applied mathematics in 2007.

She came to ARO in 2009 as the first Manager for the Biomathematics Program.

Circadian Rhythm Monitoring and Regulation

Scientific Challenge

Misadaptation to the Earth's 24-hour pattern of daylight and biological rhythms, called circadian misalignment, has potential detrimental consequences ranging from increased sleepiness and decreased attention span during the day, lower productivity, and gastrointestinal disorders, to long-term health problems such as an increased risk for cancer, diabetes, obesity, and cardiovascular disorders; some of these problems are also closely associated with PTSD. Service members are at particular risk for circadian rhythm misalignments, due in part to mission schedule, travel across time zones, and irregular sleep cycles.

Action

Upon her arrival at ARO Dr. Pasour quickly became involved in the DARPA FunBio program and steered the first follow-on program toward research aimed at gaining a clear understanding of the role and effects of time in and on human physiology and biological functions. Leveraging her involvement as the COR of the resulting DARPA Biochronicity program, she teamed with a scientist at the US Army Medical Research

This success supports these ARL Core Technical Competencies

Human Sciences



Computational Sciences



SUCCESS

IAI and RPI have developed a novel, low-cost, non-obtrusive wearable system that will increase the health, alertness, and productivity of warfighters who are disrupted by excessive, abnormal shifts in work or flights across multiple time zones or who suffer from PTSD.

RESULTS

- ▶ New Circadian Rhythm Monitoring and Regulation Device (CMR)
 - ▶ Beginning commercialization of the CMR System, selling 40 devices to NIH
 - ▶ System currently being tested for treating PTSD symptoms
-

and Materiel Command (Jason Ghannadian) to formulate an STTR extending and leveraging the literature on circadian rhythm and coupling it to the advance in wearable/embedded device technologies to develop an integrated circadian rhythm regulation device. Although the use of both light and sound to realign circadian phase were proposed and funded as Phase I projects, she found the efforts to use light to realign circadian phase undertaken by the researchers/developers at Intelligent Automation, Inc. (led by Dev Tolani), and their academic partners at the RPI Lighting Research Center (Mark Rea and Mariana Figueiro) to be the most sound scientifically and this group was funded through Phase II.

Result

The resulting Circadian Rhythm Monitoring and Regulation Device (CMR) is based on mathematical models that complemented work by a former Biomathematics Program PI (Danny Forger). Specifically, the RPI team developed a model of human circadian phototransduction that provides the ability to estimate circadian stimulus (CS) from a light source with any power spectral distribution and use CS as input to the circadian system model to quantify the effectiveness of various light sources on the circadian system. Modifications to the model of human circadian entrainment by Kronauer et al, specifically the use of CS as input to the model, facilitate customization of this model for use-cases of interest to the DoD. This is a novel, low-cost, non-obtrusive wearable system that will increase the health, alertness, and productivity of warfighters who are disrupted by excessive, abnormal shifts in work or flights across multiple time zones or who suffer from PTSD.

Field data have been collected and successfully demonstrated the ability of the model to predict phase shifting of dim light melatonin onset (DLMO) after a lighting intervention. IAI has developed the second generation of CMR sensors, based on the team's observations on the performance of the sensors. These sensors will be used in an Army-funded project (COR: Marti Jett, MRMC) for testing the efficacy of the CMR system, to improve sleep hygiene in populations with PTSD. IAI has started commercialization and transition of the CMR System, selling 40 devices to NIH. CMR sensors could also play a role in the URBAN program, (COR: Mr. Chad Haering, NSRDEC) which provides a novel way for dismounted soldiers wearing health sensors, position location devices, etc., to collect, record and analyze data streams more quickly and accurately. Moreover, the command psychologist for the 480th Intelligence, Surveillance and Reconnaissance Wing (ISRW) at Joint Base Langley-Eustis (Lt Col Alan Ogle, USAF) has expressed interest in conducting tests using the device.

Way Ahead

Building on Navy-funded studies conducted by the RPI researchers, IAI is addressing the broader issues of circadian misalignment and its effects on warfighters' cognitive readiness through investigating the integration of the circadian rhythm regulation device into Army informational systems such as ArmyFit and the Defense Health Management System Modernization (DHMSM) program and is also pursuing collaboration opportunities with DoD researchers and academic sleep scientists and researchers.

IAI also won a Phase I for another STTR that I co-authored with MRMC (POC: Marti Jett), which complements the capabilities of CMR in combating PTSD and incorporates correction of circadian rhythm disruption, gives recommendations for physical and mindfulness exercises using innovative sleep-wake and activity and arousal detection models, and uses goal-oriented, game-based interventions to enhance user engagement.

Computational Cortical Network Model

Scientific Challenge

Electrical stimulation of the brain is used for therapeutic and diagnostic clinical reasons. Previous descriptions of electric field interactions with cortical neurons have used passive excitable neural structures which exhibit no realistic underlying firing behavior. These models describe gross changes in the neuronal response but are lacking a more accurate and detailed understanding of the interaction of electrical stimulation with active and connected neurons.

Action

In the case of multiscale brain dynamics, the relationship between cellular changes at a lower scale and coordinated oscillations at a higher scale is unclear; resolving this mystery is especially needed in cases of mild TBI in which the more obvious morphological changes common to moderate and severe TBI cases is not present. ARO Biomathematics PI Stan Anderson at Johns Hopkins had developed a calibrated, biologically realistic computational model of normal and epileptic cortex using multi-compartment neuronal representations and an applied external electric field. The model Anderson and his team developed is unique and offers several advantages compared to existing models, including allowing the study of how the effects of stimulation vary across neuronal populations in various neuron types. In addition, the high density of neurons in their model, compared to densities in similar, previously studied models, permits the quantification of how electrode size affects the number of recruited neurons.

This success supports these ARL Core Technical Competencies

Human Sciences



Computational Sciences



SUCCESS

Collaboration between ARL and academic researchers for the first time established how the large-scale deficiencies in sensory processing that are found in mTBI cases can result from neuronal damage at the cellular level, facilitating diagnosis and treatment of blast-induced mTBI in Soldiers.

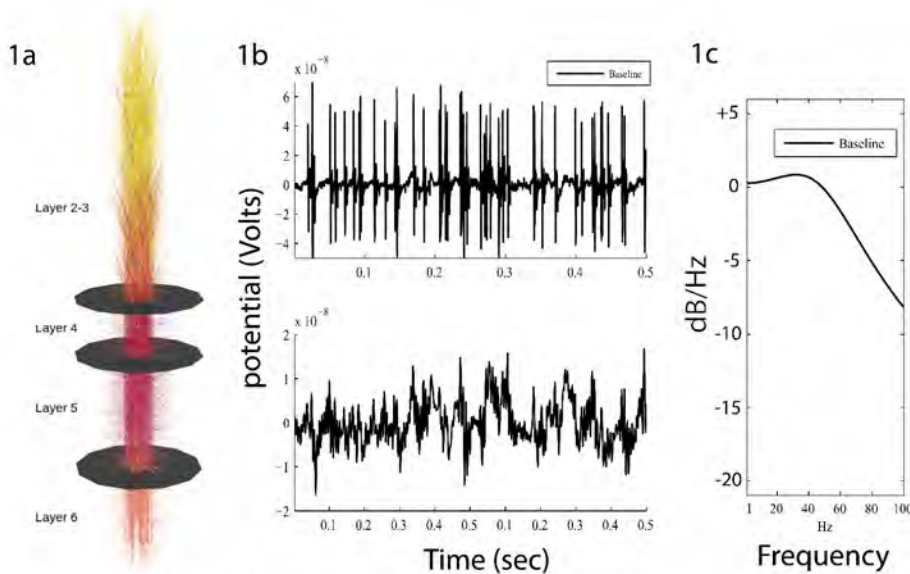


Figure 1. Overview of model and simulation output. a) Visual representation of the model, 488 showing 549 cortical neurons and layer boundaries depicted as black discs. b) Top panel shows 0.5s 489 of high-pass filtered model output for the baseline model used for detection of action potentials 490 (APs), while bottom panel plots the low-pass filtered model output simulating local field potential 491 (LFP) which resembles low frequency patterns seen in EEG. c) Parametric power spectrum estimates 492 shows power in logarithmic scale (normalized to 0 dB/Hz at -190 dB/Hz) where higher frequencies 493 have less power than lower frequencies; this result approximates $1/f$ which is similar to power 494 observed in neuroimaging methods (ECoG and EEG).

RESULTS

- ▶ 10 journal articles and 18 presentations resulting from the research
 - ▶ High-impact presentation at the Society for Neuroscience Meeting (October 2015) on identifying new robust biomarkers in ECoG/EEG that can aid in determining severity of injury
 - ▶ Computational platform that allows simulation of 9 million neurons
 - ▶ Leveraging of the cortical model through the 6.1 Cybernetics program of the Human Sciences Campaign
-

Dr. Pasour forged a collaboration between ARL and ARO Biomathematics Program PI (Stan Anderson, Johns Hopkins) to study the large-scale deficiencies in sensory processing that are found in mTBI cases.

Result

The collaboration between ARL and academic researchers resulted in the development of large-scale cortical networks, for the first time establishing how the large-scale deficiencies in sensory processing that are found in mTBI cases can result from neuronal damage at the cellular level. Performed in collaboration between ARL researchers David Boothe, Alfred Yu, Jean Vettel, and Piotr Franaszczuk and ARO funded Johns Hopkins University researchers William Anderson and Pavel Kudela, more recent research on mild traumatic brain injury published in 2017 indicates that mild traumatic brain injury due to exposure to blast could be observed as a reduction in power in the 1 to 40 Hz frequency range local field potential (see figure below). This result shows that it doesn't take very much damage to neurons to impair the brain's ability to create normal brain activity and that you can get severe impairments without being able to 'see' anything obviously amiss in the brain. These new insights about brain dynamics will facilitate diagnosis and treatment of blast-induced mTBI in Soldiers.

Figure: Overview of model and simulation output. a) Visual representation of the model, 488 showing 549 cortical neurons and layer boundaries depicted as black discs. b) Top panel shows 0.5s 489 of high-pass filtered model output for the baseline model used for detection of action potentials 490 (APs), while bottom panel plots the low-pass filtered model output simulating local field potential 491 (LFP) which resembles low frequency patterns seen in EEG. c) Parametric power spectrum estimates 492 shows power in logarithmic scale (normalized to 0 dB/Hz at -190 dB/Hz) where higher frequencies 493 have less power than lower frequencies; this result approximates 1/f which is similar to power 494 observed in neuroimaging methods (ECoG and EEG).

Way Ahead

Continuing research using Anderson's model is being conducted by a multi-disciplinary team of researchers from the Human Research & Engineering Directorate and the Computational & Information Sciences Directorate of Army Research Laboratory in the 'Timescales in Cybernetic Systems with Multiple Feedback Loops: The Role of Connectivity in Collective Dynamics and Functional Behavior' project funded through the 6.1 Cybernetics program of the Human Sciences Campaign. This work will leverage other research funded by the ARO Biomathematics Program by PI Nancy Kopell at Boston University on how neural oscillations support cognitively important neural dynamics.

BIOMATHEMATICS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Develop the mathematics and models for understanding circadian disrhythm-related illnesses, incorporating light, sleep, activity, and memory data that, if successful, is anticipated to lead to improved soldier health and performance.
- ▶ Create models and mathematical methods that take advantage of recent improvements in neurological data-gathering to bridge the gap between subjective psychological assessment and quantitative neurophysiology that if successful will facilitate diagnosis and treatment of TBI, PTSD and other Army-relevant mental disorders.

NETWORK SCIENCES DIVISION: FY18 SUCCESS STORIES

COMMUNICATIONS AND HYBRID NETWORKS PROGRAM



Dr. Derya Cansever

Program Manager, Communications and Hybrid Networks
Program Manager, Multi-Agent Network Control Program (A)
Network Sciences Division
ARO Information Sciences Directorate

Dr. Cansever completed his undergraduate studies at Bosphorus University, receiving his B.S. in Electrical Engineering in 1979. He trained as an Electrical and Computer Engineer at the University of Illinois at Urbana-Champaign, receiving his Ph.D. in Electrical and Computer Engineering in 1985.

He came to ARO in 2017 as the Manager for the Communications and Hybrid Networks Program

Interference Alignment

Scientific Challenge

Wireless spectrum is a critical and scarce commodity for the Army, as well as for the civilian sector. Therefore, maximizing the use of the available spectrum is of paramount importance. An important first step in this direction is to identify the fundamental bound on the total maximum rate that a group of users sharing the wireless medium can expect to have. In 2007, a DARPA effort unveiled a surprising result that, because of the concept of Interference Alignment, each user is simultaneously able to send at a data rate equal to half of his interference-free channel capacity to his desired receiver, even though the number of users can be arbitrarily large, thus showing that the interference channel is not fundamentally interference limited. However, this result assumes that users have exact knowledge of the channel characteristics, which is not practical. Obtaining the equivalent of Interference Alignment results under uncertain channel knowledge conditions is a very challenging task, with significant practical implications.

Action

Determining the capacity of interference networks is regarded as the holy grail of network information theory and wireless network research. Interference Alignment was invented by Professor Jafar under a DARPA grant that was managed by ARL ST Dr. Swami. In the year 2014, when Professor Syed Jafar conversed with Dr. Robert Ulman, then the Manager of the ARO Program Communications and Human Networks, with the idea of better understanding the trade-offs between these techniques and to further develop interference alignment. Dr. Ulman showed immediate interest due to his familiarity with the DARPA project. He worked with Professor Jafar to refine the concepts into a proposal and a subsequent grant. Supported by this grant, Professor Jafar obtained seminal results in Interference Alignment for realistic systems and was honored by IEEE for his contributions in this area.

In the year 2018, Dr. Cansever visited Professor Jafar for a program review of his ARO grant on Interference Alignment. During the discussions, it became apparent that the approach used in the analysis of Interference Alignment can be extended to obtain

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SUCCESS

Establishment of Generalized Degree of Freedom (GDoF) as a descriptive and flexible metric, and an illustration that many interference networks of interest have GDoF values larger than one even under channel uncertainty conditions, thus, establishing the value of Interference Alignment techniques under realistic conditions.

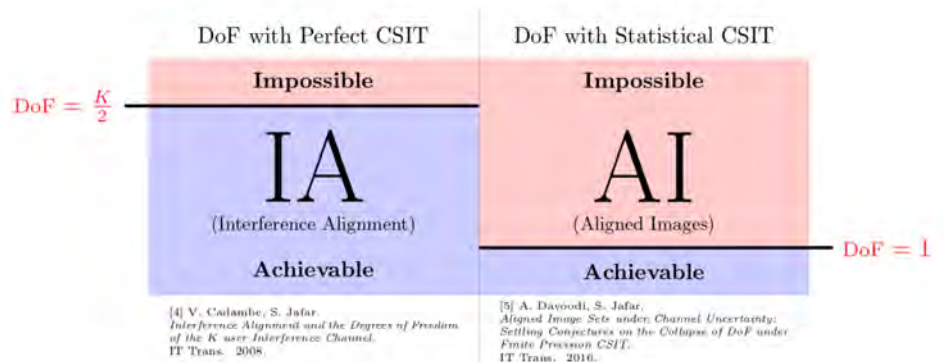
fundamental bounds on secure communications rates in the information theoretical sense. That is, security is guaranteed even against computationally unbounded adversaries, and not just asymptotically at high Signal to Noise Ratio (SNR), but at all SNR values. Dr. Cansever worked with Professor Jafar to translate these ideas into a new ARO proposal and the subsequent grant to address the next frontier of information theoretical (absolute) security in wireless communication networks.

RESULTS

- ▶ A prestigious IEEE Communications Society award made to Prof. Jafar for his foundational work in the area of Interference Alignment in wireless spectrum.

Result

Interference alignment studies have spurred much interest in the degrees of freedom (DoF) of wireless communication networks. DoF is an asymptotic value which represents a measure of the number of distinct channels available for communication in an interference network. For example, DoF for TDMA and FDM networks is one. That is, only one pair of users can communicate at a given time using the whole available spectrum. Professor Jafar and his students have shown that under idealized conditions, the DoF of K user interference channel is $K/2$, which implies that, for large K , the capacity of wireless channels can be orders of magnitude higher than what TDMA and FDM can deliver. While much progress has been made, channel uncertainty has been the biggest hurdle standing in the way of progress. This hurdle is exemplified by decade old conjectures as an open problem at the inaugural ITA workshop 2006, and subsequent conjectures by Tandon, Jafar, Shamai and Poor, on DoF being in fact equal to one, under finite precision channel knowledge, which remained unresolved for over a decade. Professor Jafar and his students produced a major breakthrough of profound significance where he settled the decade old conjecture, expressed as an ITA 2006 Open Problem, and another conjecture by Tandon, Jafar, Shamai and Poor. They characterized the DoF of broadcast networks with arbitrary number of users where the transmitter is equipped with arbitrary number of antennas, under arbitrary but symmetric levels of channel uncertainty. They showed that under these conditions, DoF will collapse to one. This is accomplished by introducing a novel "Aligned Image Sets" (AIS) approach, i.e., a combinatorial bounding of the size of the set of codewords that can be distinguished by one receiver while remaining indistinguishable at another receiver. They showed that to understand "image sets" is to understand interference in its full generality. This seemingly negative result was in fact a blessing in disguise. This result prompted a new look on DoF as a sufficiently universal metric. Professor Jafar came up with Generalized Degree of Freedom (GDoF) as a more descriptive and flexible metric, and showed that many interference networks of interest have GDoF values larger than one even under channel uncertainty conditions. This establishes the value of Interference Alignment techniques under realistic conditions.



Way Ahead

Researchers at ARL and C5ISR have received reports of this research and this work can provide guidance to the design of wireless networks in terms of their achievable capacity and assist with the performance evaluation of existing and proposed communication systems.

Army's tactical communications heavily depend on the performance of its wireless networks, which are operating in heavily congested and contested environments. This research has the potential to lead the creation of novel communication system designs that are spectrum efficient, robust and secure in most demanding use cases.

Age of Information

Challenge

For wireless networks that share time-sensitive information, it is not enough to transmit data quickly. That data also need to be fresh, in the sense that when a decision is about to be made, it must be based on the most current information. Consider the many sensors in a in a battlefield. The age of that data may vary, depending on how frequently a sensor is relaying readings. In an ideal network, these sensors should be able to transmit updates constantly, providing the freshest, most current status for every measurable feature of relevance to the mission. But there's only so much data that a wireless channel can transmit without completely overwhelming the network, especially in congested and contested spectrum environments that the Army will face in tactical operations. Then, the question is how a wireless network of constantly updating sensors can minimize the age of information that is received at the points of decision? Furthermore, how can this goal be accomplished with minimal to no coordination among the sources of data which may be dispersed over a wide area?

Action

Scheduling under deadline constraints is a challenging problem in dynamic ad-hoc wireless networks and has been the subject of one ongoing ARO grant by professors Hou and Kumar at Texas A&M University who made seminal contributions to the area. Dr. Cansever originally championed this research topic in 2014 when he was the Chief Engineer of the Communication Networks Division in Army CERDEC. The goal was to ensure the effectiveness of fire control systems where target location information will no longer be useful after a certain deadline. Dr. Robert Ulman, the Manager of the Communications and Human Networks Program in 2016 discussed this promising and important research topic with Dr. Modiano, who submitted a white paper with new insights for this problem. After some suggestions, Prof. Modiano was encouraged to submit a proposal.

Results

Professor Modiano and his students started their research by modeling a basic network, which consists of a single data receiver, such as a central control station, and multiple nodes, such as several data-transmitting drones. They posed the question: Which node should transmit data at which time, to ensure that the network receives the freshest possible data on average, from all nodes, without overloading its wireless channels. Then, they came up with a fundamental bound that indicates that one cannot possibly have a lower age of information than this value. That is, no algorithm could be better than this bound, and then they showed that their algorithm came close to that bound, so it is near-optimal. At the same time, the algorithm is simple and easy to implement in real time, so it is of practical significance.

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SUCCESS

A new theory for Age of Information in wireless networks has been established with profound impact on design of protocols to ensure timely delivery of information.

RESULTS

- ▶ 2018 ACM MobiHoc Best Paper Award for paper, "Optimizing Information Freshness in Wireless Networks under General Interference Constraints," authored by Prof. Eytan Modiano, Prof. Sertac Karaman and Mr. Rajat Talak.
-

Professor Eytan Modiano, along with his students, Igor Kadota and Abhishek Sinha, reported these results in a paper: "Optimizing Age of Information in Wireless Networks with Throughput Constraints" which received a 2018 INFOCOM Best Paper Award. IEEE INFOCOM (International Conference on Computer Communications) is the premier conference on networking, with over 1500 submissions and 300 accepted papers this year. It is a major venue for researchers to present and exchange significant and innovative contributions and ideas in the field of networking and closely related areas.

Subsequently, Professor Modiano took over the challenge to extend the above results in complex but realistic settings where source and destination nodes are placed in arbitrary networks under general interference constraints and time varying links. They considered the average age of information and the average of all the peaks of age in the network as the metrics of interest. They obtained simple scheduling policies that are optimal, or nearly optimal. When fresh information is always available for transmission, they show that a stationary scheduling policy is peak age optimal. They also prove that this policy achieves average age that is close to the optimal average age. In the case where fresh information is not always available, and packet/information generation rate has to be controlled along with scheduling links for transmission, they prove an important separation principle: the optimal scheduling policy can be designed assuming fresh information, and independently, the packet generation rate control can be done by ignoring interference. These findings pave the path for the development of practical and sophisticated network protocols and mechanisms to optimize the timely delivery of critical information in congested and contested wireless networks.

Way Ahead

Researchers at ARL and C5ISR have received reports of this research and this work can provide guidance to the Army's mission critical networks such as fire control and future Internet of Battlefield Things (IoBT) networks. This research forms a foundation for some of the ongoing work in the ARL CRA on IoBT and it was also a source of inspiration for the MURI program on the Age of Information.

Future warfare will depend on timely delivery of critical information in heavily congested and contested environments. This research has the potential to lead the creation of novel communication system designs that could provide information superiority for the Army.

COMMUNICATIONS AND HYBRID NETWORKS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Determine fundamental limits on the capacity and secrecy in shared wireless networks that if successful, will enable future technologies that will maximize the use of available spectrum in congested and contested environments while ensuring secure communications.
- ▶ Develop methods for timely gathering, delivering and processing of critical battlefield information that, if successful, will enable information superiority and situational awareness for command control.
- ▶ Achieve reliable quantum networking capabilities that if successful, will enable sensing of Army critical entities with unprecedented accuracy, and totally secure communications capabilities.



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Distributed Systems Optimization and Control

Scientific Challenge

Networks and distributed systems will play an increasingly fundamental role on the battlefield and in other operating theaters of interest to the U.S. Army, where success relies critically on integrity and availability of networked resources. Despite redundancy in numbers, protected communication, and supervised operation, studies and real-world incidents have demonstrated how capable adversaries can disrupt networked operations by observing the behavior of a few units, spoofing exchanged messages, and tampering with coordination protocols. Crucially, it is the networked coordination among the units that introduce these vulnerabilities, which have neither been analyzed nor considered in the design, implementation, and operation of networked systems. Furthermore, observing and optimizing large scale interconnected systems are challenging due to delays, actuator saturation and disturbances. The goal is to understand salient properties of distributed systems, their vulnerabilities and develop tailored control mechanisms.

Action

A previous Manager of the Multi-User Network Control Program Dr. Alfredo Garcia recognized the value of distributed control of networked systems for the Army and encouraged the development of several projects in this area. In particular, when he met with Professor Fabio Pasqualetti, he encouraged him to work on a proposal in this area, which led to a successful project on the design and operation of secure multi-agent networks. Discussions between Dr. Pasqualati and Dr. Cansever, in 2019, on networks found in human brains, and the underlying mechanisms used in their control, led to a research topic that has the potential to further inspire novel control mechanisms in networked systems.

Result

Professor Fabio Pasqualetti and his students observed that that several complex natural and man-made systems are fragile: as their size increases, arbitrarily small and localized alterations of the system parameters may trigger system-wide failures. Examples are abundant, from perturbation of the population densities leading to extinction of species in ecological networks, to structural changes in metabolic networks preventing reactions, cascading failures in power networks, and the onset of epileptic seizures following alterations of structural connectivity among populations of neurons. While fragility of these systems has long been recognized, convincing theories of why natural evolution or technological advance has failed, or avoided, to enhance

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Establishment of fundamental trade-off between controllability and robustness in interconnected systems, based on work in modeling brain networks.

RESULTS

- ▶ Best paper award at 2019 American Control Conference given to Dr. Pasqualati and his student.

robustness in complex systems are still lacking. They showed that a fundamental tradeoff exists between fragility of a complex network and its controllability degree, that is, the control energy needed to drive the network state to a desirable state. Analytical and numerical evidence indicate that easily controllable networks are fragile, suggesting that natural and man-made systems can either be resilient to parameters perturbation or efficient to adapt their state in response to external excitations and controls. This forms the basis for an important design principle that identifies a fundamental trade-off between the controllability and robustness in interconnected systems.

In an extension of this work, Dr. Pasqualetti showed that a similar trade-off exists between the robustness and degree of accuracy of complex systems, with applications in the robustness of machine learning algorithms. He identified a fundamental and previously unknown tradeoff between the accuracy of binary classification algorithms and their sensitivity to manipulated data. In particular, they casted a binary classification problem into an hypothesis testing framework, parametrized classification algorithms – including those based on machine learning techniques – using their decision boundaries, and showed that the accuracy of the algorithm can be maximized only at the expenses of its sensitivity. This tradeoff, which applies to general classification algorithms, cannot be improved by simply tuning the algorithm.

Way Ahead

Despite recent successes, machine learning algorithms are known to be vulnerable to sophisticated attacks where small, unnoticeable to humans type of changes to images can cause total failure in their operation. This research sheds new light towards the resolution of this problem in that it identifies a fundamental trade-off between the accuracy and the robustness of classification algorithms used in machine learning. Dr. Brian Jalaian in ARL and his colleagues are conducting research on robust machine learning and I informed him about the fundamental trade-off results by Professor Pasqualetti. I believe that this research could lead to novel robust machine learning approaches and it represents an example where a disciplined approach using control theoretical tools can shed additional light on challenging engineering problems.

Co-evolutionary Complex Networks

Challenge

Tactical communication networks play an essential role in Command, Control, Communications, Computing, Cyber, Intelligence, Surveillance, and Reconnaissance (C5ISR) systems. Equally important is the increasing role of autonomous systems (e.g., mobile sensors, unmanned vehicles, and robot teams) operating under networked architectures for sensing, computation, and mission execution. Beyond engineered networks, social networks provide a framework for dissemination of ideas and beliefs, formation of allegiances and coalitions, and distributed coordination and collaboration. Similarly, biological networks provide insights stemming from processes such as selective pressure to help model network evolution or contagion/epidemic dynamics to model network sustainability or resilience. In short, the sciences of engineered, social, and biological networks all contribute towards the realization of efficient operation of complex networked systems. Analysis of how such complex networks interact with each other and impact their evolution over time can shed additional light on the understanding complex systems and organizations.

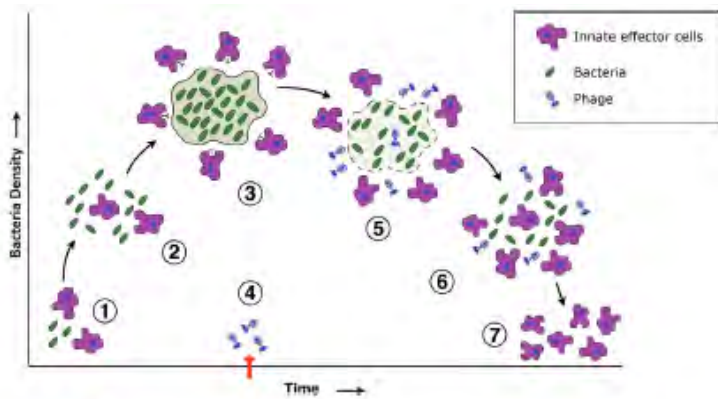
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Action

The previous Manager of the Multi-User Network Control Program Dr. Alfredo Garcia recognized the value of analyzing interacting complex networked systems and when he met with Professor Weitz, he encouraged him to develop a proposal in this area, which led to an innovative a multi-disciplinary project integrating theory, computational models, and model-experiment feedback to understand how pathogens, and in particular viruses of microbes, influence and control the fate of individual hosts, populations, and networked ecosystems.

Results

Viruses of microbes are ubiquitous in human and environmental microbiomes, with viral abundances typically exceed tens of millions per milliliter. Yet rather than asking how viruses and microbes coexist in the environment, their work began with a simple premise: could strategic deployment of viruses be used to control infections caused by multi-drug resistant (MDR) pathogens? To address this question, they developed a novel, nonlinear dynamic model of virus-microbe interactions in an immunological context and predicted a synergistic regime in which viruses and the mammalian immune system could eliminate MDR pathogens together, even if neither could do so alone. This theory stimulated new, in vivo experimental work using immunomodulated animal hosts by collaborators at the Institute Pasteur (at no cost to the ARO grant), leading to the confirmation of immunophage-synergy in which phage therapy is effective in immunocompetent but not innate immunodeficient hosts. In particular, Dr. Weitz and his collaborators in Louis Pasteur Institute in France, have made a major scientific discovery that demonstrates the efficacy of using bacteriophage (phage), a virus that invades a bacterium and causes it to disintegrate, for controlling antibiotic-resistant bacterial infections to improve Soldier physical resilience. By integrating in vivo experiments and newly developed mathematical models, the researchers showed that bacteria are eliminated by complementary action of both phage and the immune system together, when neither phage nor the immune response can eliminate the bacteria acting alone. This contrasts with the prevailing view that phage therapy effectiveness relies only on bacterial vulnerability to phages and not on a subject's immune response. The results also indicate that phage therapy could be effective in subjects with weakened immune systems, such as Soldiers under high physical and mental stress, despite phage resistance. This research builds the foundations for improved treatment of bacterial infections that affect Soldiers.

SUCCESS

The work carried by Prof. Weitz is a first of its kind that formalizes the interaction between viruses, bacteria and immune system, along with experimental results that validate the theoretical work. Indeed the work of Prof. Weitz has breathed new life into a forgotten idea of treating bacterial infections using viruses, as an alternative to penicillin like anti-bacterial medications.

RESULTS

- Over ten publications in reputed journals across several areas of research including epidemiology and control theory.

Way Ahead

Program Managers for basic research in Multi-agent Network Control and Microbiology from ARL's Army Research Office met with Dr. Mikeljon P. Nikolich, Chief of the Department of Bacteriophage Therapeutics at Walter Reed Army Institute of Research, to discuss opportunities for collaboration and follow-on work that may lead to further advances for dealing with bacteria that have developed resistance to widely used antibiotics.

MULTI-USER NETWORK CONTROL PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Determine fundamental limits of and develop methods for distributed control in large networked systems that if successful, will support efficient implementations of the Army's goal of distributed mission control, without losing sight of the common goal that derives its operations.
- ▶ Develop methods for learning in networked control systems, such as multi-agent reinforcement learning that if successful, will drastically enhance the operational capabilities of Army's autonomous systems, and protect our soldiers from high-risk environments.
- ▶ Develop control methods that ensure the stability of quantum systems such as reliable q-bits that if successful, will enable quantum computations that can have transformative effects such as breaking previously unbreakable codes and solve optimizations problems of unprecedented scales.



Dr. Purush Iyer

Program Manager, Intelligent Information Networks
Division Chief, Network Sciences
ARO Information Sciences Directorate

Dr. Iyer earned his PhD from University of Utah, and his Bachelor's and Master's degrees from Indian Institute of Technology, Madras.

Dr. Iyer came to ARO in 2009 as Program Manager for Intelligent Systems, before which he was a Professor of Computer Science at North Carolina State University.

Algorithmic Game Theory – Theory and Applications

Challenge

Since September 11, 2001, the landscape of armed conflict has changed for the U.S. Army. While it still fights large battles (such as in Afghanistan or Iraq), it is now routinely called upon to deal with asymmetric warfare against non-state actors, and sometimes rebuild societies, all under the constraint of budget and resources. Planning, strategizing, and decision making under the constraints of budget and resources, against both state and non-state actors, can always be investigated using the prism of Game Theory (as proposed by von Neumann, Morgenstern and later by Nash). However, the beautiful theoretical frameworks built in 1940s and 1950s are not that easily applicable in practice as they do not scale well, do not account for imperfect information, and, importantly, due to not account for understanding of human behavior discovered in the second half of 20th century. Addressing these challenges will have incredible impact on U.S. Army and on society.

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Network and Information Sciences



Human Sciences



Computational Sciences

Action

ARO PM, Dr. Iyer, funded a workshop in 2011, held at Duke University, to define what needed to be solved, and also funded a summer school for students to be trained in the burgeoning area of Algorithmic Game Theory at CMU, held the summer of 2012. In the meanwhile, he published a MURI topic inviting proposals in this area, and also promoted Dr. Vince Conitzer as an ideal candidate for the Presidential Early Career Award. Building on the success of the MURI, led by Dr. Tambe since 2011, Dr. Iyer wrote a MURI topic on Network Games for FY2018 to reason at societal level, and a MURI topic in 2019 on Unified Decision Theory to model human biases and its impact on decisions made by large groups. Concomitantly, he used the Single Investigator Award to fund Dr. Tuomas Sandholm to extend Game Theory to other arenas such as interactions at the cellular level between the immune system and cancer cells.

Results

For the past eight years, ARO's Network Science Division has been investing in Algorithmic Game Theory that has led to a number of scientific advances, and transitions to US Government agencies as well as to world-wide NGOs. The primary funding mechanism for this effort has been the Multi-Disciplinary Research Initiative project "Spatio-Temporal Game Theory," led by Prof. Milind Tambe, University of Southern California, and a Presidential Early Career Award for Scientists and Engineers (PECASE) to Prof. Vince Conitzer, Duke University. These researchers have made significant contributions to the field of Algorithmic Game Theory in making it usable in practice (solving problems of scalability), and also extending it in ways that makes the framework of Game Theory realistic (by taking into account learning by agents between rounds of the game, imperfect information, human biases, etc.). While Game Theory was formulated in the 1940s and 1950s, it is typically pictured as a two-person, zero-sum game with perfect information played by agents with unbounded rationality (i.e., infinite computational resources, with no biases), which does have direct application to board games such as chess. Under such assumptions the notion of Nash equilibrium is appropriate, and scalability remains the biggest problem. However, in practical situations, the game is imperfect (with rules changing on the fly and not all information being visible) as: (a) agents learn from signals from other player and, appropriately, change strategies, and (b) importantly, agents have bounded computational resources and budgets to either defend or to attack. Consequently, notions of equilibria are replaced by analyses of medium term costs and benefits. In all of the efforts the researchers have addressed both theoretical questions and use-inspired research, leading to identification of new research problems. The ARO funded researchers have made the following advances:

Signaling: The authors studied Bayesian security games in which the defender can selectively broadcast her payoff-relevant private information, a task termed as "signaling", to affect the attacker's belief regarding the game. Most previous work in security games studies how to optimize the allocation of the defender's patrolling resources. This work explores another resource for defense – the defender's informational advantage. Utilizing informational advantage to win battles/games is not rare in history, but very few work has formally considered this problem in the literature of security games. The authors show that in Bayesian security games, selectively revealing the defender's payoff-relevant private information may result in much better defender utility than that of a silent defender. They then look at the joint design of the optimal information revelation scheme and patrolling resource allocation and propose efficient algorithms to compute the optimal solution. Experimental evaluations of the ensuing algorithms show significant benefits for the defender to utilize information. Though motivated by security games, the model and approaches are generalizable to any Bayesian Stackelberg games. The work has been transitioned to Los Angeles Metro, where random check rather than turnstiles are used to enforce proper purchase

SUCCESS

The work on Algorithmic Game Theory has been carried with great success at both the foundational level and in addressing societal problems. In particular, ARO's funding has been instrumental in advancing algorithmic techniques to deal with state explosion problem, as well as address difficult human biases decision making, thus making algorithmic game theory applicable to societal and military problems.

RESULTS

- ▶ Over 150 publications among two efforts from the past and the ongoing effort.
 - ▶ Transition of software and technology to US Coast Guards, Transportation Security Authority, LA Police Department and LA Metro Train system.
 - ▶ Transition of technology to NGOs worldwide involved in wild-life conservation.
 - ▶ Numerous AAAI and AMAAS awards for best paper, best practices and significant contribution to society for the faculty involved in these projects.
-

of tickets. Furthermore, results emanating from this work are now being used in the context of Moving Target Defense of Cyber assets, in a new MURI that started in 2017.

Learning: Previous research optimizes defenders' strategies by modeling the problem of learning by agents as a repeated Stackelberg game, capturing the special property in this domain – frequent interactions between defenders and attackers. However, this research fails to handle exploration-exploitation tradeoff in this domain caused by the fact that defenders only have knowledge of attack activities at targets they protect. The approach taken by the researcher is to address this shortcoming as: (i) formulation of the problem as a restless multi-armed bandit (RMAB) model to address exploration and exploitation. (ii) Use the notion of Whittle index policy to capture the transfer of knowledge when the defender discovers an attacker's action, leading to reset of plans by the attacker to derive two sufficient conditions for indexability and an algorithm to numerically evaluate indexability. (iii) Design of binary search-based algorithm to find Whittle index policy efficiently. The technical results were used in the context of transition of scheduling algorithms to NGOs working on Tiger preservation in South East Asia and preservation of elephants in Uganda (which were being killed for ivory).

Abstractions: As more resources, local information (such as topography) and multiple adversaries are taken into account the size of the constructed game grows. Finding symmetry in the game tree becomes important. Using opportunistic crimes as a running example, Dr. Tambe and his team aim to characterize the interaction between officers and opportunistic criminals as a game with discrete targets. By merging similar targets, they obtain an abstract game with fewer total targets. The team then used real world data to learn and plan against opportunistic criminals in this abstract game, and then propagate the results of this abstract game back to the original game. The work was tested on two large-scale urban problems: a university campus and a city, with high prediction accuracy, which in turn allowed them to build strategies for planning use of scarce resources. More recently, Dr. Sandholm has shown to build abstractions and reason about sub-tree games in imperfect information games in the context of six-player Texas Hold 'Em Poker, which advances the state of art in significant ways.

Way Ahead

The work that was carried out over the past eight years has now led to a slew of new ongoing research and applications. ARO PM Dr. Iyer in an effort to lift these techniques to reason about state actors, and the non-state actors embedded within them, defined a MURI topic in 2018 to bring hybrid methods at play, by calling for synergizing work that combines Mean Field Games (which apply to an infinite number of agents of identical capability) and Discrete games that apply to a small number of players, possibly different from each other in major way. In particular, he has been pushing for mathematical formalism that would allow abstraction and refinement to be defined and reasoned about so that inferences regarding macro level observations at the level of society can be related to local micro-level observations at small group level (especially adversarial groups). This MURI was awarded, in 2018, to a group led by Dr. Mingyan Liu (University of Michigan) and the work is ongoing. In the meanwhile, he has been an advisor to Mr. Ted Senator, DARPA DSO PM, for a newly constituted DARPA program that aims to bring Game Theory to military planning and decision making. The ARO PM, Dr. Iyer, is not only advising the DARPA PM on the science but also potential opportunities for transitions.

Inferring Hidden Network Structure

Challenge

The problem of inferring latent structures in social networks has attracted significant attention in recent years, as these are important for understanding adversarial communities in, say, large mega-cities. The questions then are whether one can: (a) establish limits to computational efficiency vs. accuracy trade-off; and (b) exploit traditional mathematical logic based techniques of structure-based decomposition to yield fast methods.

Action

Using single investigator grants Dr. Iyer initiated a project with a Statistical Mechanics expert to answer the first question and has recently initiated a project with two theoretical computer scientists to answer the second question.

Results

Recently, a phase transition has been discovered in the network community detection problem below which no algorithm can tell which nodes belong to which communities with success any better than a random guess. Most result on network detectability transition so far have been limited to the case where the communities have the same size or the same average degree. Recently Dr. Galstyan and his group have considered more general scenario where the sizes of different blocks or the average degrees within blocks are different. This type of asymmetry enables them to assign nodes to communities with better-than-random accuracy by simply examining their local neighborhoods. They use the cavity method from statistical physics, and show that this asymmetry suppresses the detectability transition completely for networks with four groups or fewer. When the number of groups is >4 , however, the detectability threshold persists up to a critical amount of asymmetry, but disappears beyond (Figure 1). They find that the critical point in the latter case coincides with the point at which the local information in the network percolates, causing a global phase transition from a less-accurate solution to a more-accurate one.

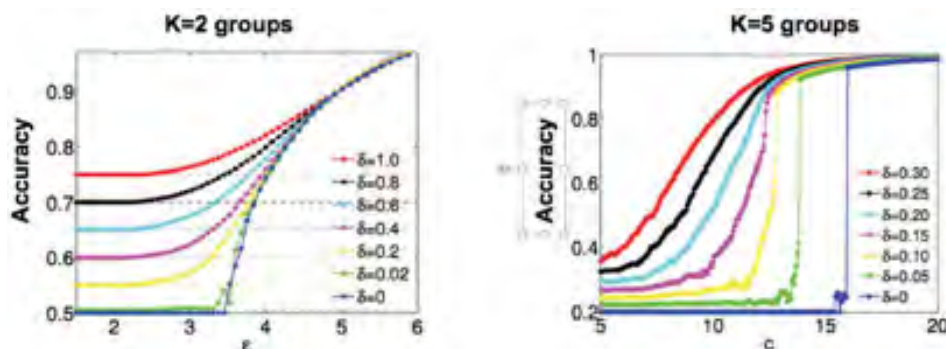


Figure 1. Detectability transition in network inference. For $K=2$, detectability transition completely disappears; for $K=S$, it persists but up to a critical point; beyond this point local information percolates, causing a global transition from a less-accurate solution to a more-accurate one

In another development, they have been working on information-theoretic tools for analyzing and extracting meaningful structures from complex data. Specifically, their goal was to analyze multi-modal brain data by using a novel unsupervised machine learning method, Correlation Explanation (CorEx), to identify groups of biomarkers that

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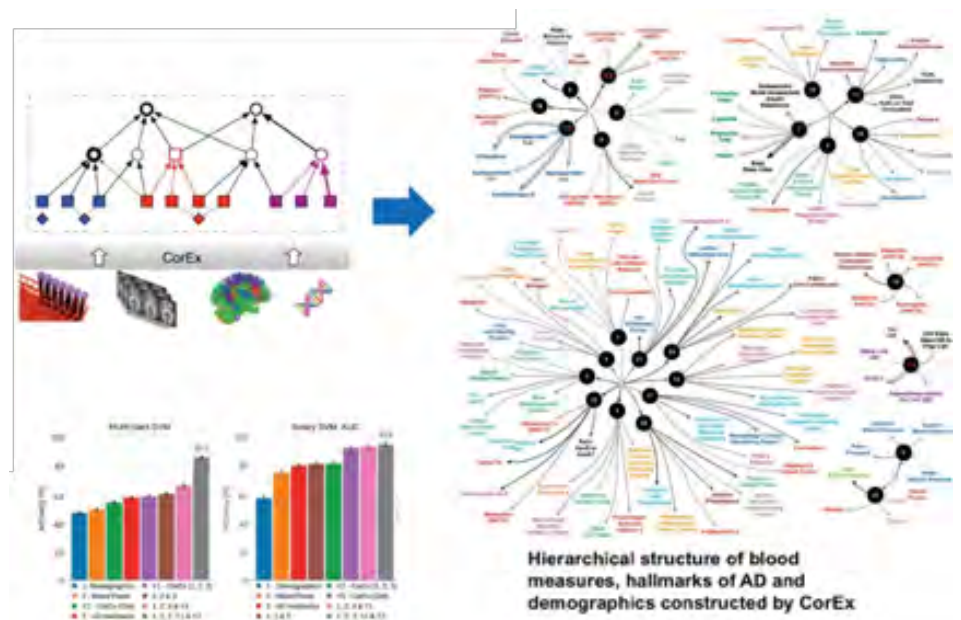


Figure 2. The schematics of the problem setup (upper left); the hierarchical latent structure discovered by CorEx (right); and the diagnostic prediction accuracy with and without CorEx features

have high multivariate mutual information, and to reconstruct latent factors that explain these correlations. Figure 2 shows the latent hierarchical structure they discover when applying CorEx to data from 829 participants - 231 cognitively normal elderly, 397 with mild cognitive impairment (MCI) and 201 with Alzheimer's Disease (AD). This data is a part of the Alzheimer's Disease Neuroimaging Initiative (ADNI), which is a large multi-site longitudinal study to evaluate biomarkers of AD.

The main result demonstrates that by combining nonlinear CorEx latent factors with groups of potential biomarkers, they are able to better predict which of the three diagnostic groups a given person belongs to (Figure 2, bottom-right). In particular, they found that dynamic brain changes and cognitive decline were associated with disease, and with lipoproteins, insulin-related markers, and immune cells in the blood - revealing links between diverse set of predictors. In summary, their findings are useful for understanding latent disease mechanisms and stratifying groups of people for inclusion in preventative and interventional drug trials.

Way Ahead

The theoretical bounds of the current work provide guidance on what is possible. However, much more work is necessary to employ decomposition techniques from theoretical computer science and mathematical logic literature to reason about large graphs, which just started.

INTELLIGENT INFORMATION NETWORKS PROGRAM –CURRENT SCIENTIFIC OBJECTIVES

- ▶ Establish framework for reasoning about adversaries to derive strategies. Furthermore, devise algorithms that accounts for human biases and is effective and efficient, viz., deals with explosive growth in state space of game representations. If these goals are successfully met then U.S. Army will have the ability to devise strategies in complex war situations.
- ▶ Establish framework for deriving fundamental limits and design of efficient algorithms for reasoning about large networks by exploiting local structure and semantics, which, if successful, will provide unprecedented situational awareness capabilities in mega-cities, the battleground of the future.
- ▶ Devise Natural Language Processing frameworks for processing and extracting meaningful information, in a graphical form, with the goal of automating decisions and inferences, which if successful, will provide unprecedented capability to fuse information across entire battle units from after-action reports.

SOCIAL AND COGNITIVE NETWORKS PROGRAM



Dr. Edward T. Palazzolo

Program Manager, Social and Cognitive Networks
Network Sciences Division
ARO Information Sciences Directorate

Dr. Palazzolo completed a double major in Communication and Psychology in 1997 at the State University of New York at Buffalo where he earned his B.A. He completed his M.A. in Communication at the State University of New York at Buffalo in 1999 and went on to earn his Ph.D. in Communication from the University of Illinois at Urbana-Champaign in 2003.

Dr. Palazzolo joined ARO in 2014 as the Program Manager for the Social and Cognitive Networks Program.

Toward Predictive Modeling Deviant Cyber Flash Mobs: A Socio-Informatics Driven Hypergraph Framework

Challenge

Scientists have a nascent understanding of the relationship between coordinated cyber activities and real world actions. Further, there is a weak understanding of deviant forms of emerging sociotechnical behavior and the necessary conditions that lead to the emergence of Deviant Cyber Flash Mobs (DCFMs) and subsequently their actions.

Action

A principle thrust of the Social and Cognitive Networks (SCN) program is focused on Computational Social Science (CSS) to create verifiable models of networked human behavior by bridging social sciences theories with computer science techniques and engineering precision. The SCN Program Manager (PM) seeks to identify critical gaps in CSS research which also have a direct impact for the Army and Joint Operations. Toward that end, the SCN PM identified a pre-tenured faculty member working on deviant cyber flash mobs (DCFMs). DCFMs are cyber flash mob behavior among

This success supports these ARL Core Technical Competencies

Network and Information Sciences



Human Sciences



Computational Sciences



SUCCESS

Dr. Agarwal and his research team successfully developed a conceptual model based on the social science theory of collective action to explain Deviant Cyber Flash Mobs (DCFM) behavior and developed a conceptual framework to predict the success or failure of a DCFM.

RESULTS

- ▶ Research methodologies for identifying and countering cyber threats transitioned to NATO and FBI
- ▶ Cyber forensic methodologies transitioned to ONR, DARPA, and NATO, to be explored further through customer funding
- ▶ ARO-funded investigator named as Priority Partner for DHS's Criminal Investigations and Network Analysis (CINA) Center of Excellence (COE)

deviant groups to recruit, train, and arm attackers with malicious code to coordinate cyber-attacks. Such behaviors are observed in dark corners of the internet where groups coordinate and disseminate misinformation or even spread propaganda to subvert democratic principles and institutions. DCFMs pose significant risks to social, political, and economic stability.

Result

This research effort advanced our nascent understanding of the relationship between coordinated cyber activities and real world actions. More specifically, this research expands our understanding of deviant forms of emerging sociotechnical behavior by identifying necessary conditions leading to the emergence of DCFMs and subsequently their actions, by identifying hidden relationships within and among different deviant groups using social cyber forensics, and by building predictive models of cyber flash mob behaviors. This was accomplished by developing a conceptual model based on the social science theory of collective action (see Figure 1) to explain DCFM behavior, utilizing social media data on extremist/violent cyber flash mobs, extracting complex relations and represented in a hypergraph construct, and conducting a power analysis of key members. Additionally, the research team developed a conceptual framework to predict the success or failure of a DCFMs.

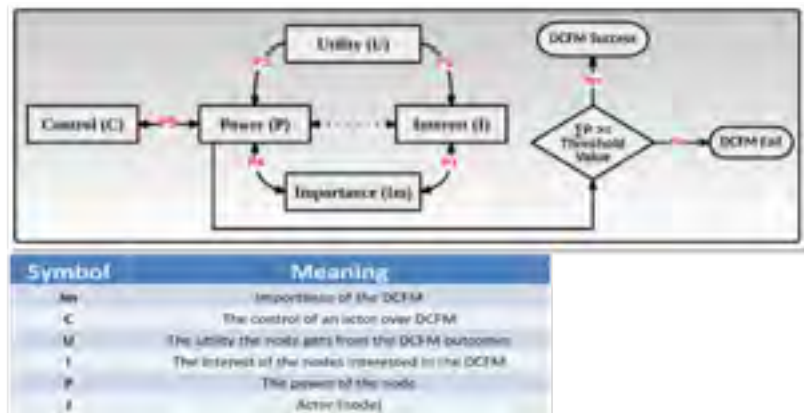


Figure 1. Logical Framework for the Formation of Deviant Cyber Flash Mobs based on Collective Action Theory

The researchers used this framework to identify most powerful actors for ISIL propaganda dissemination, anti-NATO propagandists, and deviant hackers networks (black hat hackers) on Twitter (see Figure 2), thus demonstrating the initial effectiveness of their theoretical model on real world data. Additionally, they developed Focal Structure Analysis (FSA) tool to identify key groups in a network that are collectively more powerful than most powerful individuals. This tool has been made public for adoption and utilization by academics and practitioners.

By leveraging a strong social science theory with computational techniques, this research team has created a powerful methodology to predict the success or failure of deviant cyber flash mobs as well as their likelihood to incite extremist actions. Through understanding DCFM behavior from a predictive theoretical lens, the Army is better situated to defend against such actions.

Parameter	Method of Estimation
Control (C)	In-Degree Centrality
Interest (I)	$(\text{Number of retweets} + \text{mentions}) / (\text{total number of tweets})$
Power (P)	$\text{Control} * \text{Interest}$

The top 10 powerful actors of ISIL on Twitter

Powerful Actors	# of Tweets	# of Mentions and Retweets	In-Degree Centrality	Power
shamir@twee	11,297	82	2992	1.428
abnawp	10706	32	2980	1.247
scpr@twee	812	69	138	129.67
asli@twee	5999	15	2983	5.01
trac@twee	2010	11	2901	7.40
khajal@twee	265	32	1043	36.76
thaw@twee	2257	72	1096	63.73
jah@twee	245	19	2983	155.33
ahmadMusaJibri1	0	0	0	0
omni@twee	698	82	2980	294.95

Figure 2. Top 10 powerful actors of ISIL on Twitter and power parameters used in the conceptual framework. Notes: red arrows indicate scores for actual/known foreign fighters; ahmadMusaJibri1 account was deleted by Twitter.

Way Ahead

This research methodology and results have been briefed to the FBI, DHS, US Cyber Command, and NATO. These advancements will assist Cyber Intel Analysts in identifying social media accounts responsible for coordination of attacks, predict future uprisings and attacks with the intent to mitigate action prior to disruption, and support cyber security strategies dealing with DCFM behaviors at a fundamental social and behavioral level.

Network Science of Teams

Challenge

This research program is focused on discovering the fundamental principles governing human teaming activities that support designing and maintaining high performance teams. It addresses the challenges of a lack of quantified models for cognitive dimensions of teams and that there is no known specific “recipe” for the design of high performance teams.

Action

The Social and Cognitive Networks (SCN) program seeks to predict emergent phenomena in teams and organizations by creating new measures, models, and theories that capture cognitive and behavioral processes of networked human systems to provide commanders and soldiers with tools and techniques to explore their decision option space for improved decision-making. This line of research is critical for the Army and will have transformational impact on how the Army designs and assembles teams in the form of squads and staffs and how those teams plan and execute their missions. More specifically, this research will lead to a paradigm shift, in appropriate units (e.g., Civil Affairs and Cyber Security), away from the universal, interchangeable soldier, to an elite force focused on knowledge management principles centered on the interdependencies between tasks, knowledge expertise, people and relationships.

Towards that end, the SCN Program Manager (PM) stood up a research thrust focused on Team Science. Within that thrust, the SCN PM initiated a 5-year, Multidisciplinary

This success supports these ARL Core Technical Competencies

Human Sciences



Network and Information Sciences



Computational Sciences



SUCCESS

The interdisciplinary work between social science and engineering led to an axiomatic model of team-based network dynamics for opinion evolution through team interaction and task coordination.

University Research Initiative (MURI) research effort on the Network Science of Teams called QUANTA: Quantitative Network-based Models of Adaptive Team Behavior. This research is led by six Principle Investigators (PIs) from University of California Santa Barbara, University of Southern California, Massachusetts Institute of Technology, and Northwestern University and spans multiple disciplines including the social sciences, computer science, business, engineering, and public health. Their work is organized around three research foci: (1) teams as networks of interacting entities, (2) analysis and models of dynamic team behavior, and (3) network science of teams-of-teams known as multi-team systems (MTSs).

To amplify the investment in this MURI research, the SCN PM coordinated relationships between this MURI team and other funded research efforts and other Army units. Notable coordination includes with the Army Research Institute (ARI), Fort Bragg's 92nd Civil Affairs Battalion, and Army Training and Doctrine Command (TRADOC). The SCN PM coordinated additional funds from ARI to co-fund a complimentary team science effort focused exclusively on the cognitive dimension of team science. This co-funded work looks at the tenants of Collective Intelligence and Transactive Memory Systems for predicting team performance based on unobtrusive measures.

RESULTS

- ▶ Established and transitioned methods to collect Soldier data from Civil Affairs Battalion
- ▶ Academic laboratory sent student for summer internship funded through ARL-CISD
- ▶ Results in unobtrusive measures of TM systems transitioned to Army Research Institute for subsequent funded research

Results

Now in its fourth year, this research team has significantly advanced the network science of teams. A foundational accomplishment with long-term future utilization is their work on opinion dynamics. Specifically, the interdisciplinary work between social science and engineering led to an axiomatic model of team-based network dynamics for opinion evolution through team interaction and task coordination. Figures 1 and 2 provide the high-level overview of the problem formulation and influence dynamics for quantifying and representing collective learning in a simulated six-person team.

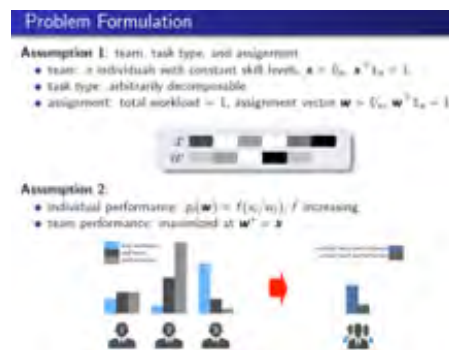


Figure 1. Opinion dynamics problem formulation and assumptions

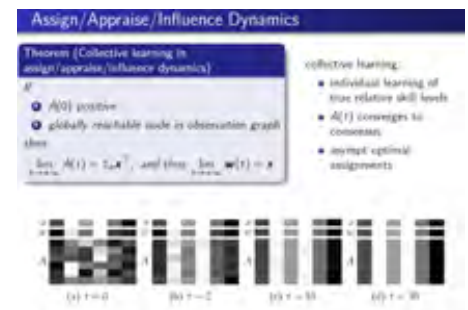


Figure 2. Collective learning in influence dynamics

Additionally, and at the direction of the SCN PM, the Network Science of Teams MURI team expanded their research foci beyond human teams to human-agent teams to study the impact of intelligent agents working alongside humans. Once such study under this MURI effort developed a framework for humans working with machines to make big decisions: predicting science that fails to replicate. Creating human-machine teams with particular conditions to synergistically complement the strengths of human minds and unbiased efficiency of machine data processing. Using natural language processing (NLP) to quantitatively transfer journal text into machine understandable representation and applying neural network learning algorithms on journal performance, they created a hybrid model to help humans identify bias and errors and make better decisions in predicting the reproducibility of science in journal articles. Using this methodology, they successfully predict whether the experimental results can be replicated and showed that the machine-only model can achieve around 6% better prediction performance than human identified metrics; moreover, the human-machine hybrid model achieves 9.5% better prediction performance.

Way Ahead

Special Operators in the 92nd Civil Affairs Battalion invited the MURI team to collect data from them with respect to their knowledge networks, communication networks, and opinion dynamics. This unique data will be utilized to build both customized and generalizable models of multi-team systems centered on unique knowledge missions. Moreover, the MURI scientists will have an opportunity to brief the 92nd's Non-Commissioned Officers (NCOs) and Officers once the data collection and analysis is complete. Lastly, the SCN PM developed a strong connection with TRADOC for not only sharing team science research findings, but, most importantly, for assisting in the development of best practices from this research for the creation of new Army Doctrine based on findings from these research and other SCN efforts.

SOCIAL AND COGNITIVE NETWORKS PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ The Social and Cognitive Networks (SCN) program seeks to predict emergent phenomena in teams and organizations by creating new measures, models, and theories that capture cognitive and behavioral processes of networked human systems that, if successful, will provide commanders and soldiers with tools and techniques to explore their decision option space for improved decision-making.
- ▶ The Computational Social Science (CSS) thrust seeks to create verifiable models of networked human behavior by bridging social sciences theories with computer science techniques and engineering which, if successful, will have an impact on Army and joint operations by providing support for decision-making.

TECHNOLOGY INTEGRATION AND OUTREACH DIVISION: FY18 SUCCESS STORIES

EDUCATION OUTREACH PROGRAM



Ms. Jennifer Ardouin

Program Specialist, Educational Outreach
Technology Integration & Outreach Division
Information Sciences Directorate

Ms. Ardouin completed her Bachelor of Science degree in psychology from the University of Maryland, European Division, Heidelberg, Germany in 1991 and earned a master's degree in Industrial and Organizational Psychology from Capella University, Minneapolis, Minnesota in 2004. Ms. Ardouin pursued her career interests through active duty U.S. Army service and state and federal government service.

She came to ARO in June 2017 as Manager of the Army's High School Apprenticeship Program (HSAP) and the Undergraduate Apprenticeship Program (URAP) and various other STEM outreach activities.

The Army's Education Outreach Program STEM Initiatives

Challenge

According to the American Affairs Journal (Spring 2019/Volume III, 1) America's current STEM crisis is not only a threat to our economic and scientific prowess but may well be a threat to our National security. To that point, STEM education outreach supports the recently published 2018 White House STEM Strategy report's three overarching goals critical to fortifying our Nations' future STEM success and global prowess - preparing the STEM workforce for jobs of the future, increasing the diversity of the STEM workforce, and expanding STEM literacy across the population.

The Army's Education Outreach Program's (AEOP) strategy of exposing students at all grade levels to STEM, even as early as kindergarten, through related hands on activities, competitions, apprenticeships and scholarships. AEOP not only creates an interest and deeper understanding of STEM but ideally establishes a pathway to advanced STEM education and occupational pursuits. At a minimum, this portfolio of STEM programs, prepares young citizens to effectively interface with future scientific and technological discoveries.

Actions

In the year 2018, ARL-ARO funded high school and undergraduate students in university partner laboratories nationwide in paid summer apprenticeships through the Army's High school Apprenticeship Program (HSAP) and the Undergraduate Research Apprenticeship Program (URAP). Ms. Ardouin's management of the apprenticeship programs included; collaboration with ARO PMs for HSAP/URAP proposal evaluation and her subsequent screening and distribution of student applications, coordination

This success supports
these ARL Core Technical
Competencies



Human Sciences

with university partners for student placement and administrative support before, during and after summer apprenticeships contributed to the success of AEOP's STEM outreach efforts. In this same year, her planning and coordination of STEM outreach activities and collaborations with internal and external partners resulted in ARL-ARO supporting underrepresented and disadvantaged NC youth during the U.S. 2020 RTP Science, Technology, Engineering and Mathematics (STEM) Expo.

Results

Through the Army Education Outreach Program (AEOP) portfolio, and in collaboration with ARO, the Army supported 114 high school and undergraduate students through 8-10 week apprenticeships designed to ignite curiosity and interest in real-world research. Apprentices worked in university laboratories, across the Nation and alongside world-class researchers where they participated in hands-on Army-funded research. It is believed that this increased their STEM literacy but also provided them with scientific proficiencies and laboratory skills that could be extended to their high school and undergraduate studies.

In further support of the Nation's STEM goals, Army participation in the 2018 U.S. 2020 RTP STEM Expo where 400 underrepresented and disadvantaged NC youth attended presentations and demonstrations led by ARO-ARL staff. Students learned how STEM research directly benefits the Nation through scientific discoveries which directly protect and equip American warfighters on and off the battle field. Additionally, expo attendees participated in brief mentoring sessions with ARL-ARO scientific staff that focused on the importance of STEM in our daily lives while advising students on how they might prepare academically for future STEM occupations, all while highlighting their careers of DoD STEM professionals. This event also enabled students to learn about, access and leverage the AEOP portfolio to enhance their STEM savvy through STEM enrichment activities, competitions, apprenticeships and academic scholarships.

During 2018, both accomplishments supported the 2018 White House STEM Strategy goals critical of preparing the future STEM workforce, increasing diversity in STEM and expanding STEM literacy.

Way Ahead

In order to further align with the Nation's STEM strategy, it is necessary to nurture existing partnerships, explore and establish new collaborations among National and community STEM partners and continue to leverage ARL- ARO and AEOP resources. While there is an overarching need to increase the number of STEM opportunities for youth, there is also the need to establish a level of diversification among participants which include disabled students, youth in rural areas and first-generation college students.



Finally, the incorporation of workforce development strategies into existing outreach programming is key to expanding the scope beyond STEM literacy to creating an intentional pathway for those youth who are interested in pursuing STEM careers. The expansion and refinement of existing STEM outreach efforts is critical to ensuring that the future workforce has a level of STEM literacy and expertise that is essential to our Nation's future readiness and global influence.

EDUCATION OUTREACH PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Introduce students to the Army's interest and investment in science and engineering research through associated educational outreach efforts.
- ▶ Through Army funded apprenticeships, provide hands-on research experience for high school and undergraduate students, anticipated to lead to student career exploration and promote interest in STEM fields of study.
- ▶ Grow the scale of high-quality mentorship experiences for students who will benefit from the expertise of world-class scientists and engineers as a mentor for professional and academic development.
- ▶ Support the preparation of students for the 21st century workforce by providing opportunities for continued research development and interests.

ARO SBIR AND STTR PROGRAM



Ms. Nicole R. Fox

Program Specialist, ARO SBIR/STTR Program
Technology Integration and Outreach Division
Information Sciences Directorate

Ms. Fox completed her B.A. in Business Administration at Bay Path University in 1997.

She came to ARO in 2010 as a contracted Program Specialist for the Army STTR program and was promoted to a government position as the ARO SBIR/STTR Program Manager in 2011.

ARL/ARO participates in the Small Business Innovation Research (SBIR) and the Small Business Technology Transfer (STTR) Programs, and is the lead for the Department of the Army's STTR Program. Congress established the SBIR Program in 1982 and the STTR Program in 1992 to provide qualifying small businesses with opportunities to participate in government-sponsored research and development (R&D). ARO uses these programs to advance scientific discoveries in the basic research base through technology innovation partnerships with small business.

The overarching goals of the SBIR and STTR programs are: (1) stimulate technological innovation, (2) increase small business participation in federal R&D, (3) increase private sector commercialization of technology developed through federal R&D, and (4) foster and encourage participation in federal R&D by businesses that are owned by women and socially and economically disadvantaged individuals. The STTR Program has the additional requirement that small companies must partner with an academic or other qualifying non-profit research institutions to work collaboratively to develop and transition emerging technical ideas from the laboratory to the marketplace. In FY18, ARO awarded \$23 million in SBIR and STTR contracts, an increase of 15% over \$20 million in FY17.

Pathogen Specific Antimicrobial Coatings for Fabrics

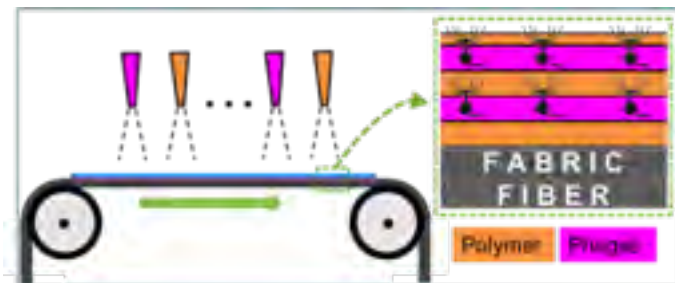
Challenge

Antimicrobial treatment of military textile systems is intended to provide enhanced protection to the Warfighter in the field by preventing colonization of harmful bacteria that cause problems such as odor, dermatitis, impetigo, cellulitis, and other skin irritations. Bio-derived antimicrobial coatings offer selective elimination of targeted bacteria without effecting commensal bacteria required for skin health. Phages, the viruses of bacteria, can uniquely offer specificity against targeted bacteria. By judicious selection of phages and host matrices.

Action

In the year 2015, a STTR topic was developed through Ms. Fox's oversight, entitled "Advanced Fibers for High Efficiency Capture and Release of Human Cellular Material for Forensic DNA Analysis." Through several topic revisions, instruction, and guidance by Ms. Fox, along with the two topic authors, Drs. Stephanie McElhinny (ARO) and Brigid O'Brien (USAF) a successful topic was published in the FY15.A Army STTR BAA. After careful reviews by the technical evaluation team lead by Dr. McElhinny, proposal selections were made and the Phase I cycle began. Through Ms. Fox and Dr. McElhinny's continued oversight and guidance Giner, Inc. was selected for a Phase II.

It was believed the primary result from the successful completion of this project would be the development of bio-derived antimicrobial textile coatings to fight against bacteria that cause odor and skin irritation. The resulting coatings will have the potential to eliminate the targeted pathogenic bacterial colonies without affecting the beneficial skin flora. A wide array of clothing segments that provides advanced fabrics to armed services, field workers, and athletics will benefit from this application.



Result

Giner, Inc. has developed a phage-based antimicrobial fabric coating that is effective in eliminating harmful skin bacteria, *Staphylococcus aureus*, which is the leading cause of skin and soft tissue infections (SSTI) in military personnel. The coating is processed on nylon/cotton fabric blends using an aqueous multilayer assembly method and consists of phages, bacteria-killing viruses, embedded within a polymer host matrix. Giner's coating technology, which was recently recognized with a TechConnect Defense Innovation Award at the 2017 Defense Innovation Summit, eliminates >99.9% of *S. aureus* without disrupting the beneficial skin microbiome. The applied coating is durable enough to withstand laundering cycles and is applied to 'next-to-skin' fabrics using a roll-to-roll coating process, making it a scalable and cost-effective method of preventing *S. aureus* colonization. The key technology concepts are: 1) the phages uniquely offer specificity against targeted harmful skin bacteria with minimal impact on beneficial skin microbes; 2) Giner's novel process enables durable and conformal antimicrobial coatings that can be applied to a wide variety of fabric materials; and 3) the coatings can be optimized for maintenance of antibacterial effects due to the facile genetic manipulation of phages.

This success supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Protection Sciences



This success supports these ARL Core Technical Competencies



Materials and Manufacturing Sciences



Network and Information Sciences



Protection Sciences

Way Ahead

The development of an advanced fiber for high recovery collection and release of forensic biological samples will increase the reliability of genomic forensic analysis and enable the extraction of actionable forensic information from evidence with limited cellular material. The civilian sector would also significantly benefit from the developed technology and could transition for use in federal, state, and local forensic laboratories, as well as the medical sector where the collection of biological specimens is routine for clinical diagnostics. This directly supports the Defense Forensic Science Center's mission of providing forensic laboratory support to Department of Defense investigative agencies and its mission to provide expeditionary forensic laboratory services in support of Overseas Contingency Operations.

DeepRadio: Deep Learning for Wireless Communications and Security

Challenge

Department of Defense (DoD) operations critically rely upon efficient, robust, resilient and secure wireless network communications. Recent emergence of stealth (silent or low-signal) attacks, such as emulating legitimate behaviors or randomizing their footprints, are difficult to detect by the conventional intrusion detection systems. Such stealth attacks can damage communication systems at different levels such as increasing message delay, reducing network throughput, and causing loss of information confidentiality or data integrity. A novel comprehensive framework of defense solutions must be designed to combat this broad spectrum of potential attacks that have recently evolved into a more stealth form to minimize their exposure to traditional attack defense systems.

Action

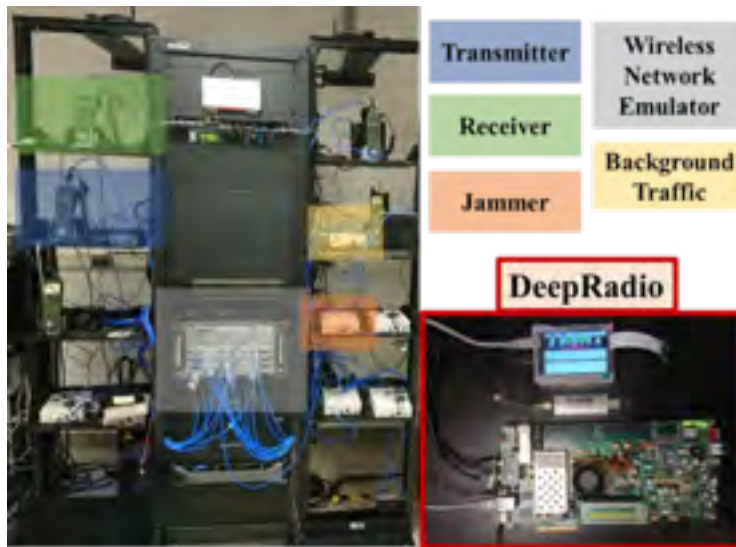
In the year 2016, a STTR topic was developed through Ms. Fox's oversight, entitled "Quantification model and systems for assessing and developing resilient wireless communication operation". Through several topic revisions, guidance, and instruction, Ms. Fox along with the two topic authors, Drs. Cliff Wang (ARO) and Hasan Cam (CISD) a successful topic was published in the FY16.A Army STTR BAA. After careful reviews by the technical evaluation team lead by Dr. Wang, proposal selections were made and the Phase I cycle began. Through continued oversight and guidance by Ms. Fox and Dr. Wang, IAI was selected for a Phase II.

It was believed that IAI would design and implement the Quantification, Analysis, Defense, and Evaluation System (QADE) prototype for secure and resilient wireless communication operations. The key innovation is to jointly integrate intelligent and comprehensive attack and mitigation capabilities, impact and resiliency quantification for wireless stealth attacks, radio programming focused on wireless security operations, high-fidelity simulation and radio experimental evaluation through emulation tests.

Result

Intelligent Automation, Inc. (IAI) developed the DeepRadio technology to provide reconfigurable embedded implementation of deep neural networks as a stand-alone radio platform for characterizing the RF spectrum environment in real time and adapting to spectrum dynamics. DeepRadio uses deep learning to detect and classify

RF signals (tactical and commercial waveforms as well as cognitive jammers), identify spectrum opportunities, and reconfigure the software-define radio (SDR) transceiver. Each DeepRadio device is an integrated unit consisting of a SDR front-end, an embedded processor, and a field-programmable gate array (FPGA). Deep neural network architecture is reconfigurable and supports adaptation to spectrum dynamics, including topology, channel, interference, and traffic effects. The outcome is real-time and accurate characterization of the RF spectrum, spectrum efficiency improvement, and support signal co-existence on busy spectrum bands. Ft. Dix field test of DeepRadio with tactical and commercial radios demonstrated the effectiveness of DeepRadio in detecting RF interfering sources and mitigating their effects on wireless communications. In the field test, DeepRadio successfully learned the behavior of a dynamic jammer (that does not transmit continuously and is hard to detect) using a deep neural network model. Consequently, DeepRadio predicted with high accuracy (>85%) when the jammer intends to jam the spectrum. Using this information, DeepRadio suspends traffic flow transmission until it predicts the spectrum is reliable, reducing packet loss rate over jammed channels and boosting reliability of tactical communications.



Way Ahead

The proposed QADE radio software product has tremendous potential in both military and commercial technologies, which introduces enhanced security, resilience and situational awareness to support wireless communications. IAI's initial focus will be to transition the QADE prototype to relevant DoD programs, focused on tactical radios and waveforms and networking programs of record. QADE has direct applications in commercial communication systems, such as cellular communications (5G), satellite communications, Wi-Fi and mobile cloud systems, sensor and vehicular networks, public safety and emergency communications systems. In particular, QADE has the strong potential in enhancing the resiliency of the commercial communication systems and supporting secure and robust interoperability over unlicensed spectrum.

This success supports these ARL Core Technical Competencies



Materials and Manufacturing Sciences



Network and Information Sciences



Protection Sciences



Human Sciences



Ballistics Sciences



Computational Sciences



Propulsion Sciences

ARO HBCU/MSI PROGRAM



Ms. Patricia Huff

Program Specialist, Historically Black Colleges and Universities (HBCU) and Minority-Serving Institutions (MSI)
Technology Integration & Outreach Division
Information Sciences Directorate

Ms. Huff is a graduate of Howard University receiving her B.A. degree in Broadcast Management in 1987. Her professional activities and accreditations include: Master Certified Facilitator and Moderator (Qualitative Researcher).

Prior to joining ARO in 2012, Ms. Huff worked for more than a decade in the federal government at the National Oceanic and Atmospheric Administration (NOAA). She went on to work as a Marketing Research Analyst for Potomac Electric Power Company (PEPCO) and later became the owner and Chief Executive Officer (CEO) of a marketing and communications consulting company.

ARO Hosts DoD Workshop for HBCU/MSIs

Challenge

The Army wants to build a stronger research network in the Historically Black Colleges and Universities (HBCUs) and Minority-Serving Institutions (MSIs) academic community that leads to a better understanding of our research requirements, a platform to share best practices and lessons learned, and the ability to make data-driven recommendations for program improvements, as well as the ability to identify real challenges to improved quality for our performance partners that can lead to real and innovative solutions to address them and measure our success.

The Army has developed a strategic plan for engaging HBCU/MSIs to help diversify their research portfolio. In developing this strategy, we focused on addressing some areas of identified concern among our many stakeholders. We recognize that we need to challenge and address the perspective that only highly equipped and funded research institutions are awarded grants or that the process requires full time grant writers on staff or a high overhead funding needs. Therefore, our challenge was to create an interactive, informative, and engaging outreach events to expand the competitiveness and research capacity at HBCUs/MSIs. Provide an opportunity for this academic community to gain a better understanding of DoD funding opportunities, priorities, and processes to develop competitive proposals in response to DoD funding opportunities.

Action

On 19 Jun 18, ARO in partnership with the Office of the Under Secretary of Defense for Research and Engineering (OUSD (R&E)) hosted a workshop in Research Triangle Park, NC to provide technical assistance on DoD research proposal writing for the HBCUs/MSIs. Panels and break-out sessions included participants from seven federal agencies (e.g., AFOSR, ONR, DARPA, NSF) and 15 private sector businesses, as well as Technical Program Managers who spent time networking with attendees.

Result

This event was attended by over 210 registered participants from across the country, representing 25 HBCUs, and 10 MSIs. Participants (from academic leadership and researchers to sponsored program officials) received assistance in developing competitive proposals in response to DoD funding opportunities. The knowledge gained

by their attendance, the breakout sessions dialogues, and their interactions with the DoD program managers are expected to increase the number of opportunities available to the HBCUs, MIs, and their students. This event supported the Army Modernization Priority of Soldier Lethality and the ARL Core Competency of Network and Information Sciences.

Way Ahead

ARO will continue the dialogue initiated with the HBCU/MSI representatives at the event to further develop areas of shared scientific interests to bolster HBCU/MSI participation in DoD funding and research opportunities.

Partnership Research Initiative (PRI) Program

Challenge

The PRI Program was established as the next phase of what was previously known as Partnership in Research Transition (PIRT) Program that ended in FY16. The focus of the PRI Program is to advance innovative basic research leading to potential technology development in areas of strategic importance to the Army by bringing competitively selected Historically Black Colleges and Universities (HBCUs) and Minority-Serving Institutions (MIs) research teams into existing ARL Collaborative Research Alliances (CRAs) and Collaborative Technology Alliances (CTAs). The CTAs and CRAs are large collaborative centers focused on developing and transitioning research in Army critical areas. Four PRI projects from HBCUs/MIs joined the CTA/CRA consortia in early FY17.

Action

In FY18, the New Mexico Institute of Mining and Technology collaborated with Multiscale Modeling of Electronic Materials (MSME) CRA by investigating how Uncertainty Quantification techniques and Optimization algorithm can be used to complete the pipeline for robust design of nanoparticles. The City College of New York contributed to Cognition and Neuroergonomics (CaN) CTA by focusing on measuring the relevance of peripheral stimuli to neural reliability via experiments in combined EEG and eye-tracking during passive free viewing of films. The University of Texas at El Paso collaborated with Cyber Security CRA by designing and running behavioral game theory experiments on group decision making. Also, North Carolina Agricultural & Technical State University contributed to Materials in Extreme Dynamic Environments (MEDE) CRA with experiments to understand the effects of loading conditions such as temperature (from ambient to 773 K) and strain rate ($10^{-3} \text{ s}^{-1} \sim 10^3 \text{ s}^{-1}$) and their coupled effects on the mechanical properties and microstructure evolution of Mg-alloys.

Way Ahead

Continue to encourage greater HBCU/MI participation in university and industry led research teams in high interest scientific areas of Army interest.

ARO HBCU/MSI PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Expand participation of HBCU/MIs in ARO Core research programs through innovative outreach and program design.
- ▶ Enhance capacity of HBCU/MIs to compete effectively for ARO research grants.
- ▶ Provide outreach and research experiences to students at HBCU/MIs to increase awareness of Army research and career opportunities.

This success supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Network and Information Sciences



Protection Sciences



Human Sciences



Ballistics Sciences



Computational Sciences



Propulsion Sciences



RESULTS

- ▶ Highly innovative and collaborative research is being conducted by HBCU/MIs with ARL CTAs and CRAs, making scientific advances with potential to impact warfighter capabilities through follow-on technology development.

ARMY SMALL BUSINESS TECHNOLOGY TRANSFER (STTR) PROGRAM



Mr. Michael J. Smith

Program Manager, Department of the Army STTR program
ARO Information Sciences Directorate

Mr. Smith completed his B.S. in General Engineering at the United States Air Force Academy, Colorado Springs CO in 1987 and his MBA at West Coast University, Los Angeles CA in 1994.

He came to ARO in 2018 as the Program Manager for the Dept of the Army STTR program. Previously, he was the Dept of the Army SBIR Program Manager (2010 to 2017).

Since 1992, the Congressionally-mandated STTR program has provided Army-wide research and development opportunities for small business/research institution partnerships, with \$35M in annual funding in FY18. The Army STTR Program is diversified across all ARL core competencies (avg. funding percentages): Materials/ Mfg Sciences (24%), Computational Sciences (10%), Ballistics Sciences (3%), Human Sciences (3%), Propulsion Sciences (8%), Network and Information Sciences (27%) and Protection Sciences (11%). Other investment areas include Biomedical, Nuclear and Space platforms.

The following table lists the Army-wide STTR investments in 2018:

Organization	Number of Topics	Number of Ph 1 Projects (\$M)	Number of Ph 2 Projects (\$M)	Total FY18 STTR Investments (\$M)
CCDC – Aviation and Missile Center	1	2 (\$0.3)	5 (\$3.0)	\$3.3
CCDC – Armaments Center	1	2 (\$0.3)	3 (\$1.5)	\$1.8
CCDC- Army Research Lab (ARL) / Army Research Office (ARO)	14	30 (\$4.5)	22 (\$13.6)	\$18.1
CCDC – C5ISR Center	1	2 (\$0.3)	6 (\$3.2)	\$3.5
CCDC – Chem Bio Center	3	4 (\$0.6)	3 (\$2.0)	\$2.6
Corps of Engineers - ERDC	1	2 (\$0.3)	2 (\$1.0)	\$1.3
Medical Research & Development Command (MRDC)	1	3 (\$0.5)	1 (\$0.5)	\$1.0
CCDC – Soldier Center	2	4 (\$0.6)	2 (\$1.0)	\$1.6
CCDC – Ground Vehicle and Systems Center	1	2 (\$0.3)	3 (\$1.5)	\$1.8
FY18 TOTAL	25	51 (\$7.7)	47 (\$27.3)	\$35.0

Army STTR Program Partnership with Army Special Operations Command (USASOC) for Rapid Prototyping

Action

The Army's STTR program rapidly prototypes innovative technologies through small business/research institution partnerships to address a wide variety of opportunities to provide warfighter capabilities in all S&T ARL core competencies.

Result

In the year 2018, Simulation Technologies (SimTech) and the Univ of Alabama-Huntsville (UAH) commercialized an innovative technique (Obscure) for obscurant generation that adheres to the physics of a simulation, while achieving required simulation execution times. In the Army STTR Ph1 and PH2 efforts, SimTech developed complex scene flow field representation for obscurant particles, demonstrated the ability to inject obscurants at known mass rates, and established the correct thermal behavior of obscurant particles. The obscurant particle system software was developed and demonstrated for a number of scenes. The turbulent flow was compared to real-world data from the previously used voxel files and showed similar statistical characteristics while being able to operate in a "real" simulation time environment. Furthermore, the attenuation factors of the generated obscurants were studied and shown to be controllable to a much higher fidelity than previous voxel versions. Under an 5-year, Indefinite Delivery/Indefinite Quantity (IDIQ) STTR Phase 3, \$20M contract, SimTech/UAH will provide Obscure simulations as part of the larger DoD government simulations package used to evaluate missile system designs and performance. Obscure will become part of the Army Aviation and Missile Common Scene Generator (CSG) and future new scene generator technologies. These scene generators are interfaced with the integrated flight simulation (IFS) software that missile vendors supply to the government for evaluations of missile designs during varying development phases of the missile.

Way Ahead

In 2019, Army STTR has teamed with US Army Special Operations Command (USASOC) to pilot a rapid-response, prototyping-transition program, bringing innovative technologies direct to the warfighter. This ARO-USASOC partnership will involve all phases of R&D life cycle processes: requirement definition, vendor selection, prototype delivery, and follow-on testing and procurement/sustainment. In September 2019, ARO-USASOC will co-host an Industry Day, allowing small businesses and universities from across the nation to learn more about these USASOC warfighting special topics, as well as provide a forum for better teaming partnerships among the Industry Day participants, with anticipated stronger proposals and more innovative ideas/solutions for warfighter vetting.

The resulting USASOC special topics will yield \$12M in STTR PH1 and Ph2 investments in 2019.

This success supports these ARL Core Technical Competencies

Protection Sciences



Materials and Manufacturing Sciences



ARMY STTR PROGRAM—CURRENT SCIENTIFIC OBJECTIVES

- ▶ Army STTR program office is aligning investment portfolios with the Army Futures Command (AFC) modernization priorities via Critical Focus Teams (CFTs)-identified S&T needs and other AFC mission areas. Army STTR will also be coordinating with the AFC University Technology Demonstration Division (UTDD) as a transition-bridging partner for all innovative STTR prototypes developed but prior to fielding/sustaining with using commands.

ARO SPECIAL PROGRAMS: FY18 SUCCESS STORIES

ARO SCIENTIFIC SERVICES PROGRAM (SSP)



Dr. Brian Ashford

Program Manager, Scientific Services Program
Special Assistant to the Director
Army Research Office

Dr. Ashford completed his undergraduate studies at the University of Central Florida, receiving his B.S. in Electrical Engineering. He trained as a Computer Scientist at the Virginia Commonwealth University, receiving his Ph.D. in Computer Science in 2001.

He came to ARO in 2005 as the Special Assistant to the Director and became Program Manager for Scientific Services Program in 2009.

Ground Vehicle Operating System Build Project Supporting PEO Ground Combat System Tactical Combat Development System Research For Vehicle Support Device Architecture Hardening

This success supports
these ARL Core Technical
Competencies



**Materials and
Manufacturing Sciences**



Computational Sciences

Challenge

The Ground Vehicle Operating System (GVOS) team requires a thorough understanding of the security needs and the ability of the computer architecture to meet security goals and to meet Assessment and Authorization objectives. Specifically, the GVOS team identified a need to both research and investigate the security architecture, security design and the Security Enhanced Linux (SELinux) security policy. The effort was focused on the GVOS base Operating System and the Cross Domain Solution (CDS) hardware spin distribution to analyze and provide recommendations. The effort employed a value engineering project approach that focused on replacing the implemented enterprise based distribution architecture with an optimized embedded architecture that by its end design would be more flexible/scalable and modularized for both ease of use and allow for improved future improvements.

Action/Results

In 2016, a task using the SSP IDIQ was initiated with the effort to assess and evaluate a prototype Security Enhanced (SE) Maintenance Support Device (SE MSD) for the GVOS. The results of this activity were to develop a recommended architecture for implementation in the next phase of this research. To accomplish this a Technical Performance Measurement (TPM) analysis was conducted resulting in the decision to migrate to a newer version (2.0) along with developing, testing and installing an upgrade to the existing BIOS that would mitigate found vulnerabilities in operation.

Way Ahead

The next objective in this effort will be the actual creation of a new GVOS Base OS with updated BIOS. To accomplish this further research and investigation into the security architecture elements looking specifically at the GVOS targeted system hardware and software architecture spins. This analysis will be from a technical security perspective to provide guidance on how to optimally meet the security requirements of the system. These elements will then be assessed and evaluated to ensure defense in depth

security. To accomplish these goals a further evaluation of the system architecture and design will be needed. For development and implementation, the creation along with evaluation will be necessary to incorporate the final design that will ensure that the SELinux security policy and resulting system design are defensible from an Authorization and Assessment (A&A) perspective. The results will then be able to provide an optimized embedded Linux spin OS distribution for Tactical CDS class Line Replaceable Units (LRUs) that is flexible and modularized for use.



CHAPTER 4 | ACTIVE MURIS

This chapter provides a brief summary of all ARO MURIs that were active in FY18, organized according to the year the MURI began. Each MURI is driving fundamental studies that will also impact one or more ARL Core Competencies, as indicated in the following table.

TABLE OF CONTENTS FOR ARO ACTIVE MURIs WITH LINKS TO ARL CORE TECHNICAL COMPETENCIES

ARL CORE TECHNICAL COMPETENCIES (CTCs)

A brief description of each Core Technical Competency is provided after the table.

The CTCs are abbreviated as follows.

- ▶ Materials and Manufacturing Sciences (**M**)
- ▶ Computational Sciences (**C**)
- ▶ Ballistics Sciences (**B**)
- ▶ Human Sciences (**H**)
- ▶ Propulsion Sciences (**P1**)
- ▶ Network and Information Sciences (**N**)
- ▶ Protection Sciences (**P2**)

MURI Title	Pg #	M	C	B	H	P1	N	P2
New Start MURIs beginning in FY18								
Ab-Initio Solid-State Quantum Materials: Design, Production, and Characterization at the Atomic Scale	216	●					●	●
Multiscale Integration of Neural, Social, And Network Theory to Understand and Predict Transitions from Illness to Wellness	217				●			●
Multiscale Network Games of Collusion and Competition	217				●			●
New Materials from Dusty Plasmas	218	●						●
Quantum Control Based on Real-Time Environment Analysis by Spectator Qubits	219	●	●				●	
Science of Embodied Innovation, Learning, and Control	220				●	●		
Stimuli-Responsive Control of Protein-Based Molecular Structure	220	●						●
Towards a Multiscale Theory on Coupled Human Mobility and Environmental Change	221				●			●

MURI Title	Pg #	M	C	B	H	P1	N	P2
Active MURIs that began in FY17								
Abelian Bridge to Non-Abelian Anyons in Ultra-Cold Atoms and Graphene	222	●					●	●
Adaptive Self-Assembled Systems	222	●						●
Data-Driven Operator Theoretic Schemes to Prediction, Inference, and Control of Systems	223			●		●	●	
Dissecting Microbiome-Gut-Brain Circuits for Microbial Modulation of Cognition in Response to Diet and Stress	224				●		●	●
Realizing Cyber Inception: Towards a Science of Personalized Deception for Cyber Defense	224		●		●		●	
Semantic Information Pursuit for Multimodal Data Analysis	225		●				●	
Active MURIs that began in FY16								
Closed-Loop Multisensory Brain-Computer Interface for Enhanced Decision Accuracy	225		●		●		●	
Defining Expertise by Discovering the Underlying Neural Mechanisms of Skill Learning	226		●		●			
Discovering Hidden Phases with Electromagnetic Excitation	226	●					●	
Modular Quantum Systems	226		●				●	
Multimodal Energy Flow at Atomically Engineered Interfaces	228			●		●	●	
Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery	229	●				●		●
Spin Textures and Dynamics Induced by Spin-Orbit Coupling	229	●					●	
Socio-Cultural Attitudinal Networks	230				●		●	●
Active MURIs that began in FY15								
Advanced 2D Organic Networks	230	●					●	
Emulating the Principles of Impulsive Biological Force Generation	231	●		●		●		
Engineering Exotic States of Light with Superconducting Circuits	231		●				●	
Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications	232		●					
Imaging and Control of Biological Transduction Using Nitrogen Vacancy Diamond	233	●					●	●
Multi-Scale Responses in Organized Assemblies	233	●						●
Network Science of Teams	234				●		●	●
Noncommutativity in Interdependent Multimodal Data Analysis	235		●				●	
Active MURIs that began in FY14								
Attosecond Electron Dynamics	236			●		●		●
Force-Activated Synthetic Biology	236	●						●
Innovation in Prokaryotic Evolution	237		●		●			●

MURI Title	Pg #	M	C	B	H	P1	N	P2
Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials	237	●	●			●		
Multistep Catalysis	238	●				●		●
New Theoretical and Experimental Methods for Predicting Fundamental Mechanisms of Complex Chemical Processes	239	●				●		●
Ultracold Molecular Ion Reactions	240	●				●		●
Understanding the Skin Microbiome	240		●		●			●
Active MURIs that began in FY13								
Adversarial and Uncertain Reasoning for Adaptive Cyber Defense: Building the Scientific Foundation	241		●				●	●
Artificial Cells for Novel Synthetic Biology Chassis	241	●						●
Control of Complex Networks	242						●	
Materials with Extraordinary Spin/Heat Coupling	243	●				●		
Nanoscale Control, Computing, and Communication Far-from-Equilibrium	243		●			●		
Non-Equilibrium Many-Body Dynamics	244	●					●	
Theory and Experiment of Cocrystals: Principles, Synthesis, and Properties	244	●		●		●		
Active MURIs that began in FY12								
Associating Growth Conditions with Cellular Composition in Gram-negative Bacteria	245				●			●
Coherent Effects in Hybrid Nanostructures	245	●					●	
Evolution of Cultural Norms and Dynamics of Socio-Political Change	246		●				●	
High-Resolution Quantum Control of Chemical Reactions	247	●		●		●		
Multivariate Heavy Tail Phenomena: Modeling and Diagnostics	247		●					
Simultaneous Multi-Synaptic Imaging of the Interneuron	248				●		●	●
Surface States with Interactions Mediated by Bulk Properties, Defects, and Surface Chemistry	248	●				●	●	
Translating Biochemical Pathways to Non-Cellular Environment	249	●						●

ARL CORE TECHNICAL COMPETENCIES (CTCs)

The ARL technical strategy provides a comprehensive vision of the future technical landscape and is a critical component of its Research Management and Leadership Strategy. Key aspects of ARL's technical strategy are the seven Core Technical Competencies (CTCs) that guide the laboratory in identifying the scientific, technical, and analytical areas of vital importance to the Army of the future. These Core Technical Competencies

guide the laboratory in identifying and answering critical research questions in support of the Army's strategy for Multi-domain Operations and the required Army Functional Concepts. A brief summary of each CTC is provided in this section.

ARO's programs support each of the CTCs; however, as noted in CHAPTER 1, ARO's mission represents the most long-range Army view for changes in its technology, with system applications often 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities.



MATERIALS AND MANUFACTURING SCIENCES

Research in this CTC drives the discovery and creation of superior materials and devices needed to enable lasting strategic land power dominance. The future Army will require materials with unprecedented properties rapidly manufactured, grown, synthesized, and produced cost-effectively to enable highly mobile, information reliant, lethal, and protected Army platforms. This technology enables the Army to execute real-time, point-of-need design and fabrication thereby increasing agility and logistical efficiency from the microscale to the infrastructure scale.



COMPUTATIONAL SCIENCES

This CTC focuses on advancing the fundamentals of predictive simulation sciences, data intensive sciences, computing sciences, and emerging computing architectures to transform the future of complex Army applications. Foundational research in artificial intelligence and machine learning will enable autonomous cross-domain maneuver warfighting concepts with intelligent agents that rapidly learn, adapt, and reason faster than the adversary to fight and win in contested, austere, and congested environments.



BALLISTICS SCIENCES

This CTC focuses on gaining a greater understanding and discovery of mechanisms and on generating concepts and emerging technologies that support kinetic lethality. Knowledge and concepts gained will lead to unprecedented enhancements in weapons range, precision, and lethality for the mounted and dismounted Soldier against a spectrum of manned and unmanned ground and aerial combat systems.



HUMAN SCIENCES

This CTC focuses on identifying, creating, and transitioning scientific discoveries and technological innovations underlying Human Behavior; Human Capabilities Enhancement; and Human-System Integration that are critical to the U.S. Army's future operational superiority. Foundational research in human agent teaming provides human agent teams with the capability to perform as well as Soldier teams but with greater team resilience, faster, more informed team decision making, and reduced numbers and risk to Soldiers.



PROPULSION SCIENCES

This CTC focuses on gaining a greater fundamental understanding of advanced mobility and maneuver technologies that enable innovative vehicle configurations and subsystems architectures – critical to the future Army's movement, sustainment, and maneuverability. Foundational research in tactical unit energy independence enables energy-intelligent autonomous squad support systems that lighten the Soldier load, providing a more maneuverable, sustainable, and lethal force and intelligently monitor and distribute power on the move, reducing dismounted Soldiers' cognitive and physical load.



NETWORK AND INFORMATION SCIENCES

This CTC focuses on gaining a greater understanding of emerging technology opportunities that support intelligent information systems that perform acquisition, analysis, reasoning, decision-making, collaborative communication, and assurance of information and knowledge. Understanding gained through these research efforts will lead to technological developments that make it possible to manage, utilize, and maintain trust in information flows and geospatial situational awareness within the battlespace.



PROTECTION SCIENCES

This CTC focuses on gaining a greater understanding and discovery of mechanisms and generating concepts and emerging technologies that support protection systems that adapt to evolving threats, and the mechanisms of injury affecting the Warfighter. Foundational research in understanding and manipulating the physics of failure will lead to technologies that enable a broad array of resilient kinetic and non-kinetic protection systems and focuses on precise and accurate knowledge of materials/system failure for protection overmatch.

This project supports these ARL Core Technical Competencies



Materials and Manufacturing Sciences



Network and Information Sciences



Protection Sciences

OVERVIEW OF ACTIVE ARO MURIs

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES. These projects constitute a significant portion of the basic research programs managed by ARO; therefore, all of ARO's active MURIs are described in this section.

ACTIVE MURIS THAT BEGAN IN FY18

Ab-Initio Solid-State Quantum Materials: Design, Production, and Characterization at the Atomic Scale

The MURI topic authors and co-managers of this project are Dr. Pani Varanasi, Materials Science Division, and Drs. T.R. Govindan and Paul Baker, Physics Division

This MURI began in FY18 and was awarded to a team led by Professor Dirk Englund at the Massachusetts Institute of Technology. The goal of this MURI is to develop novel solid-state host materials with unique color centers exhibiting extraordinary quantum properties at room temperature (low spectral diffusion, long coherence times, etc.), determine the composition- processing- defect- property relationships governing these unique properties, and explore new concepts in quantum science (e.g., multi-photon states) enabled by these new materials. In the long term, discoveries from this MURI may lead to several key quantum technologies, including single and entangled-photon emission, quantum sensors, and quantum memories.

Significant progress has been achieved in understanding and utilizing the quantum properties of optically addressable nitrogen-vacancy (N-V) color centers in a diamond for quantum sensing and communication; however, further advances have been severely limited by difficulties in achieving exact placement of N-V centers, light collection due to the high refractive index of a diamond, large scale integration, and low qubit yield. Superior solid-state host materials such as 3D wide bandgap (WBG) semiconductors (e.g., SiC, ZnO.) and recently discovered atomically thin two dimensional (2D) van der Waals materials (e.g. h-BN, WSe₂). With varieties of optically addressable color centers (far beyond N-V centers) are very attractive alternatives to advance this science. In addition, these alternative materials could also offer new opportunities not yet accessible such as multi-photon states, interactions between color centers and non-linear quantum optics.

The MURI team will employ extensive expertise in ab-initio calculations, 2D materials fabrication and manipulation, 3D atomic imaging, and quantum spectroscopy to enable an integrated feedback loop of ab-initio design, fabrication, imaging, and characterization of quantum materials at the atomic scale. The team is also developing first-of-a-kind tools for reconstruction of 3D and 2D materials fully at the atomic scale and is developing revolutionary tools for nanometer-scale and even atomic-scale fabrication of quantum emitter systems. Lastly, the team will develop revolutionary chip-integrated quantum devices, including for quantum error corrected memories, entanglement-assisted sensors, and superradiance/sub-radiance control.

Multiscale Integration of Neural, Social, And Network Theory to Understand and Predict Transitions From Illness to Wellness

The MURI topic authors and co-managers of this project are Dr. Edward T. Palazzolo, Network Science Division, and Dr. Frederick Gregory, Life Sciences Division

This MURI began in FY18 and was awarded to a team led by Professor Emily Falk at the University of Pennsylvania. The goal of this MURI is to identify and model the coevolutionary dynamics of neural, cognitive, and social networks as people transition between illness and wellness while engaged in rapid integration treatment modalities. In the long term, discoveries from this MURI may reveal the neural and social network mechanisms involved in the transition from illness to wellness, and identify specific mechanisms that can be efficiently targeted to identify and alter the trajectory of adverse behavior (e.g., substance abuse) that may impact an individual's or team's safety.

Network science advances in social network analytics and brain connectomics allow for greater understanding of network effects impacting mood and brain states. New mathematical and statistical models allow for unprecedented analysis of information dissemination and decision making. Recent research shows the impact of complex interactions between people's behavior and the route of messages through their social networks with respect to smoking behaviors, obesity, and the spread of happiness. Likewise, studies exploring mindfulness show measurable impact on human behavior as well as communication patterns between several brain regions. With greater understanding of the impact of social network connections (such as family, friends, healthcare teams, and weak ties) on the behavior of individuals embedded in society, attention must be turned to developing a foundational science to quantify how individuals' bodies and minds are impacted by such social forces and vice versa. Neuroscience advances in mapping human neural activity can now be combined with social and cognitive network research to understand how people are connected to others and the causal impact of messages from their social network on changes in their brain states. These advances are relevant to understanding individuals who suffer from a variety of conditions such as PTSD, depression, anxiety disorder, substance abuse/addiction, and fibromyalgia/chronic pain.

This project is developing a multiscale model of intra-individual (i.e., neural, cognitive, physiological) and extra-individual (i.e., social) processes using an experimental manipulation of mindfulness and hypnosis, and characterizes interactions between baseline social network resources and regulatory strategy on dynamic neural responses and controllability, and downstream cognitive, physiological, and behavioral outcomes. The team will also experimentally perturb social network structure to further validate and refine the model.

Multiscale Network Games of Collusion and Competition

The MURI topic authors and co-managers of this project are Drs. Purush Iyer and Edward Palazzolo, Network Science Division

This MURI began in FY18 and was awarded to a team led by Professor Mingyan Liu at the University of Michigan. The goal of this MURI is to create a new compositional Game Theory framework for characterizing dynamics of interaction between multi-genre networks that could potentially share members or have weak links. In the long term, discoveries from this MURI may lead to new methods to drive improved agility of DoD responses to a broad spectrum of real-world security risks, as risk heterogeneity is fundamentally tied to scale, spanning nation states, and lone-wolf actors.

This project supports these ARL Core Technical Competencies

Human Sciences



Protection Sciences



This project supports these ARL Core Technical Competencies

Human Sciences



Protection Sciences



This project supports these ARL Core Technical Competencies



Materials and Manufacturing Sciences



Protection Sciences

Advances in scalable algorithmic techniques have made Game Theory a practical tool in a number of security related applications, especially in the context of adversaries and defenders modeled in a two-party game. In practical situations, however, there are social networks that underlie adversarial and defender groups, respectively, with potential weak links between members of opposing groups which are effectively used by both groups to infiltrate the other. Examples include the use of double-agents in infiltrating gangs and non-state adversarial groups, targeting of weak members in herd of deer, targeting of specific T-cells in tumors, etc. The dynamics of networks on networks is an ill understood problem, especially the use of weak links in strategic decisions. Furthermore, there are situations, such as in modeling adversarial groups embedded in an ally's host population, where the need to consider multi-party interactions at multiple scales becomes important. The host population while agreeing that the adversarial group is a threat to society is nevertheless sympathetic to the issues raised by the adversarial group. In such cases, an intuitive strategy might be to influence the sentiment of the masses while targeting individuals in the adversarial group with each success (or failure) of the defender resulting in a weakening (or emboldening, respectively) of the adversarial group. A meaningful mathematical analysis would require a multi-scale framework in which both coarse grained model (e.g., of the host population) and fine-grained model (of the social network of adversaries) need to be reasoned about.

This project is addressing the notion of abstraction and refinement in the context of network games, a class of n-party games where the network structure among the participants play a role in distributed strategies. The research is addressing inference and decision/control problems. The inference problems involve studies to identify multi-scale network structure from potentially incomplete observational data. The decision/control problems involve the design of effective control and intervention schemes at appropriate levels of the network in order to induce desirable individual as well as group behaviors.

New Materials from Dusty Plasmas

The MURI topic authors and co-managers of this project are Dr. Michael Bakas, Materials Science Division and Dr. James Parker, Chemical Sciences Division

This MURI began in FY18 and was awarded to a team led by Professor Uwe Kortshagen at the University of Minnesota. The goal of this MURI is to elucidate and control plasma-material dynamics, concomitant with complementary novel consolidation strategies, to realize robust plasma-based synthesis of 3-dimensional free-standing macrostructures via controlled consolidation of a wide range of discrete dust particles. In the long term, discoveries from this MURI may lead to directed energy applications, and advanced metamaterials with responsive properties for sensing and protection.

Research over the last decade has demonstrated that plasmas offer a means of levitating and manipulating "dust" particles of any material into controlled organized structures (i.e., plasma "crystals") of up to tens of centimeters in size. Concurrently, magnetic plasma confinement chambers have shown abundant material accumulation and fast convective transport. This accumulation motivated advances in the understanding of plasma magnetohydrodynamics (MHD), in addition to accurate predictions of the spatial distribution of dust particles and their individual trajectories. These efforts provide the scientific basis to realize a new paradigm in custom material design: consolidation of 3D free-standing materials and structures from plasma "dust." As plasmas can be created from any element and any material can be arranged in a plasma crystal, novel chemical reactions can be identified incorporating the free electrons, ions, and neutrals of a plasma to enhance manipulation and consolidation.

The MURI team is pursuing these studies at four highly interconnected levels: synthesis of particle building blocks, consolidation of these building blocks into macroscopic materials, materials design and characterization, and overarching theory and simulation. At the synthetic level, research will focus on advancing the state of the art from the current level of producing particles with homogeneous chemical composition of well-known phases to particle materials with nonequilibrium phases and composed of heterostructures. At the plasma consolidation level, the team will focus on controlling agglomeration to assemble macroscopic materials and elucidating the new physical mechanisms that will be encountered when incorporating dust crystals into free-standing macroscopic materials. Materials characterization will focus on establishing processing-structure-property relationships and on demonstrating new material design paradigms on testbed photonic materials.

Quantum Control Based on Real-Time Environment Analysis by Spectator Qubits

The MURI topic authors and co-managers of this project are Dr. T.R. Govindan, Physics Division and Dr. Samuel Stanton, Mechanical Sciences Division

This MURI began in FY18 and was awarded to a team led by Professor Kenneth Brown at Duke University. The goals of this MURI are to discover and devise approaches in which new, sensing “spectator” qubits enable real-time characterization and verification of classical environmental factors which, when uncontrolled, decohere qubits, and to develop optimal statistics and computer science-based techniques for collecting and analyzing spectator qubit data. In the long term, discoveries from this MURI have broad applicability to all areas of quantum information science, which is of great interest to DoD for potential needs in logistics, optimization, and the quantum simulation of materials.

A multidisciplinary focus on qubit physics, materials, fabrication, and operation has resulted in orders of magnitude improvements in key qubit performance metrics. Concurrently, new computer science, statistics, and engineering-based control techniques (such as Hamiltonian parameter estimation, machine learning, and robust control of classical fields) have enabled novel quantum control and feedback approaches. The time is opportune to expand the necessary multidisciplinary approach to a systems view of a complex quantum system operating in a classical environment by integrating the new control, feedback, and sensing concepts with qubit physics to provide the next order of magnitude improvement in qubit performance. Currently, in state-of-the-art, the qubit classical environment is rarely fully characterized during qubit operations in a qubit focused, rather than an integrated, system-focused experiment.

Qubits often provide the most sensitive and precise measurements of the variability and noise in the classical environment in which they operate and, consequently, have recently been developed as high-performance sensing and metrology tools. Recent quantum sensing advances provide the opportunity for real-time control of the qubit classical environment via a novel combination of qubit sensing, statistics, machine learning, and control approaches. In the new paradigm, qubit sensor-based characterization and verification of classical control fields conducted by a distinct set of “spectator” qubits located in the vicinity of the data qubits is visualized.

The MURI team is exploring this new paradigm by investigating the potential role of spectator qubits to quantify noise in quantum systems in real time and developing control strategies for high-performance operations that can be updated based on this information. The team will aim to characterize the noise using three methods: classical detectors, sensing with the data qubit, and real-time measurement of an integrated spectator qubit.

This project supports these ARL Core Technical Competencies

Computational Sciences



Network and Information Sciences



Materials and Manufacturing Sciences



This project supports these ARL Core Technical Competencies



Propulsion Sciences



Human Sciences

This project supports these ARL Core Technical Competencies



Materials and Manufacturing Sciences



Protection Sciences

Science of Embodied Innovation, Learning, and Control

The MURI topic author of this project is Dr. Samuel Stanton, Mechanical Sciences Division

This MURI began in FY18 and was awarded to a team led by Professor Daniel Koditschek at the University of Pennsylvania. The goal of this MURI is to explore the emergence of embodied learning and control within natural and synthetic systems operating in uncertain and changing environments to develop a methodology that predicts statistical synchronization patterns between intrinsic nonlinear dynamics, sensing, and actuation to enable real-time model learning and adaptation. In the long term, discoveries from this MURI may lead to new paradigms to design and develop agile and dexterous autonomous systems capable of operating in any terrain and under battlefield conditions.

Progress in agile robotics has been limited by control methods reliant on optimization about linearized passive dynamics and nearly ideal sensing. A robot's mobility depends on its capacity to move energy from a store to its mass center along the right degrees of freedom at the right time by actuating appendages toward the periphery where it meets the environment. Because there is a premium on getting this work done quickly, power (the rate at which actuators can move Joules) is a first scarce resource. The information required to direct these outward flows appropriately must also be generated from some prior memory combined with feedback decisions made using real-time streams. Moreover, since the purposes of mobility are inevitably linked to the robot's knowledge about the environment as well as the task, its ability to bring information from the periphery inward to the core at adequate rates inevitably presents a challenge simultaneous with and dual to its management of outward power flows.

A key focus of this research is to uncover the design of morphology, mainly the nature of limbs and body and their endowment with actuation and perceptual resources to promote effective interaction between energy and information streams over contrasting scales of length and time. The project also aims to discover how to evolve, use, and revise this endowment to achieve goal directed mobility and create new solutions to sensorimotor limitations and challenges represents the second focus.

Stimuli-Responsive Control of Protein-Based Molecular Structure

The MURI topic authors and co-managers of this project are Dr. Stephanie McElhinny, Life Sciences Division, and Dr. Dawanne Poree, Chemical Sciences Division

This MURI began in FY18 and was awarded to a team led by Professor Milan Mrksich at Northwestern University. The goal of this MURI is to enable dynamic control over the motion of protein domains via incorporation of stimuli-responsive dynamic bonding chemistries (excluding disulfide/thiol linkages) to control protein function. In the long term, discoveries from this MURI may lead to engineered enzymes that provide a readily accessible supply of molecules that are currently difficult or impossible to produce or protein biomaterials with tunable mechanical properties for broad applications from antibiotics to optical storage materials.

In biological systems, function is determined by structure. This structure-function relationship is particularly striking for proteins, where function is not solely determined by a static structure but is also dependent on dynamic motions of subdomains within the folded protein. The most commonly observed domain motions are hinge and shear motions that occur in response to ligand binding, such as the hinge closure of hexokinase upon binding of glucose. To realize the full promise of engineered biological systems, mechanisms to exert dynamic control over protein structure are critical to enable regulation of protein activity.

Chemists have recently demonstrated incorporation of non-natural chemical functional groups into proteins that support synthetic bonding chemistries, including novel protecting groups that provide control over the accessibility of bonding moieties using applied external stimuli. Moreover, a variety of dynamic chemical switches have been recently developed for synthetic polymer systems, expanding the range of dynamic bonding chemistries that could be used for protein engineering. In recent years, a variety of dynamic bonding schemes have been introduced into synthetic polymer systems that enable triggered structural changes in response to applied stimuli, such as light, changes in pH, mechanical stress, and redox conditions. In these structurally dynamic polymers, macroscopic changes originate from a change in the polymer's molecular architecture through the controlled formation/breakage of bonds, providing a linkage between molecular structure and macroscopic properties that is not typically inherent in synthetic polymer systems. These dynamic chemical switches provide an opportunity to bring structural, and thus functional, control to protein biopolymers.

The MURI team is employing these biological and chemical principles to design reversible covalent chemistries that can be used to regulate the conformations of protein-based structures and combine experimental and computational approaches to design and demonstrate large-scale conformational changes in protein-based structures in response to an applied stimulus.

Towards a Multiscale Theory on Coupled Human Mobility and Environmental Change

The MURI topic authors and co-managers of this project are Dr. Lisa Troyer, Life Sciences Division, and Dr. Derya Cansever, Network Science Division

This MURI began in FY18 and was awarded to a team led by Professor Rachata Muneeppeerakul at the University of Florida – Gainesville. The goal of this MURI is to create a theory integrating environmental change, human social system dynamics, and the corresponding interdependencies, to create and validate predictive models that capture these dynamics to anticipate the trajectory of environmental change and human effects on these changes. In the long term, discoveries from this MURI may lead to new tools to advance situational awareness and facilitate operational decision making, including the identification of emerging regions of potential conflict and risk.

Large-scale environmental changes such as floods, earthquakes, and droughts, can drive social mobility, which often precipitates new population migration patterns that in turn affect health, crime, and sociopolitical instability as humans relocate to access critical resources. However, the ability to model, theorize, and predict the interdependencies among environmental change and human social system dynamics remains a scientific challenge. Successful models of social-natural interdependence must account for the unique temporal/spatial scales of those systems, the factors determining action, and the natural and social constraints placed on those actions. These requirements pose substantial analytic challenges that no single discipline has been able to overcome.

This project is modeling population dynamics as movements of people over multilayer networks, each with interdependencies between natural environments and social institutions (e.g., governance structures, religious belief systems, kin networks). There will be four case studies that develop the modeling through natural disasters (e.g., hurricane), degrading economic systems (e.g., inflation), and two cases that integrate natural disasters and natural crises to capture secondary pushes that accelerate migration. Consequently, the project captures a range of effects across systems, including the ability to contrast sudden shocks and gradual degradations. An important feature of the modeling and testing approach is the use of Bayesian frameworks to assess the relative contributions of global sensitivity measures and expert opinion inputs on prediction of migration pathways.

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ACTIVE MURIS THAT BEGAN IN FY17

Abelian Bridge to Non-Abelian Anyons in Ultra-Cold Atoms and Graphene

The MURI topic authors and co-managers of this project are Drs. Paul Baker and Marc Ulrich, Physics Division, and Dr. Pani Varanasi, Materials Science Division.

This MURI began in FY17 and was awarded to a team led by Professor Andrea Young at the University of California - Santa Barbara. The goal of this MURI is to unambiguously realize new systems exhibiting the physics of anyons and to verify their topological protection against decoherence.

The unparalleled potential capabilities of quantum sensors and quantum computers hinge upon finding systems that can be well controlled and robust against decoherence. Anyons are quasiparticles with fractional quantum statistics that can exist in low-dimensional systems and whose topological properties allow one to create quantum states that are protected from many sources of decoherence. The experimental evidence of the fractional quantum Hall effect (FQHE) was a landmark demonstration of topological order and fractional (anyonic) statistics in a two-dimensional electronic system. However, the fragility of the FQHE states, in which interesting anyons can exist, have prevented this approach from advancing despite decades of improvements in material quality. On the other hand, the recent experimental realization of Majorana modes by several groups provides an important scientific opportunity to explore these intriguing quasiparticles and provides a possible pathway to realize more general anyonic systems. Advances in 2D materials, including topological surface states, new measurement capabilities, and recent theoretical progress in analyzing strongly correlated systems are rapidly advancing toward additional breakthroughs. This MURI effort will include studies of intrinsic anyons alongside extrinsic, synthetic approaches. The realization of these new robust states can pave the way for advances in universal decoherence free quantum sensors and computation as well as provide materials with currently unachievable properties that can be explored scientifically.

Adaptive Self-Assembled Systems

The MURI topic authors and co-managers of this project are Dr. John Prater, Materials Science Division and Dr. Dawanne Poree, Chemical Sciences Division.

This MURI began in FY17 and was awarded to a team led by Professor Anna Balazs of the University of Pittsburgh. The goal of this effort is to develop experimental and theoretical approaches to integrate microscopic forms of self-organization with a scalable means of additive 3D fabrication.

Recent research related to the bottoms-up assembly of material has demonstrated the feasibility of using tailored short-range interactions to drive the assembly of functional clusters and macromolecular assemblies that are capable of performing basic functions such as catalysis, energy harvesting, color change and actuation. However, it is not currently possible to go beyond basic functionality and establish hierarchically ordered systems that display complex functional integration and dynamic system response. In particular, multifunctional structures with specifically targeted properties and robust feedback and control mechanisms that can embody aspects of emergent behavior and robust reconfiguration remain well beyond reach. This effort aims to establish the knowledge and expertise base needed to enable the design and directed assembly

of nano-building blocks into complex, hierarchical 3D architectures capable of long-range control over multifunctional behavior and smart/dynamic responses using an additive 3D material assembly approach. The research is organized around three major thrusts: (i) assembly of microscale musculoskeletal frameworks, (ii) transduction of energy to enable functionality, and (iii) additive manufacturing of large-scale dynamic material systems. If successful, the research will enable the development of artificial "smart" materials and structures that exhibit tightly coupled capabilities for sensing environmental cues and then transducing energy to perform useful, situation-specific dynamic responses.

Data-Driven Operator Theoretic Schemes to Prediction, Inference, and Control of Systems

The MURI topic authors and co-managers of this project are Drs. Samuel Stanton and Matthew Munson, Mechanical Sciences Division.

This MURI began in FY17 and was awarded to a team led by Professor Igor Mezic of the University of California at Santa Barbara. The objective of this MURI is to develop a spectral decomposition theory that encompasses elements of ergodic theory, geometric theory of dynamical systems, and functional analysis via the spectral theory of linear infinite dimensional operators, control theory, machine learning for inference, prediction, and uncertainty analysis.

The MURI team approach will be to study systems in which there exists a model (e.g., the Navier-Stokes equation for fluid flow) as well as systems with no model (e.g., data streaming either from physical sensors or unstructured data). In both cases the team will develop efficient methods to extract the correct descriptive variables via spectral properties of associated operators. The main theory topics to be pursued will expand the current reach of spectral expansion analysis: 1) Stability theory for general attractors; treatment of continuous spectrum; 2) Uncertainty analysis and spectral expansion theory of the Perron-Frobenius operator for observable evolution; 3) Extensions to inference, prediction and control; 4) Spectral expansions for finite-time analysis; and 5) Non-smooth systems. The main numerical analysis topics to be pursued will expand the current reach of spectral expansion analysis: 1) Proofs of convergence of finite-dimensional approximations to spectral objects of the infinite-dimensional Koopman and Perron-Frobenius operators; 2) Algorithms for finite-time analysis in nonautonomous and control systems; 3) Algorithms for extraction of finite-dimensional models from data for inference, prediction and control; 4) Rigorous utilization of machine learning algorithms in spectral expansion theory; and 5) Utilization of spectral expansion theory for development of next-generation, real time computational tools for complex physics; applications to vortex dynamics. Finally, the team will investigate experimental and data analysis topics to expand the current reach of spectral expansion analysis: 1) Network monitoring problems arising in cybersecurity; 2) Experiments in locomotion for a class of hybrid oscillators; 3) Experiments on finite-time vortex stability; and 4) Experiments on one of the most vexing continuous spectrum problems - turbulence in fluid-structure interactions leading to large deformations. All of these areas span DoD interests such as helicopter dynamics, robotics, and cybersecurity. The developments in this MURI will lead to massive changes in design, data inference, and control of systems possessing a very broad set of nonlinear features.

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Dissecting Microbiome-Gut-Brain Circuits for Microbial Modulation of Cognition in Response to Diet and Stress

The MURI topic authors and co-managers of this project are Drs. Frederick Gregory and Robert Kokoska, Life Sciences Division.

This MURI began in FY17 and was awarded to a team led by Professor Elaine Hsiao at the University of California - Los Angeles. The objective of this MURI effort is to investigate how the community of microorganisms naturally residing in the human gut (i.e., the gut microbiome) alters cognitive performance in response to nutritional and physical stress.

Recent studies from several laboratories reveal that the responses of the human microbiome, and specifically the gut microbiome, responds to environmental factors (e.g., diet and stress) in a way that modulates host brain activity and behavior (Magnusson, et al., 2015) (Tillisch, et al., 2013) (Bravo, et al., 2011). The objective of this MURI is to uncover gut microbiome influence on host neurobiology, develop a layered cellular and systems-level model and theory of cognitive and behavioral control by commensal gut microorganisms and extract integrated neural, endocrine, immune and gut microbial interaction principles governing nutrition and physical stress response.

This MURI, if successful, will provide sophisticated predictive tools available to the academic community and DoD upon which more comprehensive biological studies could be performed to more completely understand causative effects throughout this complex networked system. These models have the potential to far exceed current state-of-the-art by offering a currently unavailable analytical framework for future discoveries. The long-term potential applications could be the rational design of probiotic regimens to ameliorate symptoms of anxiety-like disorders including PTSD, methods to manipulate the gut microbiome to affect human performance without the need for genetically engineering the human host. Outcomes of this MURI would also direct whole-force recommendations to the Army Surgeon General's Performance Triad and Brain Health Campaigns.

Realizing Cyber Inception: Towards a Science of Personalized Deception for Cyber Defense

The MURI topic authors and co-managers of this project are Dr. Cliff Wang, Computing Sciences Division and Dr. Lisa Troyer, Life Sciences Division.

This MURI began in FY17 and was awarded to a team led by Professor Milind Tambe at the University of Southern California. The goal of this MURI research is to gain scientific understandings to significantly advance the state of art in learning and modeling of adversarial mental states and decision processes, to create metrics quantifying information effectiveness in driving cognitive state change under the deception context, and to build an integrated framework of deception composition and projection methods to successfully manipulate adversaries' mental state and decision-making process to our advantages.

The research focuses on an innovative and comprehensive study of adaptive cognitive modeling, cyber deceptive game theory, and deception and monitoring systems. The effort consists of three major thrusts. The first thrust is focused on Deception and Monitoring Systems. Ultimately deceptive strategies developed by higher-level reasoning about the attacker must be realized in a system in such a way that the deceptions are convincing and their effects on the attacker can be effectively monitored. The second thrust is focused Cyber Deceptive Game Theory. Game theory provides a mathematical framework for modeling the interactions between defenders and

attackers in cybersecurity, which is an important foundation for developing a science of security. Developing game-theoretic models and algorithms for cybersecurity will allow richer modeling of adversarial interactions, a deeper understanding of deception and information manipulation tactics, and more effective response strategies. And finally, the third thrust is focused on Cognitive Modeling. Cognitive models provide a computational representation of human cognitive processes, their detailed mechanisms and limitations, and the knowledge upon which they operate. By taking advantage of human bounded rational decision behavior, where humans make decisions according to the constraints on the environment of their own cognitive limitation, the team will build a personalized model of adversary behavior.

Semantic Information Pursuit for Multimodal Data Analysis

The MURI topic author and manager of this project is Dr. Liyi Dai, Computing Sciences Division.

This MURI began in FY17 and was awarded to a team led by Professor Rene Vidal of Johns Hopkins University. The goal of this research is to establish the theoretical foundation for context and principles of information physics for data analysis that provide an analytical framework and computation algorithms for the characterization, analysis, and understanding of information content in multimodal data.

The proposed information-theoretic framework for characterizing information content in multimodal data combines principles from information physics with probabilistic models that capture rich semantic and contextual relationships between data modalities and tasks. These information measures will be used to develop novel statistical methods for deriving minimal sufficient representations of multimodal data that are invariant to some nuisance factors as well as novel domain adaptation techniques that mitigate the impact of data transformations on information content by finding optimal data transformations. The computation of such optimal representations and transformations for classification and perception tasks will require solving nonconvex optimization problems for which novel optimization algorithms with provable guarantees of convergence and global optimality will be developed. The uncertainty of such information representations derived from multimodal data will be characterized via novel statistical sampling methods that are broadly applicable to various representation learning problems. The information representations obtained from multiple modalities will be integrated by using a novel information theoretic approach to multimodal data analysis called information pursuit, which uses a Bayesian model of the scene to determine what evidence to acquire from multiple data modalities, scales, and locations and to coherently integrate this evidence. The proposed methods will be evaluated in various complex multimodal datasets, including text, images, video, cellphone data, and body-worn cameras.

ACTIVE MURI'S THAT BEGAN IN FY16

Closed-Loop Multisensory Brain-Computer Interface for Enhanced Decision Accuracy

The MURI topic authors and co-managers of this project are Dr. Cliff Wang (initially managed by Dr. Liyi Dai), Computing Sciences Division and Dr. Frederick Gregory, Life Sciences Division.

This MURI began in FY16 and was awarded to a team led by Professor Maryam Shanechi at the University of Southern California. The goal of this research is to create new methodologies for modeling multimodal neural activity underlying multisensory

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processing and decision making, and to use those methodologies to design closed-loop adaptive algorithms for optimized exploitation of multisensory data for brain-computer communication.

This research effort will contribute to the development of a new closed-loop brain-computer interface (BCI) framework for enhancing decision accuracy. The framework will collect multimodal neural, physiological, and behavioral data, decode mental states such as attention orientation and situational awareness, and will use the decoded states as feedback to adaptively change the multisensory cues provided to the subject, thus closing the loop. To realize such a framework, the effort will make fundamental advances on four fronts, constituting four research thrusts: (1) modeling multisensory integration, attention, and decision making, and the associated neural mechanisms; (2) machine-learning algorithms for high-dimensional multimodal data fusion; (3) adaptive tracking of the neural and behavioral models during online operation of the BCI; and (4) adaptive BCI control of multisensory cues for optimized performance. Complementary experiments with rodents, monkeys, and humans will be conducted to collect multimodal data to study and model multisensory integration, attention, and decision making, and to prototype a BCI for enhanced decision accuracy. The modeling efforts will span Bayesian inference, stochastic control, adaptive signal processing, and machine learning to develop: (1) novel Bayesian and control-theoretic models of the brain mechanisms; (2) new stochastic models of multimodal data and adaptive inference algorithms for this data; and (3) novel adaptive stochastic controllers of multisensory cues based on the feedback of users' cognitive state.

Defining Expertise by Discovering the Underlying Neural Mechanisms of Skill Learning

The MURI topic authors and co-managers of this project are Dr. Frederick Gregory, Life Sciences Division and Dr. Virginia Pasour, Mathematical Sciences Division.

This MURI began in FY16 and was awarded to a team led by Professor Scott Grafton at the University of California – Santa Barbara. The goal of this MURI is to uncover the temporal dynamics of neural substrates and cognitive processes engaged during skill learning and generate a definition of expertise based on the underlying neurocognitive computational advantages generated through learning.

Neuroscience, social psychology, and education are providing insights into neural and cognitive processes involved during skill learning which show structural and functional differences in multiple brain regions when compared between 'experts' and 'novices.' Typically, these comparisons involved a novice time point and an expert time point because of the difficulty measuring intracranial brain activity over the course of skill learning. Novel materials now enable long-term implantation of high density neural recording devices in humans and animal models. Emerging engineering breakthroughs enable spike and local field potential recording from multiple neuroanatomical sites in the brain simultaneously. However, a major analytical barrier prevents easily linking this high density data with data acquired through existing non-invasive electrophysiology techniques and other tools for determining structure-function relationships like magnetic resonance imaging.

The objective of this research is to develop tools and techniques that can both predict and explain from a neurobiological perspective why there are differences among individuals in their ability to develop expertise. The future force demands expert soldier performance across many tasks. In the long term, this basic research effort will provide a critical foundation for developing training methods based on computational and network neuroscience that are grounded in neurophysiology and neuroanatomy.

Discovering Hidden Phases with Electromagnetic Excitation

The MURI topic authors and co-managers of this project are Dr. Marc Ulrich, Physics Division and Dr. Pani Varanasi, Materials Sciences Division.

This MURI began in FY16 and was awarded to a team led by Professor David Hsieh at the California Institute of Technology. The goal of this project is to create new electronic states of matter that are unobtainable through conventional solid-state synthesis, which in the long term may lead to enhancements of electronic, optical, magnetic, and thermal material properties that would lay a foundation for future technology in many areas.

Nascent research has demonstrated unique phases that are not adiabatically accessible from the known phase diagram. Recent discoveries have involved photo-excitation of a material with an ultra-short pulse which non-adiabatically induces a phase distinct from that existing elsewhere on the ground state phase diagram. Examples include a non-equilibrium superconducting state in a BCS superconductor, a ferromagnetic state in an antiferromagnetic oxide, and a unique metallic state in a thin film of a dichalcogenide. The team is attempting to employ excitations across the entire electromagnetic (EM) spectrum, including with extremely high pulsed fields to design, realize, and manipulate new phases and responses in strongly correlated materials. Specifically, the team will focus on realizing new correlated states via the following approaches: (1) EM stimulated, bond selective, tuning of charge hopping parameters; (2) direct EM modification of magnetic exchange, order, and frustration; (3) continuous EM control of dimensionality and hybridization; and (4) EM excitation across kinetic barriers to realize metastable states that are thermodynamically inaccessible. Using these non-equilibrium methods, they will aim at realizing some of the most sought-after phenomena in condensed matter physics including collective charge/current ordered phases, bandwidth controlled metal to Mott insulator transitions, quantum disordered magnets such as valence bond solids and highly entangled quantum spin liquid states, and low dimensional and quantum critical electron liquids with no quasiparticle description.

Modular Quantum Systems

The MURI topic authors and co-managers of this project are Dr. T.R. Govindan, Physics Division and Dr. T. Curcic, AFOSR.

This MURI began in FY16 and was awarded to a team led by Professor Christopher Monroe at the University of Maryland – College Park. The goal of this research is to discover and explore modularity concepts for extensibility of small high-performance multi-qubit systems to larger systems with reduction of operational complexity.

A paramount challenge in exploring physical systems (qubits) suitable for quantum information processing has been the contradictory requirement for precise manipulation of a quantum state on demand while maintaining strict isolation from the environment. Significant progress has been made in addressing this challenge. Coherence in several physical qubit types has improved by orders of magnitude. High fidelity fundamental quantum logic operations have been demonstrated. This progress has extended to multi-qubit systems involving a few (order ten) qubits. Progress continues to be made in improving coherence and fidelity. In parallel, advances have been made in connecting physically separated qubits. Key to these rapid advances has been a multi-disciplinary approach involving physics, materials science, control engineering, computer science, and mathematics, among other fields. A scientific challenge to further progress in the field has been the difficulty to add qubits and increase system size, while maintaining coherence and high-fidelity operations. System size needs to be increased before useful functionality can be explored and realized. Adding qubits increases the complexity of interactions between the qubits and makes layout, fabrication, and quantum control for high fidelity operations extremely challenging. Additional unwanted interactions

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introduce new qubit degrees of freedom to entangle with the environment and degrade coherence and fidelity. Modularity is a general scientific approach to address such complexity in which the system is decomposed into repeatable blocks with well-defined and controlled interfaces and interactions between the blocks and has been applied successfully to classical systems. Here, a module can be envisaged as a functional group of qubits and an interface. Exploring modularity for complex quantum systems is nascent but provides a potential extensible approach in which small numbers of high performance qubits can be extended to groups of high performance qubits and interfaces capable of precise manipulation within the group, between groups when required, and isolation from the environment and other groups.

Any quantum information processing system must balance the need for coherent control of the many interacting qubits necessary for a large-scale quantum system with decoherence rates that generally grow with system size. The objective of this research is to investigate a modular approach to constructing multi-qubit systems suitable for quantum information processing, to determine whether a modular system can achieve this balance and study the associated costs and benefits of taking the approach. In the long term, this research may overcome barriers and lead to new capabilities in the logistics, optimization, and the quantum simulation of materials.

Multi-modal Energy Flow at Atomically Engineered Interfaces

The MURI topic authors and co-managers of this project are Dr. Ralph Anthenien, Mechanical Sciences Division and Dr. Robert Mantz, Chemical Sciences Division.

This MURI began in FY16 and was awarded to a team led by Professor Donald Brenner at North Carolina State University (initially led by Professor Jon Paul Maria). The objective of this MURI is to bring chemistry, materials, surface science, electrochemistry, and physics together to characterize and understand short time-frame sub-nanoscale non-equilibrium phenomenon at and across materials interfaces, especially the flow, redistribution and partition of energy near the interface by devising and applying novel experimental, theoretical, and simulation approaches.

The MURI team approach will be to explore, identify, and define multiple mechanisms of energy transfer/transduction at precision-engineered interfaces. Material systems that support energy transfer through lattice/molecular vibrations, plasmon-electron coupling, and chemical reactions will be studied. The synthesis, measurement, and modeling activities are co-designed to promote extreme-non-equilibrium excitations within nano-scale geometries; to observe in situ picosecond to microsecond property responses using newly developed methods; to inform new theoretical models; and to enable accurate multiscale prediction. The plan of work explores a simple, overarching, and materials-generic hypothesis: function and failure in advanced functional materials are overwhelmingly affiliated with interfaces, where the underlying mechanisms (desirable and undesirable) are regulated by or related to energy transfer/ transduction among inhomogeneous boundaries. Observing and understanding the local processes over multiple time and length scales will improve existing and design new materials systems, and to predict their performance.

Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery

The MURI topic authors and co-managers of this project are Dr. Dawanne Poree, Chemical Sciences Division and Dr. Stephanie McElhinny, Life Science Division.

This MURI began in FY16 and was awarded to a team led by Professor Michael Jewett at Northwestern University – Evanston. The goal of this MURI is to engineer the translation machinery to accept and polymerize non-biological monomers in a sequence-defined manner using non-traditional chain growth polycondensation chemistries (beyond amide and ester linkages).

Employing only four nucleotides and twenty amino acids, a plethora of biopolymers (e.g., proteins, DNA) with precisely-defined building block sequence gives these materials the ability to fold into higher-ordered structures capable of performing a variety of advanced functions such as information storage, self-replication, and signal transduction. The ability to extend comparable molecular-level sequence control to synthetic polymers, which have a much wider range of monomeric building blocks, has many scientific and technological implications, as it would enable precise control over structure-property relationships. Recent work has demonstrated that altering the sequence of short conjugated phenylene-vinylene oligomers can significantly modulate both electronic and optical properties. While greater complexity in function is anticipated for longer chain sequence-defined polymers, chemical routes to their synthesis have remained elusive. Conversely, biology synthesizes long sequence-defined polymers with extremely high efficiency and accuracy by employing templates to provide sequence information. More specifically, the ribosome, the workhorse of the translation machinery, is very adept at sequence-defined polymer synthesis through the successive condensation of amino acids (monomers), but primarily performs a single type of chemistry—amide bond formation via a chain-growth condensation polymerization. Co-opting the natural translation machinery to accept non-biological monomers is an attractive approach to synthesize non-biological polymers with the sequence control of biology. However, this approach is limited by cell viability constraints; thus, in vitro engineering of the translation machinery may offer unprecedented freedom of design to modify and control ribosome chemistry.

The objective of this research is to engineer and repurpose the translation apparatus (including the ribosome and the associated factors needed for polymerization) to produce new classes of sequence-defined polymers. In the long term, this research may enable a broad range of disruptive technologies having significant impact on DoD capabilities. Sequence control at the atomic level will give the greatest possible control over the emergent, macroscopic behavior of oligomers and polymers, leading to new advanced personal protective gear, sophisticated electronics, fuel cells, advanced solar cells, and nanofabrication, which are all key to the protection and performance of soldiers.

Spin Textures and Dynamics Induced by Spin-Orbit Coupling

The MURI topic authors and co-managers of this project are Dr. Joe Qui, Electronics Division, Dr. Evan Runnerstrom (initially managed by Dr. John Prater), Materials Science Division, and Dr. Marc Ulrich, Physics Division.

This MURI began in FY16 and is led by Professor Kang Wang at University of California, Los Angeles. The team consists of researchers from University of California, Irvine, California Institute of Technology, University of Nebraska, North Carolina State University, and University of Texas, Austin. The objective of this project is to strive for understanding of interfacial spin-orbit coupling (SOC) and exchange coupling in novel heterostructures and superlattices of topological insulators (TIs), 2D transition metal

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di-chalcogenides (TMDs), and ferro-(FM)/ferri-/antiferro (AFM)-magnetic materials. High quality heterostructures and superlattices containing TI/TMDs, TI/FM, and TI/AFM with the atomically sharp interface are to be synthesized and characterized, and these will constitute an ideal laboratory for enabling understanding of the interfacial SOC effects and relevant spin textures and dynamics.

This project will exploit the symmetry breaking and SOC-induced collective properties (i.e., magnetization, spin wave, and spin-orbit torque) in these heterostructures and superlattices to realize new types of topological matters such as magnetic Skyrmions, topological valley insulators, and topological spin wave (magnonic) crystals. It will also help facilitate the development of new emerging fields including spin-orbitronics, spin-valley-tronics, and axion electrodynamics. In addition, direct electrical field manipulation of spin or magnetization textures in these proposed systems through spin-orbit torque and magnetoelectric effects will be investigated for energy efficiency. The anticipated results of this project will broaden understandings of the fundamental science enabled by SOC and will establish suitable material frameworks for new spin-orbitronic devices in which multi-functional applications of spintronics for ultra-low power electronics at terahertz can be realized. This research will set a milestone in the spin-based applications by creating the knowledge base to enable novel, fast, and energy efficient technologies for communications and information processing.

Socio-Cultural Attitudinal Networks

The MURI topic authors and co-managers of this project are Dr. Purush Iyer, Network Sciences Division and Dr. Lisa Troyer, Life Sciences Division.

This MURI began in FY16 and was awarded to a team led by Professor Larry Davis at the University of Maryland (initially led by Professor V. S. Subrahmanian). The goal of this MURI is two-fold: (i) develop social science theories to understand latent communication among a small group of adversaries engaged in an effort to deceive, and (ii) develop multi-media analytics tools that formalize those social science theories as algorithms which can aid an observer who is not steeped in the local culture. While driven by practical problems, the objectives of the proposed work is not only to drive the development of new social science theories, but also to drive algorithmic advances in reasoning about joint probability distributions that arise from modeling uncertainties in human actions, speech, gestures, and intentions.

ACTIVE MURIS THAT BEGAN IN FY15

Advanced 2D Organic Networks

The MURI topic authors and co-managers of this project are Dr. Pani Varanasi, Materials Sciences Division and Dr. Dawanne Poree, Chemical Sciences Division.

This MURI began in FY15 and was granted to a team led by Professor William Dichtel at Cornell University. The objective of this research is to create stable, free-standing, single-monomer-thick 2D crystalline organic polymer nanosheets/covalent organic frameworks (COFs) with designed electronic (conductivity, mobility, charge storage), optical (resonances, nonlinearities), and structural properties.

The team will combine mechanistic studies, theory, microscopy, and spectroscopy to gain fundamental insight into the 2D polymerization processes. Specifically the team will address the challenges in 2D COF synthesis and characterization by focusing on the following three major research thrusts: (1) exploration of nucleation, bond exchange, and polymerization of 2D COFs to improve their long-range order and morphological

form and isolate 2D COFs as single crystals; (2) investigation of new conjugated linkage chemistries, topologies, and doping strategies to impart extensive electronic delocalization and useful optical and electronic properties; and (3) fabrication of new hybrid device heterostructures based on the interfacing of 2D COFs with newly emerging 2D inorganic materials such as transition metal dichalcogenides.

Emulating the Principles of Impulsive Biological Force Generation

The MURI topic authors and co-managers of this project are Dr. Samuel Stanton, Mechanical Sciences Division and Dr. Robert Kokoska, Life Sciences Division.

This MURI began in FY15 and was awarded to a team led by Professor Sheila Patek of Duke University. The objective of this MURI is to establish a unified theory for understanding biological and engineered impulsive systems. The MURI team will approach the objective using a thermodynamic framework linked to impulsive performance. This will require integrating mathematical analysis, tests of biological impulsive systems, and synthesis of impulsive materials and mechanisms. The thermodynamic framework consists of five phases: (1) chemical energy conversion in cellular biological systems that potentially circumvent the force-velocity tradeoffs of actin-myosin muscle mechanisms; (2) actuation tuned to spring loading through novel engineering implementations and informed by analyses of muscular and cellular thermodynamics; (3) potential energy storage through a diversity of biological materials, scales and geometries to inform synthetic elastic design; (4) rapid conversion from potential to kinetic energy (power amplification) – a defining feature of impulsive systems – through analyses of rate-dependence in biological materials/geometries, the mechanics of biological linkages and latches, and their directed synthesis into novel impulsive designs; and (5) environment-system interactions through rigorous tests of the effects of environmental substrates and geometries, internal dissipation and reset mechanisms for repeated use and mitigation of failure due to environmental forces. This research effort will lay the foundations for scalable methods for generating forces for future actuation and energy storing structures and materials.

Engineering Exotic States of Light with Superconducting Circuits

The MURI topic authors and co-managers of this project are Dr. T.R. Govindan, Physics Division and Dr. Joe Qui, Electronics Division.

This MURI began in FY15 and was awarded to a team led by Professor Andrew Houck at Princeton University. The goal of this MURI is to initiate significant new experimental and theoretical explorations to harness recent breakthroughs in superconducting systems and to demonstrate useful new states of light that can be brought to bear on broader goals in sensing, measurement, simulation, and computation. If successful, this research may lead to new tools for metrology, could provide key insight into non-equilibrium quantum systems, and will provide new resources for quantum communication and sensing.

Quantum optics, particularly in the domain of cavity quantum electrodynamics, provides a pathway to create and use large macroscopic quantum states with photons. Such states have been difficult to generate because atoms trapped in a cavity provide only weak nonlinearity to mediate photon-photon interactions, high photon loss introduces decoherence, low photon collection and detection efficiency decrease success probability, among other challenges. On the other hand, recent progress in superconducting qubits and high-quality microwave cavities for quantum computing has enabled orders of magnitude improvements in coherence, fast single shot high-fidelity readout, high-fidelity quantum operations, low photon loss, and better

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understanding of decoherence mechanisms. These advances have enabled early experiments that have demonstrated the creation of high-fidelity coherent states with several tens of photons. In addition, the new generation of superconducting devices opens up the opportunity for the exploration of new regimes of quantum optics involving quantum states of 100s of photons. Further advances are possible if, in addition to the physics of quantum optics, advanced microwave circuit engineering is brought to bear on the regime of low-power microwave signals to improve coherence and function, and materials science is employed to determine relationships between decoherence and defects in materials, surface chemistry, and interface quality. In turn, the superconducting systems and the quantum states created in them could also be used as sensitive probes of materials behavior, in particular of the origin and sources of decoherence and dissipation mechanisms.

The multidisciplinary research team led by Professor Houck combines the efforts of physicists and engineers who will develop the theoretical and experimental tools to establish new regimes of quantum optics using superconducting circuits. The new states of light established in this program provide new tools for metrology, could provide key insight into non-equilibrium quantum systems, and in the long term may lead to applications in quantum communication and sensing.

Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications

The MURI topic author and manager of this project is Dr. Joe Myers, Mathematical Sciences Division.

This MURI began in FY15 and is awarded to a team led by Professor George Karniadakis at Brown University. The goal of this research is to develop a new rigorous theoretical and computational framework enabling end-to-end fractional modeling of physical problems governed by conservation laws in large-scale simulations.

Despite significant progress over the last 50 years in simulating complex multiphysics problems using classical (integer order) partial differential equations (PDEs), many physical problems remain that cannot be adequately modeled using this approach. Examples include anomalous transport, non-Markovian behavior, and long-range interactions. Even well-known phenomena such as self-similarity, singular behavior, and decorrelation effects are not easily represented within the confines of standard calculus. This project seeks to break this deadlock by developing a new class of mathematical and computational tools based on fractional calculus, advancing the field in specific areas of computational mechanics. The fractional order may be a function of space-time or even a distribution, opening up great opportunities for modeling and simulation of multiscale and multiphysics phenomena based on a unified representation. Hence, data-driven fractional differential operators will be constructed that fit data from a particular experiment, including the effect of uncertainties, in which the fractional PDEs (FPDEs) are determined directly from the data.

The work is addressing the fundamental issues associated with the construction of fractional operators for conservation laws and related applications. An integrated framework is being pursued that proceeds from the initial data-driven problem to ultimate engineering applications. This general methodology will allow the development of new fractional physical models, testing of existing models, and assessment of numerical methods in terms of accuracy and efficiency. The integrated framework is based on a dynamic integration of five areas: (i) mathematical analysis of FPDEs; (ii) numerical approximation of FPDEs; (iii) development of fast solvers; (iv) fractional order estimation and validation, from data; and (v), prototype application problems.

Imaging and Control of Biological Transduction using Nitrogen Vacancy Diamond

The MURI topic authors and co-managers of this project are Dr. Frederick Gregory, Life Sciences Division and Dr. Paul Baker, Physics Division.

This MURI began in FY15 and was awarded to a team led by Professor Ronald Walsworth at Harvard University. The goal of this MURI is to further develop nitrogen vacancy nanodiamonds as non-biological quantum sensors and engineer a biological interface for actuating biological processes.

The nitrogen vacancy center lattice defect in diamond nanoparticles (NV-diamond) can retain activity in biological environments. Current applications of NV-diamond include quantum computing, nanoscale magnetometry, super-resolution imaging and atomic scale magnetic resonance imaging. These state-of-the-art applications involve NV-diamonds implanted in substrates; however recent breakthroughs have allowed isolated nano-diamond particles to be used as biosensing intracellular quantum probes for thermometry and bacterial tracking as well as extracellular quantum probes of ion channel operation. A key reason for NV-diamond sensitivity, including in the emerging biosensing applications, is that the spectral shape and intensity of optical signals from NV-diamond are sensitive to external perturbation by strain, temperature, electric fields, and magnetic fields. Biological sensory transduction relies upon highly evolved ion channel-based mechanisms that involve transducing environmental energy into a bioelectrical signal for intercellular communication. The recent demonstrations of NV-diamond's extreme sensitivity and localization now provide new research opportunities for transitioning NV-diamonds from passive sensors to novel biophysical interfaces whose perturbed energy emission can be used as a signal to control or modify sensory transducer molecular physiology and intra- and inter-cellular signaling.

This multidisciplinary project has four closely-coupled aims: (1) to optimize nitrogen vacancy nanodiamond synthesis; (2) to realize stable, biocompatible nanodiamond surface functionalizations; (3) to advance nitrogen vacancy sensitivity to chemical and biological systems; and (4) to enable nitrogen vacancy-based manipulation of biological transduction. Systematically studying the integration of nitrogen vacancy nanodiamonds with reconstituted or native ion channels will lead to greater understanding, and more importantly, will create a new paradigm for exogenous control of biological transduction events and the ability to uncover fundamental mechanisms with unprecedented spatial and temporal resolution. This endeavor may lead to significant scientific breakthroughs in understanding how to develop and control quantum systems capable of interfacing with, and controlling, biological systems. If successful, this research may improve future Army capabilities ranging from advanced artificial intelligence systems, early diagnosis and effective treatment of neurological disorders at the cellular level, novel human-machine interfaces, and antidotes to neurotoxins and pathogens.

Multi-Scale Responses in Organized Assemblies

The MURI topic authors and co-managers of this project are Dr. Dawanne Poree, Chemical Sciences Division and Dr. Evan Runnerstrom (initially managed by Dr. John Prater), Materials Science Division.

This MURI began in FY15 and was awarded to a team led by Professor Sankaran Thayumanavan, at University of Massachusetts - Amherst. The goal of this MURI is to understand how a molecular level detection can be propagated across a macroscopic material to affect a global property change that spans multiple length and time scales, and connecting these multi-scale events to realize signal amplification.

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Living systems are complex systems capable of receiving and using information, interacting with each other and their environment, and performing specific functions in response to stimuli occurring at multiple length and time scales. These sophisticated, innate behaviors are essential for survival, and can be extremely valuable in non-natural systems. A variety of synthetic systems have been engineered to respond to specific stimuli; however, the dynamics of the chemical and material processes and interactions occurring at multiple length and time scales throughout the signal-propagate-response pathway are inadequately understood to rationally design autonomous, “living” systems. The daunting challenge toward synthetic “living” systems is predictably propagating a molecular level change, generated through the selective sensing of a trigger, into a readily discernible macroscopic change in a material’s fundamental properties. This can only be addressed by developing a fundamental understanding of the chemical processes that occur at multi-scale levels – from molecular to nano to macroscopic length scales and from nanoseconds to hours. The inherent complexity involved in connecting these length scales, and the propagation and amplification of the resulting signals, requires a cohesive, multidisciplinary approach.

The integrated research plan led by Professor Thayumanavan is comprehensive and addresses each of the key elements needed to understand the fundamental multi-scale responses of adaptive systems occurring across length and time scales. The research is exploiting a variety of material platforms/approaches, including liquid crystal orientation, responsive amphiphiles, depolymerization, and biological/abiological composites with non-equilibrium molecular release to address propagation and amplification at multiple length scales. Each system approach is innovative, well-formulated, and focused on a complete understanding of the basic research principles controlling each approach. A variety of triggers will be considered throughout the effort including pH, temperature, redox, light, and enzymes. A key part of this effort is the ability to monitor dynamic changes during the cooperative reorganization processes at the interface, and this is addressed by integration of novel characterization techniques such as in situ liquid cell transmission electron microscopy. If successful, this fundamental research may ultimately enable Army-relevant technologies in stimuli-responsive systems such as self-decontaminating materials, controlled release for hazardous materials management or drug delivery, and responsive systems for self-healing and smart materials.

Network Science of Teams

The MURI topic author and manager of this project is Dr. Edward Palazzolo, Network Sciences Division.

This MURI began in FY15 and was awarded to Professor Ambuj Singh of the University of California at Santa Barbara, with participation from researchers at University of Southern California, University of Illinois at Urbana-Champaign, Northwestern University, and MIT. These seven faculty provide an excellent balance of multidisciplinary scholars from sociology, cognitive and social psychology, health and behavioral sciences, computer science, statistics, controls and dynamical systems, and network science. This MURI will advance the development of the Network Science of Teams by creating quantitative, network-based models of adaptive team behavior. This research will produce methods to optimize team performance under different contexts and resource constraints. The three thrusts of this research effort include: (i) teams as networks of interacting entities; (ii) analysis and models of dynamic team behavior over task sequences; and (iii) the network science of teams-of-teams or multi-team systems. The overarching objectives of this research are to build quantifiable informative models of team behavior as dynamical systems interacting over multiple networks, to develop rigorous models that relate interaction patterns and network evolution to task performance, to break new ground in the learning of optimal design of teams for

complex tasks, and to advance social science theories of team performance. This MURI will have a significant impact for the Army and DoD with respect to how it conducts work in teams. Results from this research may help the Army and joint forces assemble more effective teams and teams of teams, and provide guidance on task sequencing to support their highest goals.

Noncommutativity in Interdependent Multimodal Data Analysis

The MURI topic authors and co-managers of this project are Dr. Cliff Wang (initially managed by Dr. Liji Dai), Computing Sciences Division and Dr. T.R. Govindan, Physics Division.

This MURI began in FY15 and was awarded to a team led by Professor Rayadurgam Srikant at the University of Illinois at Urbana-Champaign (initially led by Professor Negar Kiyavash). The goal of this research is to establish a new comprehensive information theory for data analysis in noncommutative information structures intrinsic to hierarchical representations, distributed sensing, and adaptive online processing. Methods will be developed based on a novel theory in conjunction with the latest theories of information, random matrices, free probability, optimal transport, and statistical machine learning. They will be applied to the technical domains of causal inference, adaptive learning, computer vision, and heterogeneous sensor networks, and will be validated on real-data test beds including: (i) human action and collective behavior recognition, and (ii) crowd-sourcing in a network of brain-machine interfaces. The framework will provide answers to questions such as: What are the fundamental performance limits for noncommutative information collection and processing systems? What is the effect of side information on noncommutative information structures? How can low complexity proxies for performance be defined that approximate or bound noncommutative performance limits? How can noncommutativity of adaptive measurements be exploited to improve fusion, processing, and planning for distributed sensing systems? When do sequential or partially ordered designs offer significant performance gains relative to randomized designs like compressive sensing?

The approaches for extracting knowledge from complex irreversible partially ordered information structures include but are not limited to introduction of information divergence measures over noncommutative algebras, noncommutative relative entropy measures, and estimation techniques for such measures for high-dimensional data. Accounting for noncommutative structures will result in fundamentally new ways of fusing ordered, directed, or hierarchical organized information to support timely decisions at the appropriate level of granularity. Humans learn actively and adaptively, and their judgments about the likelihood of events and dependencies among variables are strongly influenced by the perception of cause and effect, whereas man-made systems only employ correlation-type symmetric measures of dependencies. Research will lead to the development of a theory of decentralized information sharing, causal inference, and active learning inspired by human decision making. Establishment of such a theory for sensing and data processing and application of it to grand challenges in computer vision and brain-computer interfaces will provide new capabilities, including improved time-sensitive, dynamic, multi-source information processing, actuation, and performance prediction guarantees.

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ACTIVE MURIS THAT BEGAN IN FY14

Attosecond Electron Dynamics

The MURI topic authors and co-managers of this project are Drs. James Parker and Richard Hammond, Chemical Sciences Division.

This MURI began in FY14 and was awarded to a team led by Professor Stephen Leone at the University of California - Berkeley. The goal of this MURI is to use attosecond light pulses to study the electron dynamics of atoms and small molecules.

Attosecond dynamics is a new field of scientific investigation which allows one to examine dynamics phenomena on the natural timescale of electronic processes in atoms, molecules, and materials. The timescale of microscopic dynamics in quantum systems occur at a timescale about one order of magnitude less than those for less-energetic processes, such as valence electronic transitions in molecules and semiconductor materials. A recent scientific breakthrough known as double optical gating has led to the production of broadband laser pulse widths as short as 67 attoseconds, making direct observation of a variety of electronic phenomena possible in real time. Thus, now there exist opportunities to examine a variety of electron-dynamics phenomena that arise from electronic motions in molecules on the attosecond timescale.

The objective of this research is to harness attosecond pulses of electromagnetic energy to probe matter (e.g., atoms, molecules, plasmas) at attosecond time scales for the real-time observation, control, and understanding of electronic motion in atoms, molecules, and materials. If successful, this research may lead to new synthesis methods, such as plasmonically-enhanced catalysis for the direct reduction of CO₂ to create fuels, new schemes and manufacturing methods for solar photovoltaics, nano-catalysts for fuel combustion, and high-density specific impulse propellants.

Force-activated Synthetic Biology

The MURI topic authors and co-managers of this project are Dr. Stephanie McElhinny, Life Sciences Division and Dr. David Stepp, Materials Science Division.

This MURI began in FY14 and was awarded to a team led by Professor Margaret Gardel at the University of Chicago. The goal of this MURI is to understand the mechanisms by which biochemical activity is regulated with mechanical force and reproduce the mechanisms in virtual and synthetic materials.

A critical aspect of synthetic biology systems is the targeted and controlled activation of molecules affecting biological function. Molecules can be activated by a variety of different signals, including chemical, optical and electrical stimuli, and synthetic biological circuits responsive to each of these stimuli have been successfully assembled. In recent years, the ability of mechanical force to serve as a biological signal has emerged as a unique and unexpected facet to biological activation. The rapidly growing field of mechanotransduction is beginning to reveal an extraordinary diversity of mechanisms by which mechanical forces are converted into biological activity. This field has been heavily influenced and driven through ARO-funded research, including a prior MURI (Potisek, et al., 2007) (Davis, et al., 2009) (Lenhardt, et al., 2010) (Burnworth, et al., 2014). Despite these rapid advances, mechanophores have never been incorporated into advanced synthetic material. This research area provides an exceptional opportunity to integrate biological activation by mechanical force into the growing toolbox of synthetic biology, and to establish unprecedented paradigms for the incorporation of highly specific force activation and response into new materials.

The objective of this research is to elucidate the molecular mechanisms by which living cells regulate intracellular biochemical activity with mechanical force, to reproduce and analyze these force-activated phenomena in synthetic and virtual materials, and to design and exploit optimized synthetic pathways with force-activated control. If successful, this research may dramatically influence future advances in engineered biological systems, materials synthesis and fabrication, and force-responsive and adaptive bio-mimetic material systems.

Innovation in Prokaryotic Evolution

The MURI topic authors and co-managers of this project are Dr. Micheline Strand, Life Sciences Division and Dr. Joe Myers (initially managed by Dr. John Lavery), Mathematical Sciences Division.

This MURI began in FY14 and was awarded to a team led by Professor Michael Lynch at Indiana University - Bloomington. The goal of this MURI is to model evolution in nutrient-deprived bacterial cultures, and then characterize changes in the genetic, metabolic, and social networks to create models that reflect the complexities of group evolution.

Classical Darwinian evolution selects for individuals that are better than others of their species in critical areas associated with reproductive fitness. For example, giraffes are selected for longer necks and cheetahs are selected for running speed. Similarly, single-celled organisms growing in rich media are selected for their ability to reproduce more quickly. In contrast, organisms that have run out of food can no longer simply improve at what they are already able to do; they are forced to innovate new methods to exploit previously untapped resources. In times of scarcity, even unicellular organisms rapidly evolve into complex societies with assorted subpopulations formed with unique and specialized skills. It is no longer an effective strategy to grow faster during starvation. In short, evolution during lean times requires the group to evolve as a whole, as each individual competes, cooperates, and depends on other members of the group.

The objective of this research is to develop a model of evolution in isolated independent cultures of organisms that are starving for months or years, and then model change in the genetic, epigenetic, transcriptomic, proteomic, metabolomic, and social networks to create experimentally-validated, mathematically-rigorous, and predictive models that accurately reflect the real complexities of group evolution. In the long term, the results of this research may lead to new applications for safer, economical food and water storage, new mechanisms to control and kill pathogens that will impact wound healing, diabetes, heart disease, dental disease, and gastrointestinal disease.

Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials

The MURI topic authors and co-managers of this project are Dr. Joe Myers, Mathematical Sciences Division and Dr. Pani Varanasi, Materials Science Division.

This MURI began in FY14 and was awarded to a team led by Professor Mitchell Luskin of the University of Minnesota. This research is co-managed by the Mathematics and Materials Science Divisions. The objective of this project is to develop efficient and reliable multiscale methods to couple atomistic scales to the mesoscopic and the macroscopic continuum for layered heterostructures. Layered heterostructures represent a dynamic new field of research that has emerged from recent advances in producing single atomic layers of semi-metals (graphene), insulators (boron nitride) and semiconductors (transition metal dichalcogenides). Combining the properties of these layers opens almost unlimited possibilities for novel devices with desirable, tailor-made electronic, optical, magnetic, thermal and mechanical properties. The vast range

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of possible choices requires theoretical and computational guidance of experimental searches; experimental discovery can in turn inform, refine, and constrain the theoretical predictions.

The proposed research will develop efficient and reliable strongly-linked multiscale methods for coupling several scales based on a rigorous mathematical basis. Specifically: 1) The rigorous coupling of quantum to molecular mechanics will be achieved by properly taking into account the mathematics of aperiodic layered structures; 2) The coupling of atomistic-to-continuum will be achieved by methods that can reach the length scales necessary to include long-range elastic effects while accurately resolving defect cores; 3) New accelerated hybrid molecular simulation methods, specially tailored for the weakly interacting van der Waals heterostructures, will be developed that can reach the time scales necessary for synthesis and processing by CVD and MBE; and 4) The simulations will be linked to macro and electromagnetic modelling to understand the physics and bridge to experimental investigation.

The challenge of modeling layered heterostructures will promote the development of strongly-linked multiscale models capable of handling many other materials systems with varied applications, including composites, meta-atoms (atomically engineered structures), and bio-materials that are of interest to the Army.

Multistep Catalysis

The MURI topic authors and co-managers of this project are Dr. Robert Mantz, Chemical Sciences Division and Dr. David Stepp, Materials Science Division.

This MURI began in FY14 and was awarded to a team led by Professor Shelley Minteer at the University of Utah. The goal of this MURI is to enable multi-step chemical reactions through the rational design of architectures that control the spatial and temporal pathways of precursors, intermediates, and products.

The Krebs cycle is an exquisite example of a regulated enzyme cascade which biological systems use to precisely control charge and reactant transport to produce energy for the cell. Conversely, man-made systems typically involve a series of conversions with intermediate purification steps to achieve a desired product, with yield losses that compound with each step. The current approach to achieve multi-step reactions in a single reactor is an arbitrary combination of multiple catalysts that is likely to lead to poor yield with unreacted intermediates or byproducts of reactants that have reacted with the incorrect catalysts. Recent breakthroughs in materials synthesis, such as self-assembly and lock-and-key type architectures, offer control of surface arrangement and topology that enable a much more effective approach to achieving multi-step reactions through control of spatial and temporal transport of reactants, electrons, intermediates, and products.

The objective of this research is to establish methodologies for modeling, designing, characterizing, and synthesizing new materials and structures for the design and implementation of multi-step catalysis. In particular, integrated catalytic cascades will be created from different catalytic modalities such that novel scaffolding and architectures are employed to optimize selectivity, electron transfer, diffusion, and overall pathway flux. If successful, this research will provide unique paradigms for exploiting and controlling multistep catalysis with dramatically enhanced efficiency and complexity. In the long term, the results may lead to new energy production and storage technologies.

New Theoretical and Experimental Methods for Predicting Fundamental Mechanisms of Complex Chemical Processes

The MURI topic authors and co-managers of this project are Drs. Ralph Anthenien and Samuel Stanton, Mechanical Sciences Division.

This MURI began in FY14 and was awarded to a team led by Professor Donald Thompson of the University of Missouri, Columbia. The objective of this MURI is to develop new approaches to predictive models for complex, reacting systems. It will develop supporting fundamental theory, perform supporting experiments, and validate resultant models and methods. The goal is to develop computationally efficient, predictive, accurate, robust methods to predict the molecular energy hypersurface, as well as relevant pathways and bifurcation topology for reacting coordinates.

The effort will accomplish the objectives via a comprehensive research program that will design efficient methods to predict and control the behavior of complex chemical reactions, such as combustion. Complexity is the salient challenge facing modern physical chemistry, and the proposed research will yield fundamental new methods to directly address the complexity of chemical reactions - from ab initio principles to the collective evolution of chemical populations. The research program is based on two ideas: (i) It is not necessary to describe or even know all the details, only those directly involved in the relevant pathway(s) from reactants to products, and (ii) it is essential to understand the role of fluctuations in the reaction rate, such as those that can be induced by the energetic environment and the many intermediates in combustion processes. The robust and accurate methods developed will determine the critical, emergent behaviors of complex overall reactions in non-equilibrium environments. They will accurately describe how a set of reactants undergoes sequential, branching reactions, passing through many transition states and transient species, to reach a final set of stable products. To gain an understanding of the role of fluctuations in reaction rates far from equilibrium, the researchers will focus on extracting information from the detailed dynamics of molecular species that are responsible for the fluctuations and, ultimately, the limits of traditional chemical kinetics. A synergistic approach will be undertaken for these overarching challenges that integrates the full range of rigorous fundamental theoretical methods. The specific objectives of the project leverage the complexity of kinetic phenomena, which are typically nonlinear, stochastic, multi-dimensional, strongly coupled, and can persist far from equilibrium by extreme variations in intensive properties. Some of the sub-objectives will be to: (1) fully leverage the predictive capabilities of state-of-the-art electronic structure theory; (2) Gain a better understanding of how complex chemistry occurs at a microscopic level over wide ranges of temperature and pressure; (3) Identify and control relevant dynamical variables that can be probed experimentally; (4) Elucidate the role of statistical fluctuations in energy and matter on chemistry by analyzing the underlying nonlinear dynamics and reaction networks; (5) Design tractable theoretical and computational methods with immediate experimental links and reduced dimensionality without diminishing predictive capabilities; (6) Formulate connections among complexity theories, nonlinear dynamics, network theory, and chemistry; and (7) Seek kinetic control of chemical and energetic phenomena on a macroscopic (rather than microscopic) level using nonlinear dynamics, optimal control, large deviations, and network theory.

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Ultracold Molecular Ion Reactions

The MURI topic authors and co-managers of this project are Dr. Paul Baker, Physics Division and Dr. James Parker, Chemical Sciences Division.

This MURI began in FY14 and was awarded to a team led by Professor Eric Hudson at the University of California - Los Angeles. The goal of this MURI is to design, create, and exploit molecular ion traps to explore precision chemical dynamics and enable the quantum control of ultracold chemical reactions.

Investments quantum computing and precision metrology have led to the development of molecular ion trap technology. These advances provide scientific opportunities that could be exploited to enable new methods for the study and control of chemical reactions. Recent scientific breakthroughs have been achieved in ultra-cold chemistry with neutrals, suggesting that ion chemistry would provide similar opportunities for an emerging new field. In addition, work in quantum information has led to the development of new types of arrayed micro-fabricated ion traps. Ion trap technology adds novel capabilities to molecular ion research, enabling new research opportunities in materials science, condensed-matter physics, chemistry, and biochemistry. In particular, ion traps offer dramatic improvements in chemical sensing at the single-ion level. Compared with molecular neutrals, trapped molecular ions offer interaction times much longer than what is possible in beam experiments, state preparation and readout is potentially cleaner, and Coulomb interactions with co-trapped atomic ions allow for general species-independent techniques.

The objective of this research is to develop and create molecular ion traps to exploit long interrogation time to study molecular ion chemistry, utilize extended interaction times and dipolar interactions in novel quantum control scenarios, improve chemical sensing using single-ion detection, and integrate the traps with various detectors. This research could ultimately leave to dramatically improved methods for creating and studying quantum dots, energetic compounds, biological reactions, and tools for detection of trace molecules.

Understanding the Skin Microbiome

The MURI topic authors and co-managers of this project are Dr. Virginia Pasour, Mathematical Sciences Division and Dr. Robert Kokoska (initially managed by Dr. Wallace Buchholz), Life Sciences Division.

This MURI began in FY14 and was awarded to a team led by Professor David Karig of the Applied Physics Lab at the Johns Hopkins University. The goal of this research is to develop a fundamental understanding of the forces shaping skin microbial communities across a range of spatial scales and to show how this understanding can be used to identify disease risk, predict disease outcomes, and develop tools for disease prevention.

Human skin harbors diverse bacterial communities that vary considerably in structure between individuals and within individuals over time. The extent of this variability and its implications are not fully understood, nor is it known whether it is possible to predict what types of bacteria one is likely to find on the skin of a given individual. As a result, there are no effective tools to predict individuals more likely to acquire skin bacterial infections, determine the efficacy of forensic analyses based on skin bacterial communities, nor to design novel strategies to limit the effective colonization of skin by pathogens. This project brings a variety of disciplines to bear on the problem: spatially explicit sampling, metagenomics, and bioinformatics will be used to characterize skin microbial communities at intermediate and large spatial scales. Molecular biology, analytical chemistry, and synthetic biology will be used to probe smaller-scale

processes that ultimately lead to larger-scale patterns. Ecological modeling will be used to integrate small-scale processes with large-scale patterns in order to arrive at a quantitative and predictive framework for interpreting the human skin microbiome. A series of models concentrating on four grand challenges will be built, tested and refined: (i) predicting microbiome composition based on environmental conditions, host state and microbe exposure patterns; (ii) identifying microbiome composition through volatile sensing; (iii) identifying disease risk through analysis of current state and anticipation of state changes (e.g., due to upcoming activities or events); and (iv) novel approaches for mitigating skin disease (e.g., optimal design of avoidance behavior, robustly engineered skin microbiomes). The results of this work will enable the manipulation of the skin microbiome in order to facilitate identification of allies, discourage bites of flying insects, predict skin disease, and as-yet-unimagined applications.

ACTIVE MURIS THAT BEGAN IN FY13

Adversarial and Uncertain Reasoning for Adaptive Cyber Defense: Building the Scientific Foundation

The MURI topic author and manager of this project is Dr. Cliff Wang, Computing Sciences Division.

This MURI began in FY13 and was awarded to a team led by Professor Sushil Jajodia of George Mason University. Adaptive defense mechanisms are essential to protect our nation's critical infrastructure (e.g., computing, communication, and control) from sophisticated adversaries who may stealthily observe defense systems and dynamically adapt their attack strategies. This research aims to create a unified scientific foundation to enable the design of adaptive defense mechanisms that will maximize the protection of cyber infrastructure while minimizing the capabilities of adversaries.

The research will leverage recent advances in security modeling, network science, game theory, control theory, software system and network protocol security to create the scientific foundation, which may include general models for defense mechanisms and the systems they protect as well as irrational and rational adversaries. This research will develop a new class of technologies called Adaptive Cyber Defense (ACD) that will force adversaries to continually re-assess, re-engineer, and re-launch their cyber attacks. ACD presents adversaries with optimized dynamically-changing attack surfaces and system configurations, thereby significantly increasing the attacker's workloads and decreasing their probabilities of success.

Artificial Cells for Novel Synthetic Biology Chassis

The MURI topic authors and co-managers of this project are Dr. Stephanie McElhinny, Life Sciences Division and Dr. Dawanne Poree (initially managed by Dr. Jennifer Becker), Chemical Sciences Division.

This MURI began in FY13 and was awarded to a team led by Professor Neal Devaraj at the University of California - San Diego. The goal of this MURI is to understand how biological and biomimetic synthetic cellular elements can be integrated to create novel artificial cells with unprecedented spatial and temporal control of genetic circuits and biological pathways.

The field of synthetic biology aims to achieve design-based engineering of biological systems. Toward this goal, researchers in the field are identifying and characterizing standardized biological parts for use in specific biological organisms. These organisms serve as chassis for the engineered biological systems and devices. While single-

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celled organisms are typically used as synthetic biology chassis, the complexity of even these relatively simple organisms presents significant challenges for achieving robust and predictable engineered systems. A potential solution is the development of minimal cells which contain only those genes and biomolecular machinery necessary for basic life. Concurrent with recent advances toward minimal biological cells, advances have also been made in biomimetic chemical and material systems, including synthetic enzymes, artificial cytoplasm, and composite microparticles with stable internal compartments. These advances provide the scientific opportunity to explore the integration of biological and biomimetic elements to generate an artificial hybrid cell that for the first time combines the specificity and complexity of biology with the stability and control of synthetic chemistry.

The objective of this MURI is to integrate artificial bioorthogonal membranes with biological elements to create hybrid artificial cells capable of mimicking the form and function of natural cells but with improved control, stability, and simplicity. If successful, these artificial cells will provide a robust and predictable chassis for engineered biological systems, addressing a current challenge in the field of synthetic biology that may ultimately enable sense-and-respond systems, drug-delivery platforms, and the cost-effective production of high-value molecules that are toxic to living cells (e.g., alternative fuels, antimicrobial agents).

Control of Complex Networks

The MURI topic authors and co-managers of this project are Dr. Randy Zachery, Network Sciences Division and Dr. Samuel Stanton, Mechanical Sciences Division.

This MURI began in FY13 and was awarded to a team led by Professor Raissa D'Souza of the University of California at Davis. The goal of this MURI project is to develop rigorous principles to predict and control behaviors of systems made of interdependent networks. This will be accomplished through an interdisciplinary approach synthesizing mathematical theories from statistical physics, control theory, nonlinear dynamics, game theory, information theory, system reliability theory, and operations research. The results will be informed and validated by empirical studies of real-world systems from nanoscale mechanical oscillators to collections of interdependent critical infrastructure systems, to data on coalitions and conflict in primate societies, and to longitudinal data on the evolution of political networks of nation states and task-oriented social networks in open source software. The focus is to develop new approaches that exploit network interdependence for network control, and this diversity of empirical testbeds is central to developing robust theoretical principles and widely applicable methods.

It is expected that this MURI will lead to: (i) network interventions that prevent cascades of failure in critical infrastructures; (ii) novel control schemes relying on control actions and local interventions; (iii) rigorous principles for multi-modal recovery of heterogeneous systems; (iv) shaping human social response via designed incentives that align human behavior with the capabilities of technological networks; (v) design of networks of nonlinear nanoelectromechanical oscillators that exploit coupling and nonlinearity to create coherent motion; (vi) new mathematical structures for representing and analyzing networks-of-networks, especially with respect to control theory; and (vii) fundamental bounds on controllability of interdependent networks and rigorous techniques to identify which network layers are easiest to steer.

The anticipated impact on DoD capabilities is broadly applicable to controlling a disparate collection of autonomous agents interacting through numerous networks in noisy, dynamic environments with a myriad of time-scales and length-scales. Results

can be applied to security (and restoration) of critical infrastructures, supply chains, political alliance dynamics (including upheavals such as Arab Spring), conflict, risk, social dynamics, and collective action. It is also reasonable to expect that there will be new levels of nanoscale functionality in the NEMs device developed, enabling new technologies and devices.

Materials with Extraordinary Spin/Heat Coupling

The MURI topic authors and co-managers of this project are Dr. Pani Varanasi, Materials Science Division and Dr. Mark Spector, ONR.

This MURI began in FY13 and was granted to a team led by Professor Roberto Myers of Ohio State University. The objectives of this project include understanding the structure-property relationships for coupling heat and spin current in various materials and synthesize magnetic materials with extraordinary and tunable thermal conductivity due to spins, understanding non-equilibrium phonon-magnon transport and the mechanisms behind Spin Seebeck Effect, and finally measuring and understanding phonon-magnon drag and phonon-electron drag in materials.

If successful, this project may lead to long-term applications such as temperature sensors, thermal spintronic devices, solid-state Spin Seebeck Effect-based power generators, thermal management in electronic and vehicular applications, and tunable thermal conductivity in materials via magnetic field, microwaves, and light.

Nanoscale Control, Computing, and Communication Far-from-Equilibrium

The MURI topic author and manager of this project is Dr. Samuel Stanton, Mechanical Sciences Division.

This MURI began in FY13 and was awarded to a team led by Professor James Crutchfield of the University of California at Davis. The objective of this MURI is to develop fundamental understanding to enable new synthetic nanoscale systems capable of behaving as information engines, performing tasks that involve the manipulation of both information and energy. Ultimately, a unified framework for understanding, designing, and implementing information-processing engines will be developed by a team of experts in information processing by dynamical systems, nonequilibrium thermodynamics, control theory, and nanoscale devices to search for and articulate the basic principles underlying the manipulation of information and energy by synthetic nanoscale systems. Theoretical predictions will be empirically validated in experimental nanoscale devices.

This research will enable new capabilities to: (i) quantify the intrinsic computation in nanoscale thermodynamic systems; (ii) to produce a thermodynamic theory for control and optimization of out-of-equilibrium nanoscale processes; and (iii) to accomplish experimental validation of the resulting thermodynamic principles of optimization and control of molecular agents. The results will provide a scientific foundation for future nanoscale devices with groundbreaking capabilities, ranging from efficient computation on microscopic substrates to the generation of directed motion. In the long term, this research may enable devices that can coordinate the molecular assembly of materials and novel substrates for information processing on radically smaller and faster scales. This research may lead to a new generation of faster, cheaper, and more energy efficient computing devices capable of manipulating large-scale, complex data structures, as well as self-organizing nanoscale motors capable of interfacing with the physical world with maximum power and efficiency.

This project supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Propulsion Sciences



This project supports these ARL Core Technical Competencies

Computational Sciences



Propulsion Sciences



This project supports these ARL Core Technical Competencies



Materials and Manufacturing Sciences



Network and Information Sciences

This project supports these ARL Core Technical Competencies



Materials and Manufacturing Sciences



Ballistics Sciences



Propulsion Sciences

Non-equilibrium many-body dynamics

The MURI topic authors and co-managers of this project are Drs. Paul Baker and Dr. Marc Ulrich, Physics Division.

This MURI began in FY13 and was awarded to a team led by Professor Cheng Chin at the University of Chicago. The goal of this MURI is to study fundamental non-equilibrium dynamics using cold atoms in optical lattices.

Dynamics far from equilibrium is of great importance in many scientific fields, including materials science, condensed-matter physics, nonlinear optics, chemistry, biology, and biochemistry. Non-equilibrium dynamics recently has taken on significance in atomic physics, where new tools will enable breakthroughs. In particular, optical lattice emulation is allowing one to gain insight, and potentially solve, traditionally intractable problems, including those out of equilibrium. Breakthroughs in other disciplines are also enabling a new look at non-equilibrium. In materials science, a recent pump-probe experiment enabled dynamical control of material properties (Goulielmakis, et al., 2007). Another example is in biochemistry, in determining the role that non-equilibrium phase transitions play in driven biochemical networks (e.g., canonical phosphorylation-dephosphorylation systems with feedback that exhibit bi-stability) (Qian, et al., 2006) (Ge, et al., 2011). Despite the ubiquitous nature of non-equilibrium dynamics, little scientific progress has been made due to the many challenges, including the difficulty in finding many-body systems that remain far from equilibrium on experimentally accessible time scales.

The objective of this MURI project is to discover how many-body systems thermalize from non-equilibrium initial states, and explore the dynamics of far-from-equilibrium systems. Given that non-equilibrium dynamics plays an important role in many scientific and engineering areas, such as quantum sensing and metrology, atomtronics, and quantum chemistry, this research could ultimately lead to the development of dynamic materials, devices for improved computation, precision measurement, and sensing.

Theory and Experiment of Cocrystals: Principles, Synthesis and Properties

The MURI topic authors and co-managers of this project are Dr. James Parker, Chemical Sciences Division and Dr. Pani Varanasi, Materials Science Division.

This MURI began in FY13 and was awarded to a team led by Professor Adam Matzger of the University of Michigan at Ann Arbor. This MURI team is investigating molecular co-crystal formation and the implications for controlling solid-state behavior.

The largely untapped potential for creating new molecular crystals with optimal properties is just beginning to be realized in the form of molecular co-crystallization. Co-crystallization has the potential to impact the macro-scale performance of many materials, ranging from energetic materials, to pharmaceuticals, and to non-linear optics. Unfortunately, the dynamics of molecular co-crystal formation is poorly understood. Molecular co-crystals contain two or more neutral molecular components that rely on non-covalent interactions to form a regular arrangement in the solid state. Co-crystals are a unique form of matter and are not simply the result of mixing two solid phases. Organic binary co-crystals are the simplest type and often display dramatically different physical properties when compared with the pure 'parent' crystals. A significant amount of research on co-crystal design has been carried out by the pharmaceutical industry for the synthesis of pharmaceutical ingredients. However, co-crystal design has

not been exploited in broader chemistry and materials science research areas. A recent breakthrough discovery demonstrates that co-crystallization can be used to generate novel solid forms of energetic materials.

The objective of this MURI is to develop a fundamental understanding of intermolecular interactions in the context of crystal packing, and to use the knowledge gained for the design of new co-crystalline molecular materials with targeted, optimized physical and chemical properties. In the long term, a better understanding and control of molecular co-crystallization has the potential to improve the properties of a variety of materials, including: energetic materials, pharmaceuticals, organic semiconductors, ferroelectrics, and non-linear optical materials.

ACTIVE MURIS THAT BEGAN IN FY12

Associating Growth Conditions with Cellular Composition in Gram-negative Bacteria

The MURI topic authors and co-managers of this project are Dr. Virginia Pasour, Mathematical Sciences Division and Dr. Robert Kokoska (initially Dr. Wallace Buchholz), Life Sciences Division.

This MURI began in FY12 and was awarded to a team led by Professor Claus Wilke of the University of Texas - Austin. The goal of this research is to develop methods to identify statistical association in multiple-input-multiple-output (MIMO) data using microbial growth and composition data.

To trace a microbe-causing disease to its source or to predict a microbe's phenotype in a given environment it is necessary to be able to associate the conditions under which bacteria have grown with the resulting composition of the bacterial cell. However, the input and output data complexity – multiple, heterogeneous, and correlated measurements – poses an interpretational challenge, and novel methods for analyzing, integrating, and interpreting these complex MIMO data are sorely needed. The research team is thus comprised of experts in statistics, computational biology, computer science, microbiology, and biochemistry, with the goal of producing the following outcomes: (i) development of novel linear and nonlinear mathematical methods to associate bacterial cellular composition with growth conditions; (ii) identification of the types and ranges of growth conditions that lead to distinguishable cellular composition; (iii) identification of key compositional markers that are diagnostic of specific bacterial growth conditions; and (iv) assessment of model uncertainty, robustness, and computational cost. The MURI has developed capabilities in several novel areas of data analysis and statistics such as the analysis of MIMO data, the integration of side information into regression models, and inverse optimization approaches. In addition, the types of approaches developed in this project will advance DoD capabilities in bacterial forensics and enable natural outbreaks to be distinguished from intentional attacks.

Coherent Effects in Hybrid Nanostructures

The MURI topic authors and co-managers of this project are Dr. Dawanne Poree (initially Dr. Jennifer Becker), Chemical Sciences Division and Dr. Richard Hammond, Physics Division.

This MURI began in FY12 was awarded to a team led by Professor Naomi Halas at Rice University. This MURI is investigating nanomaterials and how these materials can control the propagation of electromagnetic (EM) energy.

This project supports these ARL Core Technical Competencies

Human Sciences



Protection Sciences



This project supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Network and Information Sciences



This project supports these ARL Core Technical Competencies



Computational Sciences



Network and Information Sciences

Fundamental research involving metamaterials, quantum dots, plasmonic nanostructures, and other materials systems during the last decade has demonstrated the unique ability to selectively and actively control and attenuate electromagnetic energy from the far infrared through ultraviolet regions. The absorption frequency is dependent on shape, size, orientation, and composition of the nanomaterial. The nanoparticles act as antennae that redirect, focus or otherwise re-radiate the incoming energy. Because this is a resonance phenomenon, the media is generally transparent over a broad frequency range, with one or more resonances that absorb at specific frequencies. A goal in the control of the propagation of EM energy is the design of a material that absorbs over a broad frequency range and is transparent at one or more specific frequencies.

The objective of this research is to develop a fundamental understanding of nanomaterials to control the propagation of EM energy, with a particular emphasis on designing and investigating materials that have a broad spectrum absorption with a narrow, selective window of transmission. The MURI team is using a combination of computational, nanoscale fabrication, and characterization techniques to tailor electromagnetic properties for materials in specific, selected regions of the spectrum. The research team is focusing on designing, synthesizing, and combining nanoparticles and nanoparticle-based complexes to yield nanocomplexes exhibiting optimized coherent effects. This research may ultimately enable the design of materials with precisely-positioned transparency or absorbency windows that will impact Army applications in broadband scattering and absorption.

Evolution of Cultural Norms and Dynamics of Socio-Political Change

The MURI topic authors and co-managers of this project are Dr. Lisa Troyer (initially managed by Drs. Jeffrey Johnson and Elisa Bienenstock), Life Sciences Division, Drs. Virginia Pasour, Mathematical Sciences Division, and Dr. Bruce West, Information Sciences Directorate.

This MURI began in FY12 and was awarded to a team led by Professor Ali Jadbabaie at the University of Pennsylvania. This MURI is exploring the cultural and behavioral effects on societal stability.

Recent events involving the diffusion of socio-political change across a broad range of North African and Middle Eastern countries emphasize the critically important role of social, economic, and cultural forces that ultimately affect the evolution of socio-political processes and outcomes. These examples clearly demonstrate that radically different outcomes and chances for conditions of state stability result from the different institutional frameworks within these countries. It is well established in the social sciences that change in or evolution of institutions depends on the behavior patterns or culture of the people involved in them, while these behavior patterns depend in part on the institutional framework in which they are embedded. This dynamic interdependence of culture and institutional change means that the modeling of societal stability requires the coupling of individual modeling approaches describing such issues as trust and cooperation with models describing institutional dynamics.

The objective of this MURI is to develop fundamental theoretical and modeling approaches to describe the complex interrelation of culture and institutions as they affect societal stability. The research team is extending the cultural approaches from application to individuals, families, and villages, to address stability of the larger social group. The models developed in this MURI may ultimately provide guidance in data collection and analysis of data on local populations that can provide planners with models to anticipate the second or third-order ramifications of actions that impact local populations.

High-Resolution Quantum Control of Chemical Reactions

The MURI topic authors and co-managers of this project are Dr. James Parker, Chemical Sciences Division and Dr. Paul Baker, Physics Division.

This MURI began in FY12 and was awarded to a team led by Professor David DeMille at Yale University. This MURI is exploring the principles of ultracold molecular reaction, where chemical reactions take place in the sub-millikelvin temperature regime.

The study of ultracold molecular reactions, where chemical reactions take place in the sub-millikelvin temperature regime, has emerged as a new field in physics and chemistry. Nanokelvin chemical reactions are radically different than those that occur at "normal" temperatures. Chemical reactions in the ultracold regime can occur across relatively long intermolecular distances, and no longer follow the expected (Boltzmann) energy distribution. The reactions become heavily dependent on nuclear spin orientation, interaction strength, and correlations. These features make them a robust test bed for long-range interacting many-body systems, controlled reactions, and precision measurements.

The objectives of this MURI are to develop a fundamental understanding of the nature of molecular reactions in the nanokelvin temperature regime and to extend the cooling technique previously demonstrated by Professor DeMille (through a previous ARO award) to other molecular candidates (Shuman, et al., 2010). The researchers will focus will be on the implementation of novel and efficient laser cooling techniques of diatomic molecules, and to understand the role of quantum effects, including the role of confined geometries on molecules that possess vanishingly-small amounts of thermal energy. This research could ultimately lead to new devices or methods that explicitly use quantum effects in chemistry, such as the precision synthesis of mesoscopic samples of novel molecular compounds, new avenues for detection of trace molecules, and a new understanding of combustion and atmospheric chemical reactions.

Multivariate Heavy Tail Phenomena: Modeling and Diagnostics

The MURI topic manager is Dr. Joe Myers (initially co-authored and co-managed by Drs. Harry Chang and John Lavery), Mathematical Sciences Division.

This MURI began in FY12 and was awarded to a team led by Professor Sidney Resnick of Cornell University. The project aims to: (i) develop reliable diagnostic, inferential, and model validation tools for heavy tailed multivariate data; (ii) to generate new classes of multivariate heavy tailed models that highlight the implications of dependence and tail weight; and (iii) to apply these statistical and mathematical developments to the key application areas of network design and control, social network analysis, signal processing, network security, anomaly detection, and risk analysis.

More specifically, the researchers are investigating and developing statistical, mathematical, and software tools that will provide: (i) flexible and practical representations of multidimensional heavy tail distributions that permit reliable statistical analysis and inference, allow model discovery, selection and confirmation, quantify dependence, and overcome the curse of dimensionality; (ii) heavy tailed mathematical models that can be calibrated which clearly exhibit the influence of dependence and tail weight and which are appropriate to the applied context; and (iii) exploitation of the new tools of multivariate heavy tail analysis to enable the study of social networks, packet switched networks, network design and control, and robust signal processing.

This project supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Ballistics Sciences



Propulsion Sciences



This project supports these ARL Core Technical Competencies

Computational Sciences



This project supports these ARL Core Technical Competencies



Human Sciences



Network and Information Sciences



Protection Sciences

This project supports these ARL Core Technical Competencies



Materials and Manufacturing Sciences



Propulsion Sciences



Network and Information Sciences

Simultaneous Multi-synaptic Imaging of the Interneuron

The MURI topic authors and co-managers of this project are Dr. Frederick Gregory (initially managed by Dr. Elmar Schmeisser), Life Sciences Division and Dr. Joe Qiu (initially managed by Dr. Dwight Woolard), Electronics Division.

This MURI began in FY12 and was awarded to a team led by Professor Rafael Yuste at Columbia University. The research team is exploring how individual neurons act as computational elements.

Interneurons are highly networked cells with multiple inputs and outputs. It has been to date impossible to record all the inputs and outputs from even a single living interneuron with synaptic levels of resolution in a living brain. While there is information on the morphological, physiological, and molecular properties of interneurons as a class and on their general synaptic connections, there is still little direct information on the functional roles of individual interneurons in cortical computations, and especially not on how each synapse relates to all the others within a single cell. Coupled with tagging via fluorescent molecules and/or chromophores and genomic modifications to control co-expression, electro-optical imaging may provide a solution due to its ability to achieve subwavelength resolution across a relatively wide field of view.

The objective of this research is to explain and quantitatively model the entire set of neurotransmitter flows across each and every individual synapse in a single living interneuron, with experimental preparations ranging from cell culture systems through model neural systems. The research team will use genetically-engineered mice expressing specific labels in specific interneurons, high-throughput electron microscopy, and super-resolution imaging techniques to reveal the connectivity and the location of the synapses. This research may ultimately provide models that predict the information transitions and transformations that underlie cognition at the smallest scale where such activity could take place. These models could revolutionize the understanding of how human brains instantiate thought and may lead to applications such as neural prostheses.

Surface States with Interactions Mediated by Bulk Properties, Defects and Surface Chemistry

The MURI topic authors and co-managers of this project are Dr. Marc Ulrich, Physics Division and Dr. Pani Varanasi, Materials Science Division.

This MURI began in FY12 and was awarded to a team led by Professor Robert Cava at Princeton University. This project is exploring the recently-discovered class of materials known as topological insulators.

A topological insulator is a material that behaves as a bulk insulator with a surface that is metallic (permitting the movement of charges on its surface) due to the fundamental topology of the electronic band structure. This topological property separates it from nearly every other known phase of matter. Instead of a phase being due to a broken symmetry (such as results in crystalline, magnetic, superconducting, etc., phases), the property of metallic surfaces results from a transition between two topologically distinct phases: trivial and non-trivial. This is a parallel to the quantum Hall effect which also results from topology but it has two dramatic enhancements. First, it is not limited to two dimensions, and second, the physics should be able to survive to ambient conditions if materials are sufficiently clean. The quantum Hall effect and related phenomena require ultra-low temperatures and high magnetic fields to induce them. Topological insulators do not.

The objective of this research is to advance the discovery, growth, and fabrication of new bulk- and thin-film-based topologically-stabilized electronic states in which electron-electron interactions play a significant role. The researchers are bringing strong materials science, chemistry, and surface science approaches to bear on the study of the novel properties of topological insulators. Research in this area has great potential for long-term benefits for the Army, such as electronically-controlled magnetic memory and low-power electronics.

Translating Biochemical Pathways to Non-Cellular Environment

The MURI topic authors and co-managers of this project are Dr. Stephanie McElhinny, Life Sciences Division and Dr. John Prater, Materials Science Division.

This MURI began in FY12 and was awarded to a team led by Professor Hao Yan at Arizona State University. This MURI is exploring how biochemical pathways could potentially function in a non-cellular environment.

Cells provide a precisely organized environment to promote maximum efficiency of biochemical reaction pathways, with individual enzymatic components organized via multisubunit complexes, targeted localization in membranes, or specific interactions with scaffold proteins. The eventual translation of these complex pathways to engineered systems will require the ability to control and organize the individual components outside of the natural cellular environment. Although biological molecules have been successfully attached to inorganic materials, this process often requires chemical modification of the molecule and can restrict its conformational freedom. An alternative approach to maintain biological activity outside of the cell, while preserving conformational freedom, is to encapsulate enzymes within specialized materials or structures. Unfortunately, surface patterning of current encapsulating agents has not achieved the precision required to replicate the organizational capabilities of the cell.

The objective of this research is to develop the scientific foundations needed to design, assemble, and analyze biochemical pathways translated to a non-cellular environment using 3D DNA nanostructures. The MURI team is using DNA nanostructures to direct the assembly of selected biochemical pathways in non-cellular environments. The focus of this research is to develop the scientific foundations needed to translate multi-enzyme biochemical reaction pathways from the cellular environment to non-biological materials. The ability to translate biochemical reaction pathways to non-cellular environments is critical for the successful implementation of these pathways in DoD-relevant technologies including responsive material systems, solar cells, sensor technologies, and biomanufacturing

This project supports these ARL Core Technical Competencies

Materials and Manufacturing Sciences



Protection Sciences





CHAPTER 5 | BROAD AGENCY ANNOUNCEMENT FY18 ARCHIVE

ARO is closely involved in writing or contributing to a wide range of Broad Agency Announcements (BAAs) across DoD and the Army. However, the chief BAA used by ARO to complete its mission is often referred to as the ARO Core BAA. The ARO BAA is open for submissions at any time throughout the year. This chapter provides a direct copy of the publicly-available ARO Core BAA for reference and archival. This BAA also provides descriptions of the research interests for the ARO Core Programs

The current ARO Core BAA, as of the final day of FY18, was W911NF-17-S-0002-03 (i.e., Modification 3 of the FY17-FY22 BAA with eligible submission dates 1 April 2017 – 31 March 2022).

ARMY RESEARCH OFFICE
BROAD AGENCY ANNOUNCEMENT FOR
FUNDAMENTAL RESEARCH



W911NF-17-S-0002-03
01 April 2017 – 31 March 2022

ISSUED BY:

**U.S. Army Contracting Command
Aberdeen Proving Ground
Research Triangle Park Division
P. O. Box 12211
Research Triangle Park, NC 27709-2211**

Special Notes

1. Formatting of the Announcement

The following table provides an overview of the outline structure of this announcement:

I.							
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		1.					
			a.				
				i.			
					(1)		
						(a)	
							(i)

- 2. See Appendix 1 for a Table of Acronyms used in this announcement.
- 3. See Appendix 2 for a Schedule of Amendments. Applicants are encouraged to frequently check Grants.gov and FBO.gov for updates and amendments to this BAA.

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I. OVERVIEW OF THE FUNDING OPPORTUNITY

The purpose of this Broad Agency Announcement (BAA) is to solicit research proposals in the engineering, physical, life, and information sciences for submission to the Army Research Office (ARO) for consideration for possible funding.

NOTE: For ease of reference and clarity, the Army Research Laboratory (ARL) has two BAAs. This BAA for ARO, and another one for the ARL Directorates (Computational and Information Sciences Directorate, Human Research and Engineering Directorate, Sensors and Electron Devices Directorate, Survivability/Lethality Analysis Directorate, Vehicle and Technology Directorate, and Weapons and Materials Research Directorate).

ARO is focused exclusively on extramural basic research, and is responsible for the vast majority of ARL's extramural research programs and funding. The ARL Directorates are focused on executing in-house research programs, with a significant emphasis on collaborative research with other organizations in an Open Campus setting (Open Campus opportunities are described in detail at <http://www.arl.army.mil/www/default.cfm?page=2357>). However these in-house Directorates do fund a modest amount of extramural research in certain specific areas, and ARL's BAA describes those areas of interest.

ARL has an overarching technical strategy to support Strategic Land Power Dominance for the Army of 2030 and beyond. The strategy is based on eight Science and Technology (S&T) campaigns: Extramural Basic Research, Computational Sciences, Materials Research, Sciences-for-Maneuver, Information Sciences, Sciences-for-Lethality and Protection, Human Sciences, and Assessment and Analysis. These campaigns are structured to create discovery, innovation, and transition of technologies leading to Power Projection Superiority, Information Supremacy, Lethality and Protection Superiority, and Soldier Performance Augmentation for Strategic Land Power Dominance. Further details are described in the *ARL Technical Strategy* document (www.arl.army.mil). ARO is responsible for the Extramural Basic Research Campaign, and that Campaign is aligned with ARL Core Campaign Enablers (CCEs) as referenced in this BAA. Additional information about the Campaigns can found in the ARL S&T Campaigns document (also at www.arl.army.mil). The aforementioned documents are subject to further refinements which may result in taxonomy inconsistencies. These inconsistencies should not affect the efficacy of the BAA to present a complete portfolio of essential ARO research.

Proposals are sought from institutions of higher education, nonprofit organizations, state and local governments, foreign organizations, foreign public entities, and for-profit organizations (i.e. large and small businesses) for scientific research in mechanical sciences, mathematical sciences, electronics, computing science, physics, chemistry, life sciences, materials science, network science, and environmental sciences. Proposals will be evaluated only for fundamental scientific study and experimentation directed toward advancing the scientific state of the art or increasing Hbasic knowledge and understanding. Proposals focused on specific devices or components are beyond the scope of this BAA.

Proposals are expected to be for cutting-edge innovative research that could produce discoveries that would have a significant impact on enabling new and improved Army operational capabilities and related technologies. The specific research areas and topics of interest described in this

document should be viewed as suggestive, rather than limiting. ARO is always interested in considering new innovative research concepts of relevance to the Army. Additional information about ARO areas of interest can be found on the ARL website:

<http://www.arl.army.mil/www/default.cfm?page=29>.

In order to conserve valuable applicant and Government resources, and to facilitate determining whether a proposed research idea meets the guidelines described herein, prospective applicants contemplating submission of a whitepaper or proposal are strongly encouraged to contact the appropriate Technical Point of Contact (TPOC). The TPOCs' names, telephone numbers, and e-mail addresses are listed immediately after each research area of interest. If an applicant elects to submit a whitepaper, it should be prepared in accordance with the instructions contained in this BAA. Upon receipt, a whitepaper will be evaluated and the applicant will be advised of the results. Applicants whose whitepapers receive a favorable evaluation may be encouraged to prepare a proposal in accordance with instructions contained in this BAA. The costs of whitepapers and/or proposals in response to this BAA are not considered an allowable direct charge to any award resulting from this BAA or any other award. It may be an allowable expense to the normal bid and proposal indirect costs specified in Federal Acquisition Regulation (FAR) 31.205-18. ARO prefers proposals to cover a 3-year period and include a brief summary of work contemplated for each 12-month period so that awards may be negotiated for an entire 3-year program or for individual 1-year increments of the total program. Proposals may be submitted at any time while this BAA, including any amendments, is valid.

In accordance with federal statutes, regulations, and Department of Defense (DoD) and Army policies, no person on grounds of race, color, age, sex, national origin, or disability shall be excluded from participation in, be denied the benefits of, or be subjected to discrimination under any program or activity receiving financial assistance from the Army.

Applicants submitting proposals are cautioned that only a Contracting or Grants Officer can obligate the Government to any legal instrument involving expenditure of Government funds.

This BAA is also used to solicit research proposals for submission to the U.S. Army Research, Development, and Engineering Command (RDECOM) International Technology Centers.

All administrative inquiries regarding this BAA shall be submitted in email to: usarmy.rtp.aro.mbx.baa@mail.mil. Scientific and technical questions should be referred to the TPOCs shown following each research area of interest. Interested parties are encouraged to periodically check any of the following websites for updates and amendments to this BAA: www.grants.gov, www.fbo.gov, and the (ARL) website www.arl.army.mil/.

DAVID SKATRUD
Director
Army Research Office

(End of Section)

A. Required Overview Content**1. Agency Name**

U.S. Army Research Office

Issuing Acquisition Office

U.S. Army Contracting Command-Aberdeen Proving Ground, Research Triangle Park (ACC-APG-RTP) Division

2. Research Opportunity Title

ARO Broad Agency Announcement (BAA) for Fundamental Research for 01 April 2017 – 31 March 2022

3. Announcement Type

Amended Announcement

4. Research Opportunity Number

W911NF-17-S-0002-03

5. Catalog of Federal Domestic Assistance (CFDA) Number and Title

12.431 – Basic Scientific Research

6. Response Dates

This BAA is a continuously open announcement valid throughout the period from the date of issuance through 31 March 2022, unless announced otherwise. This announcement succeeds BAA W911NF-12-R-0012 (including all modifications) dated 15 May 2012.

(End of Section)

B. Additional Overview Information

This BAA sets forth research areas of interest to the ARO. This BAA is issued under FAR 6.102(d)(2), which provides for the competitive selection of fundamental research proposals, and 10 U.S.C. 2358, 10 U.S.C. 2371, and 10 U.S.C. 2371b, which provide the authorities for issuing awards under this announcement for fundamental research. The definitions of fundamental research may be found at 32 CFR 22.105.

Proposals submitted in response to this BAA and selected for award are considered to be the result of full and open competition and in full compliance with the provision of Public Law 98-369, "The Competition in Contracting Act of 1984" and subsequent amendments.

The DoD agencies involved in this program reserve the right to select for award all, some, or none of the proposals submitted in response to this announcement. Due to Government budget uncertainties, no specific dollars have been reserved for awards under this BAA. The participating DoD agencies will provide no funding for direct reimbursement of whitepaper or proposal development costs.

Whitepapers and technical and cost proposals (or any other material) submitted in response to this BAA will not be returned to the applicant. Unless noted in an applicant's proposal to the contrary, unsuccessful proposals will be retained for six (6) months from declination and then properly destroyed. It is the policy of participating DoD agencies to treat all proposals as sensitive, competitive information and to disclose their contents only for the purposes of evaluation.

An applicant may withdraw a proposal at any time before award by written notice or by email sent to the Government point of contact (POC) identified in Section G of this BAA.

(End of Section)

II. DETAILED INFORMATION ABOUT THE FUNDING OPPORTUNITY

A. Program Description

1. RESEARCH INTERESTS FOR U.S. INSTITUTIONS

ARL's ARO mission is to serve as the Army's principal extramural basic research agency funding research at universities, companies and not-for-profits in the engineering, physical, and information sciences. ARO's research portfolio is executed through ten scientific divisions, with titles reflecting fundamental scientific disciplines familiar to academic institutions. These Divisions directly support the ARL CCEs, which comprise the ARL Extramural Basic Research Campaign and supports all the other ARL S&T Campaigns. Additional information about the ARL S&T Campaigns can be found at the ARL website: www.arl.army.mil.

a. Physical Sciences

Research in the Physical Sciences is focused on basic research to discover, understand, and exploit physical, chemical, and biological phenomena. This research is of a fundamental nature; however, in the long term, discoveries in this area are expected to lead to revolutionary capabilities in sensing, communications, protection, wound healing, power/energy storage and generation, and materials that extend the performance of Army systems well beyond current limits.

i. Chemical Sciences

The objective of the Chemical Sciences Division is to uncover and exploit the fundamental properties and processes governing molecules and their interactions in materials and chemical systems. The Division encourages proposals that promote basic research to develop methods for accurately predicting the pathways, intermediates, and energy transfer of specific reactions, to understand the fundamental processes governing electrochemical reactions and transport of species, and to discover the relationships between macromolecular microstructure, architecture, functionality, and macroscopic properties. In addition, these efforts will likely lead to new methods for synthesizing and analyzing molecules and materials that will open the door to future studies not feasible with current approaches.

Research in the Chemical Sciences Division will reveal previously unexplored avenues for new Army capabilities while also providing fundamental results to support (i) the ARL Materials Research Campaign's goals to create multifunctional, responsive materials, and to discover and exploit materials for more efficient power generation and energy storage, (ii) the ARL Sciences-for-Maneuver Campaign's goal to identify and exploit innovations in energy sources, storage, and conversion, and (iii) the ARL Sciences for Lethality-and-Protection Campaign's goal to develop new energetic materials and predictive models of their behavior.

The Division's research programs are currently focused on five research areas that include one program focused on international research. The titles, scopes and points of contact for these

programs, each of which address general aspects of basic research in chemical sciences, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Polymer Chemistry

The goal of this Program is to understand the molecular-level link between polymer microstructure, architecture, functionality, and the ensuing macroscopic properties. Research in this Program may ultimately enable the design and synthesis of functional polymeric materials that give the Soldier new and improved protective and sensing capabilities as well as capabilities not yet imagined. This Program is divided into two research thrusts: (i) *Precision Polymeric Materials* and (ii) *Complex Adaptive Polymeric Systems*. Within these thrusts, high-risk, high-payoff research is identified and supported to pursue the Program's long-term goal.

The *Precision Polymeric Materials* thrust supports research aimed at developing new approaches for synthesizing polymers with precisely-defined molecular weight, microstructure, architecture, and functional group location. Of particular interest are research efforts that focus on novel methods for achieving sequence and tacticity control in synthetic polymers as well as enabling the synthesis of novel 2D organic polymers. Also of interest to this thrust are research efforts that explore how molecular structure influences polymer assembly into more complex, hierarchical structures as well as influence interactions with other materials (e.g., inorganic or biological materials) to render functional hybrid assemblies.

The *Complex Adaptive Polymeric Systems* thrust focuses on developing polymers that exhibit programmed molecular responses to external stimuli. Particularly of interest are research efforts related to stimuli-responsive self-immolative polymers, polymer mechanochemistry, and stimuli-mediated polymer assembly. Additionally, research focused on exploring the assembly/incorporation of multiple responsive groups into a single polymeric material system as well as the incorporation of feedback mechanisms to engender complex responsive behavior is also of interest.

TPOC: Dr. Dawanne Poree, dawanne.e.poree.civ@mail.mil, (919) 549-4238

(2) Electrochemistry

This Program supports fundamental electrochemical studies to understand and control the physics and chemistry that govern electrochemical redox reactions and transport of species, and how these are coupled with electrode, catalysis, electrolyte, and interface. Research includes ionic conduction in electrolytes, electrocatalysis, interfacial electron transfer, transport through coatings, surface films and polymer electrolytes, activation of carbon-hydrogen and carbon-carbon bonds, and spectroscopic techniques that selectively probe electrode surfaces and electrode-electrolyte interfaces. Novel electrochemical synthesis, investigations into the effect of microenvironment on chemical reactivity, quantitative models of electrochemical systems, and electrochemistry using excited

electrons are also of interest.

This Program is divided into two research thrusts, although other areas of electrochemical research may be considered: (i) Reduction-oxidation (Redox) Chemistry and Electrocatalysis, and (ii) Transport of Electroactive Species.

The *Redox Chemistry and Electrocatalysis* thrust supports research to understand how material and morphology affect electron transfer and electrocatalysis, to tailor electrodes and electrocatalysts at a molecular level, and to discover new spectroscopic and electrochemical techniques for probing surfaces and selected species on those surfaces.

The *Transport of Electroactive Species* thrust supports research to uncover the mechanisms of transport through heterogeneous, charged environments such as polymers and electrolytes, to design tailorable electrolytes based on new polymers and ionic liquids, and to explore new methodologies and computational approaches to study the selective transport of species in charged environments.

TPOC: Dr. Robert Mantz, robert.a.mantz.civ@mail.mil, (919) 549-4309

(3) Molecular Structure and Dynamics

The goal of the Molecular Structure and Dynamics program is to determine the reactive pathways and intermediates for reactions of molecules and molecular ions in gas and condensed phases at a range of temperatures and pressures, and to develop theories that are capable of accurately and efficiently describing and predicting these phenomena. In the long term, these studies may serve as the basis for the design of future propellants, explosives, and sensors. This Program is divided into three research thrusts: (i) *Reaction Dynamics*, (ii) *Computational Modeling*, and (iii) *Chemistry of Novel Energetic Materials*.

Research in the *Reaction Dynamics* thrust explores energy transfer mechanisms in molecular systems. In particular, research is focused on understanding dynamic processes such as roaming radicals, chemical reactions in solid state crystals and heterogeneous mixtures, phase transformations, kinetically stabilized versus thermally stabilized polymorphs and opportunities for control of polymorphic phase, and control of chemical processes using a variety of spectroscopic methods. Studies that yield new insights on the decomposition pathways of energetic molecules including their associated ionic states, both in the gas and condensed phases, are also of interest. The role that cations and anions play during detonation of bulk phase energetic materials is currently of high interest in the program. Proposals are especially encouraged in this area.

Research in the *Computational Modeling* thrust is focused on the development and validation of theories for describing and predicting the properties of chemical reactions and molecular phenomena in gas and condensed phases. In particular, research targeted

at the development and implementation of novel theoretical computational chemistry methods is of interest. Ideally, such methods will go beyond current theories to allow for efficient, accurate, and *a priori* prediction of thermochemical properties. Such methods may take advantage of near-ideal parallel processing on massive computer clusters, or they may seek to solve current scaling problems through novel implementation of unprecedented theories via computer algorithms. The accurate prediction of intermolecular forces for problems in solid-state chemistry, such as the prediction of x-ray crystal structures, is also of interest.

Research in the *Chemistry of Novel Energetic Materials* thrust is focused on the synthesis, characterization, and measurement of properties of novel disruptive energetic materials. For a programmatic definition, disruptive energetic materials are those which have the potential to release two to ten times the explosive power of RDX when detonated. Such novel disruptive energetic materials will likely be derived from systems which differ significantly from traditional hydrogen-carbon-nitrogen-oxygen energetic materials. To be practical, any useful EM must have a high potential energy stored within the chemical bonds and also be stable from unwanted stimulations leading to accidental detonation. This principle can be used to develop notional disruptive energetic materials, and the methods of chemical synthesis can be used to target them for development. Academic research in this area is focused on discovery and characterization.

TPOC: Dr. James K. Parker, james.k.parker30.civ@mail.mil, (919) 549-4293

(4) Reactive Chemical Systems

The goal of the Reactive Chemical Systems Program is to achieve a molecular level understanding of interfacial activity and dynamic nanostructured and self-assembled chemical systems to provide unprecedented hazardous materials management capabilities and soldier survivability. This Program supports basic research with Army relevance in surfaces, catalysis, organized assemblies, and stimuli-responsive chemical systems. This program is divided into two thrusts: (i) *Interfacial Activity* and (ii) *Synthetic Molecular Systems*.

The *Interfacial Activity* thrust supports research on understanding the kinetics and mechanisms of reactions occurring at surfaces and interfaces and the development of new methods to achieve precise control over the structure and function of chemical and biological molecules on surfaces. Specific areas of interest include adsorption, desorption, and the catalytic processes occurring at surfaces and interfaces and the interface between nanostructures and biomolecules to generate advanced materials.

The *Synthetic Molecular Synthesis* thrust supports research that imparts multi-functionality, stimuli-responsive and dynamic behavior to completely synthetic molecular and chemical systems. Research of interest includes design and development of nanostructured scaffolds and sequential catalytic systems. This thrust also supports research aimed at exploring the properties and capabilities of self-assembled and

supramolecular structures, including their functionality, and how to control assembly in different environments.

In addition, the emerging field of dynamic, responsive, multi-functional materials have great potential to provide revolutionary new capabilities. A specific technical area in this field is "targeting and triggering" in which a specific chemical (or event) is targeted (recognized) and that recognition triggers a response. Particular technical challenges of interest include selective and reversible recognition, amplification, and multi-responsive systems. Alternative approaches to selective, yet reversible, recognition are needed. Amplification includes an understanding of how to amplify the response from a single molecular recognition event to a multi-molecular response with approaches that promote chain reactions, self-amplification or cascade-type reactions within a single system. Multi-responsive systems in which specific stimuli trigger distinct responses are also of interest.

TPOC: Dr. Dawanne Poree, dawanne.e.poree.civ@mail.mil, (919) 549-4238

(5) Energy Transport and Storage (International Program)

As one of the ARO International Programs, the Energy Transport and Storage Program is focused on supporting research at institutions outside of the U.S., with the goal of building international partnerships and laying the foundational work upon which future energy storage and power generation technologies depend.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

ii. Physics

The objective of the Physics Division is to develop forefront concepts and approaches, particularly exploiting quantum phenomena, that will in the long-term have revolutionary consequences for Army capabilities, while in the nearer-term providing for existing Army needs. In support of this goal, the interests of the Physics Division are primarily in the areas described in the following subsections.

Research in the Physics Division will reveal previously unexplored avenues for new Army capabilities while also providing fundamental results to support (i) the ARL Materials Research Campaign's goals to determine how quantum processes could be harnessed for quantum memory and secure communication, and to explore and exploit recent advances in unique materials such as topologically non-trivial electronic phases, (ii) the ARL Information Sciences Campaign's goal to explore techniques, architectures, and properties that take advantage of the quantum and related effects for processing and transmitting information, and (iii) the ARL Sciences for Lethality-and-Protection Campaign's goal to identify, exploit, and protect against the effects of directed and non-directed application of energy.

The Division's research programs are currently focused on five research areas, including one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in physics, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Condensed Matter Physics (CMP)

The CMP Program strives to drive research that looks beyond the current understanding of natural and designed condensed matter, to lay a foundation for revolutionary technology development for next generation and future generations of warfighters.

Strong Correlations and Novel Quantum Phases of Matter. Understanding, predicting, and experimentally demonstrating novel phases of matter in strongly correlated systems will lay a foundation for new technology paradigms for applications ranging from information processing to sensing to novel functional materials. Interest primarily involves strong correlations of electrons, but those of other particles or excitations are not excluded. This thrust also emphasizes dynamically- stabilized electronic states and metastable phases that are not adiabatically accessible from known ground states. The Program seeks to foster novel experimental and theoretical research targeting the discovery and rational design of new quantum phases of matter, along with exploring how excitations within these phases can be probed and controlled.

Topologically Non-Trivial Phases in Condensed Matter. Topologically non-trivial states of matter beyond the quantum Hall phases have shown a remarkable opportunity to advance our understanding physics as well as provide a foundation for new technologies. This thrust seeks to expand our understanding of both single-particle mean field topological states and those with strong correlations. Discovery as well as engineering of new non-trivial phases, verification of non-trivial topologies and phase transitions between trivial and non-trivial topological states and among the latter are of interest.

Unique Instrumentation Development. Advanced studies of CMP phenomena often require unique experimental techniques with tools that are not readily available. For example, unambiguous experimental verification of predicted topologically non-trivial phases can be beyond the reach of existing techniques. The construction and demonstration of new methods for probing and controlling unique quantum phenomena is of particular interest.

TPOC: Dr. Marc Ulrich, marc.d.ulrich.civ@mail.mil, (919) 549-4319

(2) Quantum Information Science

Quantum mechanics provides the opportunity to perform highly non-classical operations that can result in beyond-classical capabilities in imaging, sensing and precision measurements, exponential speed-ups in computation, or networking. This Program seeks to understand, control, and exploit such non- classical phenomena for

revolutionary advances beyond those possible with classical systems. An overarching interest is the exploration of small systems involving small numbers of entangled particles. There are three major areas of interest (thrusts) within this Program.

Foundational Quantum Physics (FQP). Experimental investigations of a fundamental nature of quantum phenomena, potentially useful for quantum information science, are of interest. Examples include coherence properties, decoherence mechanisms, decoherence mitigation, entanglement creation and measurement, nondestructive measurement, complex quantum state manipulation, and quantum feedback. An important objective is to ascertain the limits of our ability to create, control, and utilize quantum information in multiple quantum entities in the presence of noise. Systematic materials focused research which identifies and/or mitigates decoherence mechanisms is also of interest. Models of machine learning that are based on the foundations of quantum physics are of interest. Theoretical analyses of non-classical phenomena may also be of interest if the work is strongly coupled to a specific experimental investigation, such as proof-of-concept demonstrations in atomic, molecular, and optical (AMO) as well as other systems.

TPOC: Dr. Sara Gamble, sara.j.gamble.civ@mail.mil, (919) 549-4241

Quantum Sensing, Imaging, and Metrology (QSIM). This research area seeks to explore, develop, and demonstrate multi-particle coherent systems to enable beyond classical capabilities in imaging, sensing, and metrology. Central to this research area is the exploration of small systems involving a few entangled particles. Topics of interest in this research area include the discovery and exploration of (a) multi-particle quantum states advantageous for imaging, sensing, and metrology, (b) quantum circuits that operate on multi-particle quantum states to enable beyond- classical capabilities, and (c) methods for the readout of quantum states. Other research topics of interest are: theory to explore multi-particle quantum states useful for beyond classical capabilities, quantitative assessment of capabilities and comparison to classical systems, efficient state preparation, quantum circuits for processing these states as quantum bits, readout techniques, decoherence mitigation and error-correction for improved performance, supporting algorithms as a basis for processing circuits, connections between the solution of hard computational problems and overcoming classical limitations in imaging, sensing, and metrology, entanglement as a resource, and suitable physical systems and key demonstration experiments.

TPOC: Dr. Sara Gamble, sara.j.gamble.civ@mail.mil, (919) 549-4241

Quantum Computation and Quantum Networking (QCON). Quantum computing and networking will entail the control and manipulation of quantum bits with high fidelity. The objective is the experimental demonstration of quantum logic performed on several quantum bits operating simultaneously, which would represent a significant advance toward that ultimate goal of beyond classical capabilities in information processing. Demonstrations of quantum feedback and error correction for multiple quantum bit systems are also of interest. There is particular interest in developing quantum

computation algorithms that efficiently solve classically hard problems, and are useful for applications involving resource optimization, imaging, and the simulation of complex physical systems. Examples include machine learning, parameter estimation, constrained optimization, and quantum chemistry, among others. The ability to transmit information through quantum entanglement distributed between spatially-separated quantum entities has opened the possibility for new approaches to information processing. Exploration of quantum networking of information and distributed quantum information processing based on entanglement is of interest. These include the exploration of long-range quantum entanglement, entanglement transfer among different quantum systems, and long-term quantum memory.

TPOC: Dr. T.R. Govindan, t.r.govindan.civ@mail.mil, (919) 549-4236

(3) Atomic and Molecular Physics (AMP)

Topics of interest within the AMP Program include (i) quantum degenerate atomic gases, both Bose and Fermi, their excitations and properties, including mixed species, mixed state, and molecular, (ii) quantum enhanced precision metrology, (iii) nonlinear atomic and molecular processes, (iv) quantum topological matter, (v) collective and many-body states of matter, and (vi) emerging areas. Cooling schemes for molecules are of importance for extending the range of systems that may be exploited. In addition, there is an interest in emerging areas of AMO physics such as states of topologically protected matter including but not limited to topological phases, emergent lattices in quantum gases, opto- mechanical interfaces, non-equilibrium many body dynamics, and many-body localization. Research efforts within the AMP Program fall within two thrust areas: *Advanced Quantum Capabilities* and *Novel Quantum Methods*. It is anticipated that research efforts within these areas will lead to applications including novel materials, efficient computational platforms, and exquisite quantum sensors.

Advanced Quantum Many-body Dynamics. The focus of this thrust is the development and study of strongly interacting many-body systems. The quantum simulator portion of the thrust seeks research on novel cooling, trapping, and the expansion of atomic and molecular species. The effort seeks the validation of many-body quantum theories through the development of experimental tools including quantum gas microscopes, synthetic gauge fields, mixed species, and novel interactions. Complimenting this effort will be the inclusion of foundational investigations into quantum mechanics, such as entanglement, many-body localization, topologically protected states, and entropy. To take advantage of the precision inherent in future quantum devices, these systems will need to connect to the classical world in such a manner that allows them to sample the signal of interest while remaining robust to noisy environments. Investigating how to maximize both the quality and quantity of entanglement within these systems will be a priority. General issues of quantum coherence, quantum interference, entanglement growth, entanglement purity, and non-equilibrium phenomena, as well as discovering new scientific opportunities are also of interest.

Novel Quantum Metrology. The AMP Program has a general interest in exploring

fundamental AMP that may impact future Army capabilities. This thrust is divided into two main areas: precision metrology beyond the standard limit and harnessing collective many-body states to improve quantum sensing. The Novel Quantum Metrology efforts will expand the foundations of quantum measurement into new areas that seek to exploit entanglement, spin-squeezing, harnessing collective-spin state, developing back-action avoidance measurements, and other areas that increase fundamental precision through interactions, including cavities and Rydberg atoms. It is expected that research in this thrust will complement efforts in the *Advanced Quantum Many-body Dynamics* thrust and *vice versa*. For example, collective many body states could be studied in optical lattices or quantum gas microscopes and foundational research of entanglement and topologically protected states are anticipated to provide new metrological capabilities.

TPOC: Dr. Paul Baker, paul.m.baker4.civ@mail.mil, (919) 549-4202

(4) Optical Physics and Fields

The objective of this Program is to investigate physical phenomena that will lead to a deeper understanding of the underlying physics or the discovery of new physical effects that can improve capabilities of the Army. In particular, this program emphasizes physics that will significantly improve areas such as remote sensing, information processing, light and energy transmission, interactions between light and matter, and new or emerging phenomena relating to optical physics and fields. Much of the Army's capability in sensing and information and/or energy exchange depends on light. This Program also seeks research for other long-range physical fields that can complement electromagnetic radiation.

Extreme Light. This thrust focuses on research on extreme light, meaning the examination of light in the extreme limits, such as the shortest pulses attainable and the highest intensity fields attainable. Advances in these areas require theoretical and experimental research. For example, ultrashort pulsed lasers have now achieved intensities of 10^{22} W/cm². Future applications of these pulses may include high-harmonic generation, nanolithography, particle beam acceleration and control, and light filaments. In addition, effects such as THz formation and control and broadband localized radiation from filaments are of interest. In the near future, even higher intensities are expected. Theoretical and experimental research efforts are needed to describe and understand how matter behaves under these conditions—from single particle motion and radiation reaction to the effects in materials—and how to generate these pulses and use them effectively. Pulses as short as 80 attoseconds have been produced, and the Program seeks ways to make them shorter and to understand both the physics and applications of this form of radiation. Proposals for new areas of extreme light such as relativistic optics are welcome.

Meta-Optics. This thrust pursues a fresh start in optics due to the new kinds of effects allowed by optical metamaterials. In this area, many conventional limits of optics can be broken in ways such as sub-wavelength imaging and superlensing related phenomena. It is timely to look at the quantum optics of such processes as well as research in in flat

photonics. Proposals for new areas involving discrete symmetries, such as parity-time symmetries and non-Hermitian Hamiltonians are of interest. A related area is supersymmetric optics (SO), where project are sought that use SO concepts in the design of photonic materials with new properties or capabilities. New forms of imaging using transformation optics or other novel imaging, including quantum optics, are also of interest. In general, any optical phenomena that can ultimately improve Army capabilities are sought.

Non-Electromagnetic Fields. Other forms of propagating energy have been predicted and will theoretically have properties that differ dramatically from electromagnetism. Modern theories of gravity as well as string theory predict, in addition to gravity, the existence of two other long- range fields. If these theories are correct in their predictions, this suggests applications in which these new fields may be useful for detection or communication, especially in situations where electromagnetism and optics are not useful, such as propagating through conducting media. This program seeks proposals that may lead to the detection and/or measurement of these fields.

TPOC: Dr. Richard Hammond, richard.t.hammond10.civ@mail.mil, (919) 549-4313

(5) Quantum Scale Materials (International Program)

As one of the ARO International Programs, the Quantum Scale Materials Program is focused on supporting research at universities outside of the U.S., with the goal of providing key connections with world-class researchers outside the U.S. and supporting the most forward-looking physics research.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

iii. Life Sciences

The Life Sciences Division supports research efforts to advance the Army and Nation's knowledge and understanding of the fundamental properties, principles, and processes governing DNA, RNA, proteins, organelles, prokaryotes, and eukaryotes, as well as multi-species communities, biofilms, individual humans, and groups of humans. The interests of the Life Sciences Division are primarily in the following areas: biochemistry, neuroscience, microbiology, molecular biology, genetics, genomics, proteomics, epigenetics, systems biology, bioinformatics, and social science. The results of fundamental research supported by this Division are expected to enable the creation of new technologies for optimizing warfighters' physical and cognitive performance capabilities, for protecting warfighters, and for creating new Army capabilities in the areas of biomaterials, energy, logistics, and intelligence.

Research in the Life Sciences Division will reveal previously unexplored avenues for new Army capabilities while also providing fundamental results to support (i) the ARL Human

Sciences Campaign's goals to discover and predict human cognitive, physical, and social behaviors, as well as the role of training paradigms in building expertise, and to characterize the fundamental aspects of social network dynamics involving ethics, values, trust, social-cultural, economic, and geopolitical effects, (ii) the ARL Assessment and Analysis Campaign's goal to identify human capabilities and limitations, (iii) the ARL Information Sciences Campaign's goal to develop predictive models that consider the availability of power or food sources and the potential for social unrest or insurgency activity, (iv) the ARL Materials Research Campaign's goal to exploit the evolutionary solutions created by nature and create new capabilities using synthetic biology.

The Division's research programs are currently focused on seven research areas, which includes two programs focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in life sciences, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Biochemistry

This Program emphasizes basic research focused on understanding and controlling the activity and assembly of biomolecules. Scientific advances supported by this Program are anticipated to enable the development of novel systems, materials and processes that enhance Soldier protection and performance. An overarching goal of the Program is to provide the scientific foundations to support biological activity outside of the natural biological context, including integration of biological systems with synthetic systems.

The *Biomolecular Specificity and Regulation* thrust is focused on elucidating the mechanisms by which biomolecules recognize and interact with their targets, as well as the regulatory mechanisms utilized to activate or inhibit biomolecular activity. This research thrust also includes novel engineered approaches to modulate and control biomolecular activity.

The *Biomolecular Assembly and Organization* thrust is focused on understanding the molecular interactions and design rules that govern self-assembly of biomolecules into both naturally occurring biomolecular structures and designed architectures. This research thrust also includes novel approaches to control biomolecular assembly and approaches to utilize biomolecular architectures to organize biomolecular activity and/or achieve specialized properties.

TPOC: Dr. Stephanie McElhinny, stephanie.a.mcelhinny.civ@mail.mil, (919) 549-4240

(2) Genetics

This Program supports basic research in genetics, molecular biology, genomics, epigenetics, and systems biology in areas that may enable the optimization of the

Soldier's cognitive and physical performance capabilities, increase Soldier survivability, and improve Army capabilities in areas such as biomaterials, sensing, energy, and intelligence. This Program emphasizes innovative high-risk fundamental research in areas such as identification and characterization of gene function, gene regulation, genetic interactions, gene pathways, gene expression patterns, epigenetics, mitochondrial regulation and biogenesis, and nuclear and mitochondrial DNA replication, mutagenesis, oxidative stress, and DNA repair.

The *Organismal Genetics* thrust is focused on identifying and characterizing the genetic pathways that affect warfighter survival and performance. This Program is interested in identifying and understanding the molecular factors that affect human physical and cognitive performance capabilities as well as human survival and protection under normal conditions and when affected by a variety of stressors likely to be encountered in battlefield situations, such as dehydration, heat, cold, sleep deprivation, fatigue, caloric insufficiency, pathogens, and physical and psychological stress.

The *Population Genetics* thrust is focused on understanding genetic change at a population level. Areas of interest include mechanisms of prokaryotic adaptation, social insects, modeling species distributions, plant genetics, biological components of social instability, and biological systems for sensing and detection.

TPOC: Dr. Micheline Strand, micheline.k.strand.civ@mail.mil, (919) 549-4343

(3) Microbiology

This Program supports basic research in fundamental microbiology that can help advance needs in Soldier protection and performance. There are two primary research thrusts within this program: (i) *Microbial Survival Mechanisms* and (ii) *Analysis and Engineering of Microbial Communities*.

The *Microbial Survival Mechanisms* thrust focuses on the study of the cellular and genetic mechanisms and responses that underlie microbial survival in the face of environmental stress. These stressors include extremes in temperature, pH, or salinity; the presence of toxins including metals and toxic organic molecules; oxidative stress; and cellular starvation and the depletion of specific nutrients. Research approaches can include fundamental studies of microbial physiology and metabolism, cell biology, and molecular genetics that examine key cellular networks linked to survival, microbial cell membrane structure and the dissection of relevant critical signal transduction pathways and other sense-and-respond mechanisms.

The *Analysis and Engineering of Microbial Communities* thrust supports basic research that addresses the fundamental principles that drive the formation, proliferation, sustenance and robustness of microbial communities through reductionist, systems-level, ecological and evolutionary approaches. Bottom-up analysis of information exchange, signaling interactions and structure-function relationships for single and multi-species communities within the context of planktonic and biofilm architectures is considered.

Of joint interest with the ARO Biomathematics Program, research efforts that advance the ability to work with complex biological data sets to increase understanding of microbiological systems marked by ever-increasing complexity are encouraged.

TPOC: Dr. Robert Kokoska, robert.j.kokoska2.civ@mail.mil, (919) 549-4342

(4) Neurophysiology of Cognition

The Neurophysiology of Cognition program supports non-medically oriented basic research in neuroscience, the behavioral sciences, physiology and neuroengineering that might enable the optimization of Soldier's cognitive and physical performance capabilities. An overarching goal of the program is to provide foundational knowledge of molecular, cellular and systems-level neural codes underlying cognition and performance across multiple length and time scales. Research in this program can include a broad range of methodological and theoretical approaches applied to animal and human experimental systems including electrophysiology, neuroimaging and computational neurobiology. This includes the study of the psycho-physiological implications of brain-machine interfaces, the measurement and modeling of individual cognitive dynamics and decision making during real-world activity, and identifying how neuronal circuits generate desirable computations. In the long term, research in this area may enable the development of interfaces enabling humans to more efficiently control machines, new training methods and devices to predict and optimize individual performance, and the potential restoration from injury at the neural level. Basic research opportunities are sought in two primary research thrusts within this program: (i) Multisensory Synthesis and (ii) Neuronal Computation.

Multisensory Synthesis. The Multisensory Synthesis thrust aims to understand how the human brain functions in relation to the interaction of sensory, cognitive and motor processes during its performance of real-world tasks. Research focuses on mapping, quantifying and modeling distributed neural processes, physiological processes and mind-body interfaces that mediate these features to ultimately develop better understanding of cognition for eventual application to Soldier performance.

Neuronal Computation. The Neuronal Computation thrust is focused on understanding how living neuronal circuits generate desirable computations, affect how information is represented, show robustness to damage, incorporate learning and facilitate evolutionary change. Research focuses on determining how brains structure, process and refine inputs into efficient decisions and behaviors, and how these multiscale features are altered under stresses. Cell culture, brain slice and *in vivo* models are used to develop better understanding of small and large-scale living neural networks for eventual application in Army systems.

TPOC: Dr. Frederick Gregory, frederick.d.gregory5.civ@mail.mil, +44 (0)1895-626517

(5) Social and Behavioral Science

The goal of this Program is to promote basic research on human and social behavior to

discover the theoretical foundations of behavior at all levels, from individual actors to global societies. The goals of this Program include (i) developing reliable and valid measures of social and behavioral concepts, and (ii) discovering, modeling, and testing causal theories that describe, explain, and predict human, group, and societal responses to physical, environmental, psychological, or social stimuli.

Of particular interest is research that examines (1) the interrelationships among human, social, natural, and physical systems and (2) multi-level system dynamics. Examples might include, but are not limited to: (a) understanding how change in human-made and natural environments affects migration, urbanization, change in governance systems, collective action, deviance; (b) investigating the interrelationships between individual values, group identity, and interpersonal and intergroup cooperation and conflict; (c) studying how emerging technologies impact intra- and intergroup dynamics; and (d) modeling the diffusion of values, beliefs, and influence from micro-to macro-levels of interactions among individuals, groups, and social systems along with the physical and natural contexts that impact pathways of diffusion.

Research in this program can include a broad range of methodological and theoretical approaches including empirical studies that require primary data collection, such as random control trials, quasi-experiments, laboratory and field experiments, surveys, comparative and observational studies, or the use of secondary data sources, such as media archives or area reports. Formal computational approaches are encouraged to aid in the development of testable dynamic models of individual, group, and population-level phenomena.

TPOC: Dr. Lisa Troyer, lisa.l.troyer.civ@mail.mil, (919) 549-4230

(6) Synthetic Biology (International Program)

As one of the ARO International Programs, the Synthetic Biology Program is focused on supporting research at institutions outside of the U.S., with the goal of providing key connections with world-class researchers outside the U.S. and supporting the most forward-looking studies in synthetic biology.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

(7) Human Dimension (International Program)

As one of the ARO International Programs, the Human Dimension Program is focused on supporting research at institutions outside of the U.S., with the goal of providing key connections with world-class researchers outside the U.S. and supporting the most forward-looking research in this area.

Refer to Section II.A.2 of this BAA for a detailed description of this international

research program's research goals, including the titles, scopes and points of contact for these programs.

b. Engineering Sciences

Research in the Engineering Sciences is focused on basic research to discover, understand, and exploit new material systems, mechanical systems, electronics, and earth sciences that are expected to create revolutionary capabilities for the Army. Discoveries in this area are expected to lead to capabilities in materials, the sciences for maneuver, the information domain, the sciences of lethality and protection, and Soldier performance augmentation, well beyond the limits facing today's Army.

i. Mechanical Sciences

The Mechanical Sciences Division supports research in a broad spectrum of fundamental investigations in the disciplines of fluid dynamics, solid mechanics, complex dynamics and systems, and propulsion and energetics. Though many creative and imaginative studies concentrate on a particular sub-discipline, increasingly, new contributions arise from interdisciplinary approaches such as the coupling between aerodynamics and structures, complex dynamics and systems, combustion and fluid dynamics, or solid mechanics and structures as in the structural reliability areas. Additionally, several common themes run through much of these four sub-disciplines, for example, active controls and computational mechanics. Research in such areas is addressed within the context of the application rather than as a separate subject of study. Fluid dynamics research is primarily concerned with investigations in the areas of rotorcraft wakes, unsteady aerodynamics of dynamic stall and unsteady separation, and fundamental studies of micro adaptive flow control. Solid mechanics include a wide array of research areas such as high strain rate phenomena, penetration mechanics, heterogeneous material behavior, and reliability of structures. The complex dynamics and systems area is focused on investigations in vehicle structural dynamics, and simulation and air vehicle dynamics including rotor aeromechanics. Research in the propulsion and energetics area is concentrated on processes characteristic of reciprocating (diesel) and gas turbine engines and the combustion dynamics of propellants used for gun and missile propulsion. The following narratives describe the details of the scope and emphasis in each of these sub disciplinary areas.

The Division also supports the ARL S&T Campaigns. This includes the Sciences for Maneuver Campaign through research in hydrocarbon combustion, non-equilibrium dynamical systems, unsteady separation and dynamics stall, and vortex dominated flows S&T areas, and the Sciences for Lethality and Protection Campaign through research in energetics, multi-scale mechanics of heterogeneous solids, and low-stiffness, nonlinear materials and material systems S&T areas. These efforts also contribute to lesser extent to the Materials Research and Human Sciences Campaigns through its impacted S&T areas.

The Division's research programs are currently focused on four research areas. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in mechanical sciences, are listed in the following subsections. Symposia,

conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Fluid Dynamics

Fluid dynamics plays a critical role in many Army operational capabilities. Significant challenges exist for accurate and efficient prediction of flow physics critical for improved performance and future advanced capability. Army platforms are often dominated by flows with high degrees of unsteadiness, turbulence, numerous and widely separated spatio-temporal scales, and geometrical complexity of solid or flexible boundaries. In order to gain the necessary physical insight to enable future capabilities spanning Army vehicles, munitions, medical devices, and logistics, the Fluid Dynamics program seeks to support basic research investigations of fundamental and novel flow physics. In view of the nonlinear and high-dimensional character of the governing equations, revolutionary advances in fluid dynamics research tools are also of great interest; advanced experimental methods, sophisticated computational techniques and breakthrough theoretical advances will be critical for gaining the required fundamental understanding. There are three major subareas or thrusts within the Fluid Dynamics program: Dynamics of Unsteady and Separated Flows, Nonlinear Flow interactions and Turbulence, and Flow Stability and Control. Each of these is described in detail below.

Dynamics of Unsteady and Separated Flows. Operating conditions for many Army platforms are characterized by flows featuring unsteadiness, nonlinear interactions, turbulence, three-dimensionality and flow separation. All efforts in this thrust area will require novel and aggressive strategies for examination of the interplay between disparate spatio-temporal scales, inclusion of physically significant sources of three-dimensionality, and characterization of the role of flow instabilities and nonlinear interactions across a range of appropriate Mach and Reynolds numbers. Historical management of physical complexity has often resulted in scientific approaches that result in the elimination of potentially critical flow physics. Research efforts that are capable of gaining deep understanding of highly complicated flows are likely to allow critical physics to be exploited, leading to significant performance gains for Army systems. As an example, shortcomings in understanding the details of unsteady flow separation, reverse flow phenomena, and dynamic stall continue to limit the capabilities of Army rotorcraft vehicle platforms. While much progress has been made towards unraveling these details, it has become apparent that revolutionary advances are unlikely if the full complexity of the physics is not considered.

Nonlinear Flow Interactions and Turbulence. As mentioned above, many Army relevant flows are governed by strong nonlinearities and turbulent behaviors. Historically, many analysis tools developed for linear dynamics have been applied to gain understanding of flow behaviors. While local insights can be gained through applications of these methods, the ability to provide global understanding of the evolution of flows requires new approaches that are capable of dealing directly with inherent nonlinearities. Turbulent dynamics may also benefit from new approaches based in dynamical systems

theory to push modeling frameworks beyond the notions based on Reynolds averaging and stochastic dynamics and to determine if a useful underlying deterministic structure exists. Modeling flows near walls is a continuing challenge to accurate numerical prediction of complex flows that may benefit from novel non-intrusive diagnostics to inform creative numerical and theoretical constructs capable of efficiently producing a high degree of fidelity near physical boundaries.

Flow Stability and Control. Many of the previously described flows are susceptible to initially small amplitude, but dynamically significant, instabilities that can ultimately lead to fundamental changes in global flow behaviors. Thorough understanding and prediction of these instabilities and their growth is crucial not only to maintaining robustness in the face of disturbances, but also to gain advanced control over the evolution of flows through their exploitation. Research breakthroughs in global and local stability characteristics and their subsequent manipulation are of interest. Theoretical, computational, and experimental examinations of canonical problems to enable focused studies of interactions between instability mechanisms and global flow characteristics are highly encouraged, especially those that seek nonlinear descriptions. Flow control efforts should seek to exploit understanding of these mechanisms to permit the flow evolution to be prescribed. Flow control investigations should also seek to understand not only the impact of control actuation on the flow, but should also consider strategies for closed-loop feedback control and appropriate scaling laws that lead to the potential for such strategies to transition into new capabilities in real-world flows.

TPOC: Dr. Matthew J. Munson, matthew.j.munson6.civ@mail.mil, (919) 549-4284

(2) Solid Mechanics

The goal of the Solid Mechanics Program is to investigate and understand behavior of complex material systems under a broad range of loading regimes in various environments and to develop analytical and computational methods to characterize material models which can serve as physically-based tools for the quantitative prediction and control of Army relevant material systems subjected to extreme high loading and strain rate conditions such as impact and blast. The program seeks novel approaches to innovate unprecedented systems and structures with previously unattainable properties and behaviors. Research in analytical, computational and experimental solid mechanics is sought to form the foundation for understanding these systems as well as to validate developed physical models. Understanding of failure in soft and active material systems is also of interest to the program. Such work should lead to novel ideas and concepts for revolutionary capabilities.

The understanding of the mechanics of material behavior during transition into states of damage and fracture initiation due to extreme loading, high rate loading, high-temperature variations, and repetitive loading are of interest. The program seeks the development of models of material behavior across broad spatial and temporal scales that are based on these physical processes taking place at different scales and of

establishing essential physical understanding of the relationships of the various processes taking place such that failure may be accurately predicted.

Novel experimental methods aimed to investigate and validate material models play on all scales are sought. Development of new experimental techniques is essential for solid mechanics development. In particular, the program seeks techniques to enhance the understanding of the physical processes taking place during deformation and failure in the interior of materials.

Computationally efficient methods capable of integrating the new physical relationships and models, and with the ability to predict the behavior of novel material systems in extreme conditions across a broad range of scales are sought.

TPOC: Dr. Ralph A. Anthenien, ralph.a.anthenien2.civ@mail.mil, (919) 549-4317

(3) Complex Dynamics and Systems

The Complex Dynamics and Systems Program emphasizes fundamental understanding of the dynamics, both physical and information theoretic, of nonlinear and nonconservative systems as well as innovative scientific approaches for engineering and exploiting nonlinear and nonequilibrium physical and information theoretic dynamics for a broad range of future capabilities (e.g. novel energetic and entropic transduction, agile motion, and force generation). The program seeks to understand how information, momentum, energy, and entropy is directed, flows, and transforms in nonlinear systems due to interactions with the system's surroundings or within the system itself. Research efforts are not solely limited to descriptive understanding, however. Central to the mission of the program is the additional emphasis on pushing beyond descriptive understanding toward engineering and exploiting time-varying interactions, fluctuations, inertial dynamics, phase space structures, modal interplay and other nonlinearity in novel ways to enable the generation of useful work, agile motion, and engineered energetic and entropic transformations. Further information on the current scientific thrust areas are detailed in the paragraphs that follow.

High-Dimensional Nonlinear Dynamics. Classical dynamics has produced limited fundamental insight and theoretical methods concerning strongly nonlinear, high-dimensional, dissipative, and time-varying systems. For over a century, qualitative geometric approaches in low-dimensions have dominated research in dynamics. These approaches of reduced-order-modeling of high-dimensional dynamics are often premised on empirical and statistical model fitting and are incapable of capturing the effects of slowly growing instabilities and memory. The program seeks to develop novel theoretical and experimental methods for understanding the physical and information dynamics of driven dissipative continuous systems. It also seeks novel reduced-order-modeling methodologies capable of retaining time-dependent and global nonlinearities. Novel research pertaining to the analysis and fundamental physics of time-varying nonlinear systems and transient dynamics is a high-priority.

Nonlinear Mechanical Metastructures. Another emerging area in this thrust concerns nonlinear mechanical metastructures. Emphasis is on exploiting nonlinear behavior within nonlinear mechanical lattices and lattices of nonlinear mechanical modules from the millimeter to meter scale. Proposals exploring interactions between nonlinear metastructures with fluids, especially if such interactions augment desired dynamic behavior, are strongly encouraged.

Embodied and Distributed Control, Sensing, and Actuation. This thrust develops deeper understanding, through supporting theory and experiment, of the role of embodiment and dynamics on a physical system's capability to process information and transform energy. Proposals emphasizing the mechanics and control of soft, continuous bodies are encouraged along with novel experimental paradigms leveraging programmable printed matter. Generally, this thrust strongly leverages advances in, and approaches from, sensory biomechanics, neuromechanics, underactuated systems theory, and mechanical locomotion dynamics to understand the motion of both articulated and continuum dynamical systems operating in highly-dynamic environments. The scientific principles sought, however, are not limited to biological movement and manipulation. Proposals are strongly encouraged that view morphology in an abstract sense. For example, understanding morphology as a system's symmetry, its confinement (e.g. chemical reactions), or its coupling topology.

Statistical Physics of Control and Learning. The program seeks to lay the foundations for an algorithmic theory of control and learning that goes significantly beyond the state-of-the-art in model predictive control and integrates novel learning methodologies that are not mere variations of artificial neural networks and deep learning. Additional goals of this program is to develop an experimentally tested theoretical framework for controlling and creating new types of critical dynamics, phase transitions, and universality classes by bringing together theory and physical principles in statistical dynamics with control and dynamical systems theory (controlling statistical dynamics). Topics of interest relating to this include: nonlinear control of distributions with non-Gaussian uncertainty; non-Gaussian uncertainty representations; understanding relationships between work absorption and dynamics in the presence of fluctuations leading to emergent prediction and emergent centralization; steering multi-critical interacting dynamical systems toward desired universal scaling behaviors; externally controlling the strength of stochastic fluctuations and intrinsic noise in systems that are driven far from thermal equilibrium and display generic scale invariance; and selectively targeting and stabilizing specific self-generated spatio-temporal patterns in strongly fluctuating reaction-diffusion systems. Stochastic control at the microscale to enable novel manipulation of the dynamics of synthetic and natural biomolecular machines is also of interest.

TPOC: Dr. Samuel C. Stanton, samuel.c.stanton2.civ@mail.mil, (919) 549-4225

(4) Propulsion and Energetics

Propulsion and Energetics Research supports the Army's need for higher performance propulsion systems. Future systems must provide reduced logistics burden (lower fuel/propellant usage) and safer (insensitive) higher energy density systems. Fundamental to this area are the extraction of stored chemical energy and the conversion of that energy into useful work for vehicle and projectile propulsion. In view of the high temperature and pressure environments encountered in these combustion systems, it is important to advance current understanding of fundamental processes to enable truly predictive models as well as to advance the ability to make accurate, detailed measurements for the understanding of the dominant physical processes. Thus, research in this area is characterized by a focus on high pressure, high temperature combustion processes and on the peculiarities of combustion behavior in systems of Army interest.

Hydrocarbon Combustion. Research on combustion phenomena relevant to diesel cycle engines is focused on intermittent reacting flows containing fuel injection processes, jet break-up, atomization and spray dynamics, ignition, and subsequent heterogeneous flame propagation as well. Gaining fundamental understanding of these phenomena pertaining is a major objective. Novel diagnostics for the investigation of the dense field region of the spray are of special interest. Research on heterogeneous flames requires supporting study into kinetic and fluid dynamic models, turbulent flame structure, soot formation and destruction, flame extinction, surface reactions, multiphase heat transfer, and other factors that are critical to an understanding of engine performance and efficiency. An additional consideration is the high pressure/low temperature ignition environment encountered in advanced engines, which influences liquid behavior and combustion processes at near-critical and super-critical conditions. Fundamental research is needed in many areas, including low temperature physical and chemical rate processes, combustion instability effects at low temperatures, and non-equilibrium behavior. New characterization methods to investigate kinetics and flame phenomena in-situ at high pressure are needed. New computational methods to be able to predictively model complex reacting systems are also needed. With advances in sensing, modeling, and control architectures, it is becoming possible to further optimize the performance of combustion systems. Providing the foundations for such active control is also of interest to the program.

Energetic Materials. Research on energetic material combustion processes is focused on understanding the dynamics of the planned and inadvertent ignition and subsequent combustion of these materials which are commonly used for propulsion in gun and missile systems and in ordinance. The program is also addressing the characterization of advanced energetic materials, e.g., those based on nanoscale structures and/or ingredients. Basic research is needed in several areas, including: thermal pyrolysis of basic ingredients and solid propellants; flame spreading over unburned surfaces (particularly in narrow channels); surface reaction zone structure of burning propellants; chemical kinetics and burning mechanisms; propellant flame structures; characterization of physical and chemical properties of propellants and their pyrolysis products; and coupling effects among the ignition, combustion, and mechanical deformation/fracture processes. The use of advanced combustion diagnostic techniques

for reaction front measurements, flame structure characterization, and determination of reaction mechanisms is highly encouraged, especially those able to probe surface and sub-surface reactions in the condensed phase. Also of interest are novel methods which can well characterize the ignition and burning behavior of a material utilizing only minute quantities of that material. Complementary model development and numerical solution of these same ignition and combustion processes are also essential. There is also need to understand the unplanned or accidental ignition of energetic materials due to stimuli such as electrostatic discharge, impact, friction, etc. This requires, for example, research on the processes of energy absorption and energy partitioning in the materials, the effect of mechanical damage on the ignition events, and other topics relating to the safety of energetic materials.

TPOC: Dr. Ralph A. Anthenien, ralph.a.anthenien2.civ@mail.mil, (919) 549-4317

ii. Electronics

The Electronics Division seeks to support scientific and engineering endeavors in research areas that possess the potential to define new electronic capabilities or to enhance future electronic performance. The Division is more concerned with generating basic knowledge about processes and mechanisms than creating actual devices, although prototype devices may be useful for demonstration of principle. The Electronic research sub-areas are (1) Nano and Bio- Electronics, (2) Optoelectronics, (3) Electronic Sensing, and (4) Electromagnetics and High Frequency Electronics. Proposals are sought that advance fundamental understanding of electronic and photonic processes leading to new or improved materials and devices with a strong prospect for use in future Army technology.

The Electronics Division supports many of the ARL S&T Campaigns, especially the Materials Research Campaign which is supported by all Electronics' sub-areas in novel electronic and photonic materials. The Computational Sciences Campaign is supported through novel Nano, Bio, and Optoelectronic computing, Sciences-for-Maneuver Campaign by active and passive sensing, Information Sciences Campaign by new algorithms from biosciences as well as electromagnetic discoveries, Sciences for Lethality and Protection Campaign through targeting and directed energy, and Human Sciences through understanding and interfacing electronically with biological systems.

The Division's research programs are currently focused on four research areas. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in electronics, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Biotronics

This research area focuses on the discovery and manipulation of phenomena and the creation of new processes where electronics and biology overlap at the cellular / sub-cellular level. This length scale is where the amplitudes of many types of energies (e.g.,

electrostatic, mechanical, and chemical terms) converge, and correspondingly, where electronics can have fundamental biological impacts and where leveraging electronics capabilities at the nanoscale can yield unique new understanding of the cellular and intracellular processes. New electronic structures and materials are now able to focus localized static electric and magnetic fields and electromagnetic fields at the nanoscale, which presents the opportunity to selectively address and manipulate the organelles and membranes making up the structure of the cell. Moreover, cell constituents can have a frequency dependent response to mechanical and electromagnetic excitation, resulting in unique electronically enabled and controlled biological experiments. Molecular and subcellular events at the biological interfaces or surfaces are key to downstream biological dynamics. The stimulation or manipulation of these events by electronic means provides the opportunity for unique control and experimentation that are orthogonal to existing biochemical or genetic approaches. Ion flow, which is fundamental to inter- and intra-cellular signaling and process control, is susceptible to electromagnetic influence and produces electromagnetic signatures of cellular processes. The dynamics of charged and polarized cellular components also produces minute displacement currents, and can produce very large field distributions in a confined nanoscale space (e.g., within a protein scaffold or across a lipid bilayer); both of which are subject to electromagnetic probing and analysis. The different geometries of organelles within a cell result in different electromagnetic signatures and sensitivities which can be leveraged for selective control of cellular processes. Proteins play a role in almost every cellular process. As extremely large and complex molecules, they should have electromagnetic and mechanical responses that can be exploited for control. The skeletal protein assemblies of the cell, in particular, may offer a highway for the introduction of electrical currents or mechanical vibrations. Bio-chemical or genetic alteration of the interface of the cell and its components can introduce new electromagnetic properties, for example a new capability for photosynthesis in bacteria or new electromagnetic responses. Cellular engineering of membranes, cellular organelles, and proteins by the introduction of nano-particles and bio-molecules can introduce new sensitivities and new functionality. Opto-genetics is a well-established procedure for interrogating cells. Early attempts at “magneto-genetics” have been controversial, however “electro- or RF-genetics” may offer new opportunities. There may also be inherently non-trivial quantum mechanical mechanisms linked to biological behaviors, such as navigation. Inherently quantum phenomena such as the tunneling of electrons and protons play a critical role in many intracellular processes and can be modulated or manipulated with nanoscale electric fields. This research area seeks understanding and control of inter- and intra-cellular phenomena at the micro- and nano-scale.

TPOC: Dr. James Harvey, james.f.harvey.civ@mail.mil, (703) 696-2533

(2) Optoelectronics

Research in this subarea includes novel semiconductor structures, processing techniques, and integrated optical components. The generation, guidance and control of UV through infrared signals in semiconductor, dielectric, and metallic materials are of

interest. The Army has semiconductor laser research opportunities based on low dimensional semiconductor structures (quantum dots, wells, wires, etc.) operating in the eye-safe (>1.55), 3-5, 8-12, and 18-24 microns regions for various applications, such as ladar, infrared countermeasures, and free space/integrated data links. Components and sources in the UV/visible spectral ranges (particularly < 300 nm) may be of interest as well. Research is necessary in semiconductor materials growth and device processing to improve the efficiency and reliability of the output of devices at these wavelengths.

Research that leads to an increase in the data rate of optoelectronic structures is sought. Interfacing of optoelectronic devices with electronic processors will be investigated for full utilization of available bandwidth. Electro-optic components will be studied for use in guided wave data links for interconnections and optoelectronic integration, all requirements for high speed full situational awareness. Optical interconnect components are needed in guided-wave data links for computer interconnection and in free-space links for optical switching and processing. For high-speed optical signal processing as well as potential for power scaling, research on individual and 1 or 2-D arrays of surface or edge-emitting lasers is necessary. Research addressing efficient, novel optical components for high speed switching based on plasmonics, quantum dots, metamaterials or other regimes may be of interest. Emitters and architectures for novel display and processing of battlefield imagery are important.

TPOC: Dr. Michael Gerhold, michael.d.gerhold.civ@mail.mil, (919) 549-4357

(3) Electronic Sensing

The ultimate goal of Army sensing is 100% situational awareness to include day/night, all weather, non-line-of-sight and through natural and man-made obstructions for sensing of vehicles, personnel, weapons, chemical and biological threats, projectiles, explosives, landmines, improvised explosive devices (IEDs), and motion. Novel techniques that enhance the stimulus-response characteristics of nano-structures and semiconductor devices are of interest. This includes ways to improve the absorption of the signal, conversion (transduction) of the signal to another form with higher efficiency, and techniques to lower the noise. Sensing technologies of interest to this research sub- area currently include acoustic; seismic; passive electromagnetic; magnetic, and light-matter interactions. Other technologies that meet an Army need are also welcome, however chemical, biological, and radar sensing techniques are generally funded through other sub-areas as is image processing.

Light-matter interactions at infrared and ultra-violet wavelengths are of particular interest. Efforts are sought that improve the quantum efficiency and lower the noise such that the signal to noise ratio is maintained as the temperature is increased. Research opportunities include components based on quantum confined devices and semiconductor materials operating in the infrared 1-24 microns regions as well as the ultra-violet spectral region. In both regions, fundamental studies involving growth, defects, interfaces, substrates, doping, and other electronic characteristics will be

considered. Back-of-the-envelope calculations of the detectivity or noise equivalent power should be included for proposals involving infrared and ultra-violet detection.

TPOC: Dr. Michael Gerhold, michael.d.gerhold.civ@mail.mil, (919) 549-4357

(4) Solid State and Electromagnetics

This research area emphasizes efforts to discover and create unique electromagnetic phenomena in solid-state materials and structures. Innovative research is sought in areas involving quantum phenomena, internally and externally induced stimulus, and novel transport and electromagnetic interaction effects in solid-state electronic structures. This basic research will address issues related to design, modeling, fabrication, testing and characterization to include the ability to individually address, control, and modify structures, materials and devices, and the assembly of such structures with atomic-scale control into systems. It will seek realize advanced device concepts with revolutionary capabilities.

This program will explore the latest developments in semiconductor materials and device physics, such as negative capacitance transistors, tunneling field effect transistors and ultra-wide bandgap materials. More importantly, it will emphasize scientific discoveries in the frontier of nanoelectronic materials and structures. Scientific opportunities in this research include, but are not limited to, quantum-confined structures (nano-tubes/-wires/-dots) and large-scale precise alignment and integration of these structures to create collective behaviors; 2D atomic crystals and their heterostructures; complex heterostructures of 2D crystals, topological insulators, Dirac and Weyl semimetals and other dissimilar nanoelectronic materials potentially leading to unique interfacial phenomena; spintronic, valleytronic, and mixed domain (charge/spin/quantum degrees of freedom) device concepts. Of interest are quantum transport phenomena such as ballistic transport and hydrodynamic flow, dissipationless transport in topologically protected edge states, and pseudo-relativistic transport of massless Dirac fermions. Exotic electromagnetic phenomena which require theoretical formulations beyond the well-established Maxwell's equations, such as axion electrodynamics, chiral anomaly and spontaneous symmetry breaking, are also relevant. Interfacial proximity effects in these heterostructures that lead to unique electromagnetic properties will also be considered.

TPOC: Dr. Joe Qiu, joe.x.qiu.civ@mail.mil, (919) 549-4297

iii. Materials Science

The Materials Science Division of the ARO seeks to realize unprecedented material properties by embracing long-term, high risk, high-payoff opportunities for the US Army with special emphasis on: Materials Design, Mechanical Behavior of Materials, Physical Properties of Materials, and Synthesis and Processing of Materials. Research supported by the Division seeks to discover the fundamental relationships that link chemical composition, microstructure, and processing history with the resultant material properties and behavior. The work, although basic in nature, is focused on developing new materials, material processes, and properties that

promise to significantly improve the performance, increase the reliability, or reduce the cost of future Army systems. Fundamental research that lays the foundation for the design and manufacture of multi-component and complex materials is of particular interest. Foundational research that integrates novel experimental work with the development of new predictive materials theory is also of significant interest. Furthermore, there is lasting interest in new ideas and cross-disciplinary concepts in materials science that may have future applications for the Army.

The Division supports the ARL Materials Research Campaign by aggressively seeking to extend the state-of-the-art in materials design, mechanical behavior of materials, physical properties of materials, and synthesis and processing research. It supports the ARL Sciences for Lethality and Protection Campaign with extraordinary lightweight materials, force-activated materials, stabilized nanostructured materials, manufacturing process science, novel electronics, and advanced sensory materials. It supports the ARL Sciences for Maneuver Campaign with unique materials for advanced power storage and generation and lightweight structures, in addition to low-cost manufacturing and repair processes. It also supports the ARL Computational Sciences Campaign with research efforts that integrate computational theory and precision experimental measurement to design and optimize advanced materials.

The Division's research programs are currently focused on five research areas that include one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in materials science, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Materials Design

The Materials Design program seeks to establish the experimental techniques and theoretical foundations needed to facilitate the hierarchical design and bottom-up assembly of multifunctional materials that will enable the implementation of advanced materials concepts including transformational optics, biomimetics and smart materials.

Directed 3D Self-Assembly of Materials is aimed at enabling the directed 3D assembly of reconfigurable materials, and developing viable approaches for the design and synthesis of multi-component materials incorporating hierarchical constructs and tolerant of structural defects.

Functional Integration of Materials focuses on demonstrating the predictive design and integration of functional properties and feedback control into complex multi-component systems, and developing analytical techniques for interrogating the evolution of the 3D structure and properties of material assemblies at the nanoscale.

TPOC: Dr. John Prater, john.t.prater.civ@mail.mil, (919) 549-4259

(2) Mechanical Behavior of Materials

The Mechanical Behavior of Materials program seeks to reveal underlying design principles and exploit emerging force-activated phenomena in a wide range of advanced materials to demonstrate unprecedented mechanical properties and complementary behaviors.

Force-Activated Materials focuses on the creation, design, and optimization of a broad range of robust mechanochemically adaptive materials, based on exquisite control of force-activated molecules and force-activated reactions, and on tailoring the deformation and failure mechanisms in materials to mitigate the propagation of intense stress-waves and control energy dissipation.

Mechanical Complements in Materials endeavors to create materials with the ability to facilitate extraordinary electrochemical reactions through an interdependent optimization of mechanical properties, to catalyze the discovery and demonstration of unique fiber precursors, tailored for lateral and axial interactions, toward new paradigms for revolutionary structural fibers, and to discover and optimize new atomic-scale strengthening mechanisms governing bulk mechanical behavior.

TPOC: Dr. David Stepp, david.m.stepp.civ@mail.mil, (919) 549-4329

(3) Physical Properties of Materials

The Physical Properties of Materials program seeks to elucidate fundamental mechanisms responsible for achieving extraordinary electronic, photonic/optical, magnetic and thermal properties in advanced materials to enable innovative future Army applications.

Novel Functional Materials supports the discovery of novel functional materials such as free-standing 2D materials/heterostructures/hybrids, Spin-Caloritronic materials, co-crystals, and other such materials with unique structures/compositions. The thrust focus is on the synthesis, modeling and novel characterization of these materials (organic/inorganic/hybrids) to determine unprecedented functional properties (semiconducting, superconducting, ferroelectric/multiferroic etc.).

Science & Engineering of Crystal Imperfections explores the influence (either positive or negative) of various crystal imperfections (e.g. point, line, area, volume defects etc.) on the physical properties of functional materials, and elucidates different mechanisms of incorporation during thin film growth/bulk materials processing of materials to influence the resulting extraordinary functional properties.

TPOC: Dr. Pani Varanasi, chakrapani.v.varanasi.civ@mail.mil, (919) 549-4325

(4) Synthesis and Processing of Materials

The Synthesis and Processing of Materials program seeks to discover and illuminate the governing processing-microstructure-property relationships to enable optimal design and

fabrication of nano or micro structural bulk structural materials.

Processing Induced Material Design supports research focused on innovative processing methods capable of fabricating materials with deliberate microstructural architectures and features that advance the material's properties to levels unattainable by conventional processing.

Manufacturing Process Science supports investigation into fundamental physical laws and the unique phenomena occurring under metastable and far-from-equilibrium conditions to develop revolutionary and disruptive new materials or processing methodologies.

TPOC: Dr. Michael P. Bakas, michael.p.bakas.civ@mail.mil, (919) 549-4247

(5) Innovations in Materials (International Program)

As one of the ARO International Programs, the Innovations in Materials Program is focused on supporting research at institutions outside of the U.S., with the goal of building international partnerships and laying the foundational work upon which future material technologies depend.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

iv. Earth Sciences

The Earth Sciences Division of the ARO seeks to advance understanding of the terrestrial environment for the U.S. Army with special emphasis on Earth Materials and Processes and Environmental Chemistry. Research supported by the Division seeks to explore the properties of Earth materials and chemical species to discover how they interact with their environments and respond to external forces. Knowledge of the fundamental properties of these materials, from the atomistic to the landscape scale, and their interactions with the atmosphere, hydrosphere, and biosphere are relevant to Army operations, infrastructure, and stewardship. Fundamental research lays the foundation to support a range of Army needs, including the remote characterization of land surfaces, trafficability of ground vehicles, and environmental priorities such as waste management and remediation. Furthermore, there is lasting interest in new ideas and cross-disciplinary concepts in Earth science that may have future applications for the Army.

The Division supports the ARL Sciences-for-Maneuver Campaign through advances to achieve superior remote characterization of terrain and new paradigms for change detection and maneuver. It supports the ARL Sciences for Lethality-and-Protection Campaign with the development of new approaches for protection systems that are effective, fieldable, and affordable against a broad array of threats. It also supports the ARL Human Sciences Campaign with novel predictive capabilities for energy propagation through geologic materials,

land management, and human health.

The Division's research programs are currently focused on two research areas. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in earth sciences, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Earth Materials and Processes

The Earth Materials and Processes program seeks to elucidate the properties of natural and man-made Earth surfaces, with the goals of revealing their histories and governing dynamics and developing theory that describes physical processes responsible for shaping their features.

Earth Surface Materials aims to utilize experiments, models, and theory development to describe the physical and mechanical properties and behaviors of rocks, minerals, and soil, and to exploit the properties of these materials to provide quantitative information on recent and ongoing surface processes and perturbations.

Surface Energy Budget aims to determine, at Army-relevant spatial and temporal scales, how natural and artificial surfaces (e.g., soil, sand, or concrete) store and conduct energy depending on their spatial relationships, inherent material properties, and imparted features such as moisture storage and evapotranspiration, and to determine how these surfaces affect flows in complex terrain.

TPOC: Dr. Julia Barzyk, julia.g.barzyk.civ@mail.mil, (919) 549-4379

(2) Environmental Chemistry

The goal of the Environmental Chemistry program is to understand the fate and transport of chemicals that in the long term will enable future force protection, and water treatment. This program seeks to encourage research to provide a more complete and practical understanding of chemical pathways of degradation and transformation in the environment. The research will embrace environmental complexity by including the study of multiple phases and chemicals simultaneously present. Environmental surfaces of interest are soils (e.g., clay, sediments, dust), water (e.g., surface and bulk, snow and ice structures) and films (e.g., biological and urban made). The program will identify fundamental research opportunities in two main thrusts: (i) *Chemical Fate and Transport*, and (ii) *Environmental Forensics*.

The *Chemical Fate and Transport* thrust interest is in mechanisms, thermodynamics and kinetics with a focus on experimental and theoretical approaches to investigate sorption, degradation, and photo degradation mechanisms of chemical species under environmentally relevant conditions. Of particular interest is understanding the conditions that lead to degradation and transformation of contaminants, and develop

novel speciation models of complex environmental media.

The *Environmental Forensics* thrust focuses on developing integrated experimental and computational approaches to discern chemical transformation of contaminants from source to point-of-detection and provide predictions of its future transformations in different environments and conditions. In addition, this thrust includes research to provide information about manufacturing process and location of chemicals released into the environment.

TPOC: Dr. Robert Mantz, robert.a.mantz.civ@mail.mil, (919) 549-4309

c. Information Sciences

Research in the Information Sciences is focused on discovering, understanding, and exploiting the mathematical, computational, and algorithmic foundations that are expected to create revolutionary capabilities for the future Army. Discoveries in this area are expected to lead to capabilities in materials, the information domain, and Soldier performance augmentation, well beyond the limits facing today's Army.

i. Computing Science

The principal objective of the ARO Computing Science Division is to provide increased performance and capability for processing signals and data, and to extract critical information and actionable intelligence to enhance the warfighters' situation awareness, decision making, command and control, and weapons systems performance. The Division supports research efforts to advance the Army and nation's knowledge and understanding of the fundamental principles and theories governing intelligent and trusted computing. More specifically, the Division aims to promote basic research to establish new computing architectures and models for intelligent computing, create novel data fusion and extraction techniques for efficient information processing, and build resilient computing systems for mission assurance. The results of these research efforts will stimulate future research and help to keep the U.S. at the forefront in computing sciences. The research topics described in this section of the BAA are those needed to provide the warfighters with the latest information science and technology to achieve the vision of future Army operations.

Research in the Computing Sciences Division will reveal previously unexplored avenues for new Army capabilities while also providing fundamental results to support ARL's (i) Information Sciences Campaign goal of algorithm design for object classification and scene understanding from active and passive 3D scenes and full motion video through enhanced semantic object recognition; (ii) Computational Sciences Campaign goal of large scale computing and modeling, and dynamic multi-dimensional heterogeneous data analytics, by devising scalable algorithms that effectively handle the size, complexity, heterogeneity, and multi-modality of data and by creating new hardware and software architectures for emerging and future computing systems that optimize the use of Army computational resources; and (iii) Information Sciences campaign goal of estimating adversarial dynamics and infrastructure

through new game models for capturing attacker/defender interactions and better predication of adversarial mental state (intent, capability, and decision process) to enable better cyber defense.

The Division's research areas are currently focused on five research areas that include one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in computing science, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Computational Architectures and Visualization

The Computational Architectures and Visualization program is concerned with modeling, analysis, design, and validation of computational infrastructure, both hardware and software, with special emphasis on the effect emerging and future computational architectures will have on managing, processing, analyzing, and visualizing massive data sets. This is due to the fact that the Army's ability to generate data of all types from the battlefield to the laboratory far outpaces the Army's ability to efficiently manage, process, analyze, and visualize such massive amounts of information. Emerging architectures only exacerbate the problem because the present and traditional models of computation no longer apply.

The research strategy is to focus on the effect that the technological shift to these new, advanced architectures will have on newly-developed systems and how to compute with these architectures efficiently as well as to make very large simulations and the visualization of massive data sets more interactive for the user while maintaining a high level of accuracy. As such, this programs funds innovative architectural designs of both hardware and software components and their interfaces that efficiently optimize computational resources and innovative algorithms that render massive data sets and/or massive geometric models and perform large scale Army simulations both quickly and accurately. Advances in this program are expected to lead to new computer modeling and design concepts (or paradigms) as well as software libraries that compute efficiently on these new and emerging architectures, that are scalable (usable on large-scale complex problems and able to handle massive amounts of data), and accurate (precise enough to predict and detect phenomena of interest) for both the laboratory and the battlefield. Also to be expected is the development of more efficient, interactive, and physically realistic battlefield, training, and scientific simulations.

Computational Architectures. Future computer systems will be both massively heterogeneous and parallel, implying the present and traditional models of computation will no longer be applicable. As a result, new computational theories are needed as well as mathematical abstractions and models of computation to address the difficulties associated with heterogeneous, parallel and distributed processing. Of special interest is determining how these new abstractions, algorithms, and computational processes map onto emerging computational resources of different types (e.g., multi-core, quantum, cloud, and chaotic computing, and determining which platforms are most suitable for Army applications). Other important issues to be considered for these emerging and

future architectures are programmability, language and compiler support, real-time scheduling, resource-allocation, and the development of a flexible software environment.

Visualization. Interactive simulation and visualization provides new and enhanced capabilities for the examination, exploration, and analysis of information and data critical to the Army. However, Army applications are not limited to any one type of data or computational platform. As a result, new research and techniques are needed in order to visualize and simulate complex Army data such as training for battlefield scenarios with speed and precision on any platform for superior analysis and information extraction capabilities for realistic Army simulations and full situational awareness. Specific research areas of interest are, but not limited to, computational geometry, robust geometric computing, geometric and solid modeling, interactive graphics, 3D visualization tools, verification and validation, and synthetic environments. Special emphasis is placed on making very large simulations and the visualization of massive data sets faster, more computationally efficient, and more interactive for the user while maintaining an appropriate level of fidelity and physical realism.

TPOC: Dr. J. Michael Coyle, joseph.m.coyle14.civ@mail.mil, (919) 549-4256

(2) Information Processing & Fusion

With ubiquitous data acquisition capabilities, effective data and information processing is of critical importance to defense missions. The Information Processing and Fusion program is concerned with the creation of innovative theories and algorithms for extracting actionable intelligence from diverse, distributed multimodal data to support Army operations.

Foundations of Image and Multimodal Data Analysis. Innovative research is sought concerning: (1) novel representations of multimodal data to enable the understanding of multimodal sensor data and contextual information, with particular emphasis on data in complex forms such as image or video data; (2) detection, localization, and recognition of objects and locations from image data with particular emphasis on provable performance guarantees; (3) detection of events, actions, and activities to extract activity-based intelligence, especially when no extensive training data is available; and (4) integrated approaches that enable semantic descriptions of objects and events including relations. Learning and adaptation should enable the representation at both low and high-levels, where inputs from actual users of the systems are used to improve the performance of the algorithms and the fidelity of models at all levels of the modeling hierarchy. Also of interest are methods to exploit the structure of the data, capture its intrinsic dimensionality, and extract information content of data. The development of an “information/complexity theory” and a “learning theory” specific for remote sensing, imaging data, and decision tasks is highly desirable.

Data and Information Fusion. Multimodal data acquisition systems are increasingly prevalent with disparate sensors and other information sources. This thrust seeks advanced mathematical theories and approaches for integrating multimodal data and

contextual information to provide actionable intelligence. Of particular interest are systematic and unifying approaches for data and information fusion from diverse sources. Scalable methods are needed for efficiently handling vast amounts of data. Fusion in networked environments addressing issues such as adaptive, distributed, and cooperative fusion is emphasized. Theories and principles for performance analysis and guarantees at all fusion levels to support robust data and information fusion are important to ensure successful military operations.

Active and Collaborative Sensing. Modern sensing systems typically include multiple networked sensors with communication capabilities where the whole network can be thought of as a Meta sensor that can be controlled, in addition to each individual node having some controllable degrees of freedom such as mobility for unmanned aerial/ground systems, pan-tilt-zoom for infrastructure sensors, or waveform for agile radar. Depending on the task or query, it is desirable for the system to control the data acquisition process so as to acquire the “most informative data” for the specific task or query. Consequently, of particular interest are methods that address the integration of mobility, sensor-selection, modality selection, and active observation for real-time assessment and improvements of sensing performance. Another research area of interest is performance-driven active data collection. A query is given to the system together with a desired performance bound. Where the confidence in answering the query is insufficient, the system should actively interrogate or control sensors in order to achieve the desired confidence. Such an active learning and information-driven sensor control should include the Soldier in the feedback loop.

TPOC: Dr. Liyi Dai, liyi.dai.civ@mail.mil, (919) 549-4350

(3) Information and Software Assurance

From the Army perspective, Information Assurance must provide authentic, accurate, secure, reliable, timely information to warfighters in order to achieve information dominance, regardless of threat conditions. Computing and information processes may be carried out over distributed and heterogeneous systems, which may include mobile computing and communications systems, and high performance information process systems that are inter-connected through both tactical and strategic communication systems.

Robust and Trusted Wireless Communication. Research is needed in the areas of theory, protocols, and techniques that will assure delivery of trustworthy data to support battlefield missions. Reconfigurable, survivable, and self-healing systems allow a combat unit to dynamically establish and maintain its command and communication capability under diversified and extreme battlefield situations. The Army requires a fully mobile, fully-communicating, agile, and situation-aware force that operates in a highly dynamic, network centric environment. This force consists of a heterogeneous mixture of individual soldiers, ground vehicles, airborne platforms, unmanned aerial vehicles (UAVs), robotics, and unattended sensor networks that operate in a complex wireless environment. Information theory has played a foundational role in the study of

security. Across a wide range of application domains and security objectives, information theory leads to insight to the underlying tradeoffs between security and performance. The Army seeks novel ideas in fundamental research areas such as information-theoretic security and the science of security that will provide direct guidance in the design of secure tactical wireless systems. In particular, topics of interest include new paradigms for physical layer security (ranging from confidentiality to authentication to trustworthiness in physical layer communications), the fundamental bounds in key management in distributed systems, the exploitation of key establishment and distribution protocols, and trusted information delivery and dissemination in mobile environments. The corresponding constructions that would arise from such an investigation represents a significant avenue for improving future wireless communication as well as the corresponding secrecy capacity limits that could serve as valuable guidelines in developing future systems with confidential and authenticated communications. New computing and communication protocols and techniques are needed to assure critical information processing and delivery even when such systems are under severe resource constraints or under persistent attacks.

Models and Metrics for Next Generation Survivable Systems. The field of information assurance needs a foundational science to guide the design of systems and to quantitatively measure safety and the level of assurance of complex systems that the Soldier depends upon today. Assurance principles and metrics are needed to help define, develop, and evaluate future robust and resilient systems and network architectures that would survive sophisticated attacks and intrusions with measurable confidence. The program seeks the capability to measure a complex system and to produce a scalar value that can determine the trustworthiness of that system. In addition, human users need to be in the loop for system assurance analysis. Developing human centric security-usability metrics, computational models for usable security in stressful situations, and adaptive security protocols according to perceived threats are some of the research areas of interest for improving warfighter performance while maintaining sufficient security requirements. One new challenging area of research that offers great promise in stronger system robustness is the modeling of adversaries and defender interactions, since ultimately systems need to defend effectively against their attacks. A deeper understanding and more accurate modeling of adversarial behaviors will improve future system development.

Cyber Deception. Cyber deception is a proactive technique to manipulate the mental state and decision process of the adversary so that we can degrade and mitigate their attack effectiveness. Unique aspects of cyber deception may offer more opportunities but add more complexity to model and analyze: 1) Cyber artifacts (both genuine and fake) can be created easily and are not bounded by the laws of physical space. The velocity of cyber situation change could be very high; 2) While deceptions are normally played out between a defender and an attacker, users could be directly or indirectly entangled in the game due to the nature of shared infrastructure. Usability issues or negative impact to the mission need to be considered; 3) Social and cultural aspects are important elements in the cyber deception game. Key scientific understanding is still lacking in 1) Establishing effective mental models for understanding and tracking the

adversaries' intent, capability, and decision process, and 2) deception information formulation and communication techniques, which requires new thinking in order to provide a quantifiable measure on how a given deception approach will drive mental state change. Recent honeypots/decoy experiences gave initial insights on how to engage adversaries through fake cyber artifacts, but a clear understanding of the dynamics (especially mental interactions) between attackers and defenders is missing. A better learned adversarial model will be critical to the success of cyber deception. In addition, advanced honeypot like schemes are desired to engage adversaries in order to gain understanding of adversaries so that effective deception schemes can be crafted.

Principles of Moving Target Defense. Current cyber defenses are often static and governed by lengthy processes, while adversaries can plan their attacks carefully over time and launch the attacks at cyber speeds at times of their choosing. The program seeks a new class of defensive strategies to present adversaries with a moving target where the attack surface of a system keeps changing. Although such an idea of a "moving target" is a powerful paradigm for building systems robust to security threats, many fundamental aspects associated with such a strategy need to be further investigated and understood. For example, such a "moving target" system may operate under many different contexts, ranging from the use of frequency hopping in spread spectrum to software diversification. It is critical to establish new theories and models that can provide trade-off analysis between system robustness against attacks vs. performance/usability, and quantify the risks associated with system adaptation under an adversarial setting. Ultimately the understandings and analytical models obtained will establish an important foundation for creating robust tactical systems capable of maximizing the difficulties for the adversaries to attack while minimizing the impact to system performance and usability.

TPOC: Dr. Cliff Wang, cliff.x.wang.civ@mail.mil, (919) 549-4207

(4) Intelligent Systems

Computational intelligence is becoming an important part of our life and plays a critical role in defending the nation, both in physical and cyber space. Advanced capability in learning, understanding, reasoning, and decision making are key elements of intelligent systems. However, compared to humans, machine intelligence is still at its infancy. Important issues such as robustness, adaptability, awareness, and realism are the frontier of research today. Advances in these areas will contribute to the development of intelligent systems that can greatly enhance the Army's capabilities in mobility, agility, lethality, and survivability.

Advanced Learning Theory, Methodology, and Techniques. Machine learning to build computational intelligence has been studied for the past 50 years. While great strides have been made in artificial intelligence as demonstrated by the success of Deep Blue and recently AlphaGo, compared to biological systems, machine learning still lacks the rigor, agility, and adaptation and is quite fragile to changing environment or context. This thrust focuses on establishing a theoretical foundation of machine learning. New

learning approaches will need to address both the dimensionality challenges and temporal characteristics that may be evolving continuously. In addition, new techniques must address robustness where the learning system will be able to deal with incorrect input due to noise and observation errors and potentially malicious input that aims to disrupt learning. Adaptation in learning is another major challenge. It is critical to create an advanced system that can continuously learn and evolve to changing context and environment, update its knowledge base accordingly, and dynamically adapt its reasoning, decision, and action.

Intelligent Systems for Improved Decision Making. Intelligent systems span a wide spectrum of applications, from autonomous robotics such as Unmanned Ground Vehicle (UGV) and UAV to software decision making tools for Command, Control, Communications, Computers, Intelligence, Surveillance, and Reconnaissance (C4ISR). Quite often intelligence systems are engaged in sensing, perception, reasoning and understanding, learning, collaboration, and taking actions in an autonomous way. For these systems, sensing and vision understanding functions play a key role in establishing perception and situation awareness and help perform complex tasks such as navigation. Robust networking, communication and information processing ensure mission execution and contribute to a shared knowledge base, coordination and collaborations for dynamic environments. A common trait of intelligent systems lies in their capability in processing information along with suitable context and environment to make the best decisions and to take appropriate actions. An ideal intelligence system would have a strong cognitive capability that would enable itself to deal with environmental changes, to carry out new tasks, and cope with unknown situations. Unfortunately the current generation of intelligent systems have fairly narrow scopes and are designed to perform specific tasks, thus are quite often unable to adapt to a changing environment. New research is needed to create a new intelligent system with advanced cognitive capabilities that can successfully integrate advanced learning, knowledge representation and organization, cognitive reasoning, adaptation, and autonomous action.

TPOC: Dr. Cliff Wang, cliff.x.wang.civ@mail.mil, (919) 549-4207

(5) Advanced Computing (International Program)

As one of the ARO International Programs, the Advanced Computing Program in South America is focused on supporting research at universities outside of the U.S., with the goal of providing key connections with world-class researchers outside the U.S. and supporting the most forward looking and promising research in computing science.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

ii. Mathematical Sciences

The objective of the Mathematical Sciences Division is to support research to develop a

foundational framework for the understanding and modeling of complex nonlinear systems, for stochastic networks and systems, for mechanistic models of adaptive biological systems and networks, and for a variety of partial differential equation (PDE) based phenomena in various media. These research areas focus on discovering nonlinear structures and metrics for modeling and studying complex systems, creating theory for the control of stochastic systems, spatial-temporal statistical inference, data classification and regression analysis, predicting and controlling biology through new hierarchical and adaptive models, enabling new capabilities through new bio-inspired techniques, creating new high-fidelity computational principles for sharp-interface flows, coefficient inverse problems, reduced-order methods, and computational linguistic models.

Research in the Mathematical Sciences Division will reveal previously unexplored avenues for new Army capabilities while also providing fundamental results to support ARL's (i) Information Sciences Campaign goal of image and video sampling and reconstruction through investigations of sparsity in combinations of distributions with unknown parameters; (ii) Computational Sciences Campaign goals of stochastic simulation methods, interfaces and evolving topologies, and uncertainty propagation, through investigations of fast separable methods for stochastic PDEs, of novel meshes for both front tracking and domain-fitting, and of weak-interaction processes; (iii) Computational Sciences Campaign goal of computational social sciences by establishing a general theory of crisis/change through new mathematical models that go beyond network models to incorporate morphisms as model elements; (iv) Human Sciences Campaign goals of brain networks and of cognitive and neural modeling, through investigations of neural dynamic models and their computation; and (v) Computational Sciences Campaign goal of stochastic optimization and modeling through investigations of fast separable methods for stochastic PDEs.

The Division's research programs are currently focused on four research areas. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in mathematical science, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Modeling of Complex Systems

The Modeling of Complex Systems Program is a program of fundamental mathematics-oriented research, the broad objectives of which are twofold. First, the program seeks to develop and analyze new, innovative, and robust modeling frameworks that may be adapted and generally applied across a variety of disciplines. The second goal is to develop both quantitative and qualitative models of specific complex phenomena in areas in which current models are either not fully based on first/basic principles or are based on empirical and ad hoc metrics for which the first/basic principles are not yet well known. Although they break down into more specific research directions, the three thrust areas of interest to the Modeling of Complex Systems Program are 1) development and analysis of new, general modeling frameworks, 2) geometric and topological modeling – which can be further broken down into more specific thrust areas, as noted below – and 3) small and large group social modeling and social informatics.

Metrics – in the general, non-mathematical sense of the word – are a natural part of the mathematical modeling framework. Traditional metrics, when they exist, often do not measure the characteristics in which observers in general and the Army in particular are interested. For many complex phenomena, new metrics need to be developed at the same time as new models. As is the case for the modeling effort, these metrics should preferably be in a complete mathematical analytical framework, which is to say, in part, that they should derive from the problem in question as opposed to a situation in which one forces the model to fit an *a priori* chosen metric. The research in modeling of complex phenomena supported by the Modeling of Complex Systems Program is primarily mathematical analysis and *not* numerical analysis or computational mathematics. One expects computation to play some role in any modeling endeavor, but the innovation in research carried out in the Modeling of Complex Systems program should be largely in the areas of modeling and analysis, and not in the computational techniques.

Furthermore, any modeling research effort that could be of benefit to military or intelligence applications but that might not fall directly under one or more of the program thrust areas will still be considered, particularly if the innovation in the modeling and analysis are significant and noteworthy.

The three major areas of research of the Modeling of Complex Systems Program are:

Modeling Frameworks and Analysis. Mathematical and physical modeling is fundamental to nearly every other direction of research in the physical, social, and computational sciences. A common element of modeling – even if the phenomenon in question is highly complex – is to incorporate simplifying assumptions that sacrifice realistic application and utility for computational ability. For Army and DoD applications, however, such simplifications often render the model impractical. Modeling frameworks are desired that are able to eschew the usual computational simplification assumptions and realistically capture, adequately govern and/or control, and effectively operate within the particular complexities of real world environments and phenomena, while still maintaining some degree of computational tractability. Of specific interest are causal and predictive modeling frameworks, hybrid model frameworks that capture both causal and predictive features, statistical modeling frameworks, and abstract categorical models (cf. Homotopy Type Theory).

Models of particular complex systems that address and are to be utilized for more specific purposes and objectives will be assessed within the context of one of the program's other modeling thrust areas described below. Research carried out under this section should address the general theory and analysis of mathematical modeling from a broader perspective.

Geometric and Topological Modeling. Representation of complex, irregular geometric objects and complicated, often high-dimensional, abstract phenomena, functions, and processes is fundamental for Army, DoD, and civilian needs. Such needs arise in the modeling of urban and natural terrain, geophysical features, biological objects (e.g. human

brain mapping), information flow, and many other contexts. Any research that incorporates an innovative geometric and/or topological approach to address a problem with military, defense, and intelligence applications is welcome and will be considered, but there are two specific threads that are of particular interest to this thrust of the program: 1) geometric data analysis, and 2) multiscale geometric modeling, including dynamics and physical modeling on domains with fine, complex, geometric and/or topological structure.

Geometric data analysis includes – among other subfields – topological data analysis, subspace analysis, principal component analysis, and dimension reduction techniques. Current research directions of importance to Army applications include video, audio, and image processing (i.e. mathematical signal analysis), fast and accurate face/object recognition (i.e. reconstructing and matching geometric data through queries over a database), geometrically motivated methods and structures for working effectively with large – and often real-time extracted – data sets that may be corrupted in some way (e.g. missing or distorted data), and the application of persistent homology in the detection and classification of signals by shape. For instance, although good progress has been made in this direction, real-time capture, representation, and visual reproduction of 3D terrain – not just as a height field but with multivalent height functions and clearly defined topological obstructions – obtained directly from real-time or stored point-cloud data cannot be fully achieved with current techniques like the multitude of variations of piecewise planar surfaces that are presently studied. New approximation theory that does not require the classical assumptions – primarily smoothness – and that provides structure for the many new non-smooth approximation techniques currently under investigation is required. Concurrently, research on the metrics by which we measure and evaluate the approximation is needed.

Additionally, approximation theory for information flow and other abstract phenomena in large wireless communication, sensor and social networks is also of interest. The approximation theory developed under support of this program is expected to provide building blocks for computational geometry, pattern recognition, automatic target recognition, visualization systems, information processing and network information flow.

Multiscale geometric modeling, analysis, and dynamics are of particular interest, both in the context of models of physical phenomena over real-world terrain and in the aforementioned complex, high-dimensional data structures. Models that make use of self-similar structures and recursively defined spaces (e.g. fractals, solenoids, etc.) would be of great interest in adapting or enhancing current techniques in areas such as data mining, fluid and heat flow, and search, evasion, deployment, and maneuver over complex terrain that exhibits self-similar properties (e.g. urban or mountainous terrain). Current techniques for dealing with complex dynamical processes and large, noisy, and possibly corrupted data sets could be greatly improved in both the time and efficiency realms by employing techniques from scale symmetry, which often allows one to reduce a large and unwieldy number of variables to a more manageable problem if the variables are appropriately scaled. Models that adapt self-similarity and automata theory, in particular, can oftentimes lead to mapping complex dynamical systems problems into an algebraic and/or topological category, which then may allow for entirely new tools and approaches to be used.

Homotopy Type Theory and its applications are such an area that is of significant interest in military applications.

Small and Large Group Social Modeling. Both qualitative and quantitative analytical models of social group dynamics and information flow are required for operations, training, simulation (computer generated forces) and mission planning, as well as real-time analysis, processing, and dissemination of information. Current models have limited accuracy. Research focused on mathematically justified, practically useful, computationally tractable and data-tractable models is needed. (“Data-tractable” means “does not require more data or more detailed data than is realistically likely to be available.”). Research on the metrics in which the accuracy of the models should be measured is also vitally important.

The broad term for this research pursuit would be social informatics, which is an important area in which more significant progress is needed, especially in the military and intelligence realms. Social informatics, briefly, is the study of the role played in society by information-based technology. This includes examinations of how the spread of information through technology effects social and organizational changes in society, as well as the converse – how social organization of information and use of technology to spread information are affected by social structures and practices. Modeling of the flow, dissemination, and possible evolution of belief systems and cultural factors through physical group migration or through social networking is an important tool in being able to predict where social and military issues might arise in the world. This could lead to better preparation and the avoidance of “caught-off-guard” situations in global politics and military affairs.

Included within the social informatics realm are narrower but equally important research directions. These would include – but not be limited to – the dynamics of information flow across physical groups of people as well as social/technological networks, pattern detection in information flow and language, which would lead to more efficient surveillance and pre-emptive threat detection, as well as security in information transmission. In this latter direction, new and unique data structures and encryption techniques would be hugely beneficial. Complex but tractable multiscale data structures and viable fractal or self-similar encryption techniques – which heretofore have proved to be of academic but not very practical interest – are just a few examples of many that could prove useful.

Paralleling the pursuit of social informatics, information flow analysis, and pattern recognition in information and data is the quickly developing field of deep machine learning. The Army is particularly interested in developing programming models and training algorithms that can automate as much of these processes as possible. This involves a great deal of research into pattern recognition and data analysis, as well as model analysis. The interplay between causal, data-based models and predictive modeling are of special interest and an active area of military research.

TPOC: Dr. Jay Wilkins, leonard.d.wilkins3.civ@mail.mil, (919) 549-4334

(2) Probability and Statistics

The research strategy of this program will focus on the following opportunities for crucial discoveries: innovative theories and techniques for modeling, analysis, and control of stochastic networks, stochastic infinite dimensional systems, and open quantum systems; innovative statistical theory and methods for network data analysis, spatial-temporal statistical inference, system reliability, and classification and regression analysis. Research in this area will provide the scientific foundation for revolutionary capabilities in counter-terrorism, weapon systems development, and network-centric warfare.

The program supports extramural basic research in stochastic analysis and control, and statistical analysis and methods in response to the Army's need for real-time decision making under uncertainty and for the test and evaluation of systems in development. Special emphasis is placed on methods for analyzing data obtained from phenomena modeled by such processes. The two major areas of research are described below.

Stochastic Partial Differential Equations. Research on analytical and approximation methods for solving stochastic delay and stochastic partial differential equations and their related nonlinear filtering and control problems is one of the program objectives. The Hamilton-Jacobi-Bellman theory via dynamical programming principle and/or necessary optimality conditions in terms of maximum principles have to be further developed and refined for optimal control of these infinite dimensional equations. Modeling of rare event analysis of spatial-temporal random phenomenon requires a fundamental mathematical understanding of the theory of large deviations for infinite-dimensional stochastic dynamical systems, in particular stochastic partial differential equations driven by Brownian and/or Poisson space time noises.

Measure-Valued Stochastic Processes. An emerging and mathematically challenging area is the study of measure-valued process models of stochastic networks. One of the goals of this program is to develop general tools for the study of these processes, and their application to gain insight into the performance analysis, stability, control and design of this class of network models.

Weakly Interacting Stochastic Systems. Many physical and engineering systems can be modeled as a large collection of stochastically evolving agents or particles, whose dynamics are weakly coupled by an interaction that depends only on the empirical rise to many mathematically challenging questions. Among the many areas where progress is needed, the most important include the development of a general methodology to understand the long- time behavior of the solution to the limit measure-valued stochastic equation, and a related analysis into the implications of the long-time behavior of the limit for the stability or metastability of the stochastic N- particle system. Also of interest are issues of mean-field stochastic control, game theory, and in particular the design of stochastic controls via Lyapunov function techniques and the interplay between ergodicity and controllability in the stabilization of the stochastic system.

Quantum Stochastics and Quantum Control. With technological advances now allowing the possibility of continuous monitoring and rapid manipulations of system at quantum

level, there is an increasing awareness of the applications and importance of quantum filtering and quantum control in engineering of quantum states, quantum error correction, quantum information, and quantum computation. To further understand the back action effects of measurements on quantum states and control of the system based on these measurements, novel mathematical development of non-commutative quantum stochastic calculus, quantum filtering and quantum control theory is necessary. Proposed mathematical research of this nature that has potential applications in quantum information and quantum computation is hereby solicited.

Statistical Testing and Validation of Network Models. The structure (network design), data sets and human element have a major impact on soldier performance. The need exists to develop new statistical techniques and theories to support the selection of optimal designs, validate predictive network models and modify data mining and inferential statistical techniques to use on ill-defined data and improve measurement. The research concentration areas include dynamical inference of structure in underlying models. In particular, ability to measure reaction of particular features buried in the network and not directly observable, and sequential analysis (change point detection) in networks.

Reliability and Survivability. To support future network-centric operations, the Army needs novel and efficient statistical tools for improving network reliability and survivability, and for analyzing data collected from sensor networks.

Bayesian and Non-parametric Statistics. Future emphasis in statistics on "predictive" models vice explanatory models is important. Military operations call for predictive models based on a growing base of sensor-fueled data stores. Increased computational capability is also leading statistics in a new direction, away from using "classical" results which are really approximations to avoid computational issues. This suggests a need for increased emphasis on research in areas such as robust statistics, non-parametric statistics, non-linear models etc.

Statistical Analysis of Very Large and Very Small Data Sets. The state-of-the-art in statistical methods is well adapted to elicit information from medium-size data sets collected under reasonable conditions from moderately well-understood statistical distributions. However, Army analysts frequently have very large or very small data sets sampled from nonstandard, poorly understood distributions. Very often the data available does not measure the variable of interest and gives only indirect information. Thus the variable of interest is sampled in some ill-defined fashion. One needs to look at this problem in some generality and develop new theory to handle such problems with ill-defined data.

Geometric Methods for Statistical Inference. There is a research interest in unifying mathematical frameworks to capture the space of statistical models for inference and learning purposes. Models using differential geometric insights (such as Information Geometry) to characterize the manifold of probability density functions, to conceptualize measure-valued stochastic processes as paths on such manifold, and to understand the

metric of model comparison and selection are welcome.

TPOC: Dr. Joseph Myers, joseph.d.myers8.civ@mail.mil, (919) 549-4245

(3) Biomathematics

The introduction of Biomathematics as a separate area of basic research recognizes the importance and specialized nature of quantitative methods, specifically mechanistic modeling, in the biological sciences. Biology involves a large number of entities that interact with each other and their environment in complex ways and at multiple scales. This complexity makes biomathematics a highly interdisciplinary field that requires unique and highly specialized mathematical competencies to quantify structure in these relationships. In fact, progress in mathematical models of biological systems has traditionally been achieved by making convenient simplifications; major advances in Biomathematics research continue to require removing these assumptions (for example, stationarity, ergodicity and deterministic nature) and finding ways to effectively model the essential complexity. Modeling techniques currently utilized in the field range from agent-based approaches for determining the results of individual behavior, whether those individuals be molecules, zooplankton, or humans, to multi-compartmental modeling in physiology, epidemiology and neurobiology, to network models involved in understanding ecosystem and human social dynamics, as well as encompassing both deterministic and stochastic approaches. Research in control techniques is also valuable for its potential application in militarily important areas such as bio warfare and disease spread. Exciting new opportunities to advance the field are found in high risk attempts to develop modeling techniques in areas of mathematics, such as algebra and topology, not traditionally brought to bear on biological problems, advances in Bayesian statistics, a growing recognition that the diffusion approximation is not necessarily adequate for many systems, and the availability of large amounts of complex biological data.

The ultimate goal of the Biomathematics Program focuses on adapting existing mathematics and creating new mathematical techniques to uncover fundamental relationships in biology, spanning different biological systems as well as multiple spatial and temporal scales. One area of special interest to the Program is Neuromathematics, the mechanistic mathematical modeling of neural processes. Recent advances in neuroscience provide important foundations to begin understanding how the brain works. Combined with experimental data, innovative mathematical modeling provides an unparalleled opportunity to gain a revolutionary new understanding of brain physiology, cognition (including sensory processing, attention, decision-making, etc.), and neurological disease. With this new understanding, improved soldier performance, as well as treatments for Post-Traumatic Stress Disorder, Traumatic Brain Injury, and other brain-related disorders suffered by the warfighter will be able to be achieved more effectively, efficiently, and ethically than via experimentation alone.

Thrust areas of the Biomathematics Program are as follows:

Fundamental Laws of Biology. The field of physics has long been “mathematized” so

that fundamental principles such as Newton's Laws are not considered the application of mathematics to physics but physics itself. The field of biology is far behind physics in this respect; a similar process of mathematization is a basic and high-risk goal of the ARO Biomathematics Program. The identification and mathematical formulation of the fundamental principles of biological structure, function, and development applying across systems and scales will not only revolutionize the field of biology but will motivate the creation of new mathematics that will contribute in as-yet-unforeseen ways to biology and the field of mathematics itself.

Multiscale Modeling/Inverse Problems. Biological systems function through diversity, with large scale function emerging from the collective behavior of smaller scale heterogeneous elements. This “forward” problem includes creating mechanistic mathematical models at different biological scales and synchronizing their connections from one level of organization to another, as well as an important sub problem, how to represent the heterogeneity of individual elements and how much heterogeneity to include in the model. For example, the currently increasing ability to generate large volumes of molecular data provides a significant opportunity for biomathematical modelers to develop advanced analytical procedures to elucidate the fundamental principles by which genes, proteins, cells, etc., are integrated and function as systems through the use of innovative mathematical and statistical techniques. The task is complicated by the fact that data collection methods are noisy, many biological mechanisms are not well understood, and, somewhat ironically, large volumes of data tend to obscure meaningful relationships. However, traditionally “pure” mathematical fields such as differential geometry, algebra and topology, integration of Bayesian statistical methods with mathematical methods, and the new field of topological data analysis, among others, show promise in approaching these problems. Solutions to these types of multiscale problems will elucidate the connection, for example, of stem cells to tissue and organ development or of disease processes within the human body to the behavior of epidemics.

The “inverse” problem is just as important as the forward problem. From an understanding of the overall behavior of a system, is it possible to determine the nature of the individual elements? For example, from knowledge of cell signaling, can we go back and retrieve information about the cell? Although inverse problems have been studied for a long time, significant progress has been elusive. This thrust area involves innovations in spatial and/or temporal modeling of multi-level biological elements with the goal of achieving a deeper understanding of biological systems and eventually connecting top-down (data-driven) and bottom-up (model-based) approaches.

Modeling at Intermediate Timescales. Biological processes operate at a variety of timescales; understanding the dynamics of a system at intermediate timescales, as opposed to its long term, asymptotic behavior, is critically important in biology, more so than in many other fields. For example, an epidemic is a necessarily transient phenomenon. In addition, deterministic models are an approximation that often is not good enough to be informative about the system. Yet, intermediate timescales of nonlinear dynamics with stochasticity, both internal and external, are not well

understood. This thrust area attempts to fill the gap in the basic understanding of modeling of systems, as well as their control, at intermediate timescales.

TPOC: Dr. Virginia Pasour, virginia.b.pasour.civ@mail.mil, (919) 549-4254

(4) Computational Mathematics

The research strategy of this program is to focus on the following opportunities for crucial discoveries: innovative methodologies for solving currently intractable problems that take advantage of symmetry, conservation, and recurrence, that can adapt to both the evolving solution and to the evolving run-time resource allocation of modern computer architectures; novel algorithms that accommodate different mathematical models at different scales, interacting subsystems, and coupling between models and scales; methods that incorporate nonlocality through integral operators with advantageous representations. Research in this area will ultimately lead to the development of new mathematical principles that enable faster and higher fidelity computational methods, and new methods that will enable modeling of future problems.

Scientific computation is an essential component of scientific inquiry, complementing theory and experiment, and is also an essential element of engineering in both design and in failure autopsy. Simulations in support of inquiry, design, or autopsy often require expert knowledge in order to select methods that are compatible with the assumptions of the scenario at hand, require considerable skill to properly set up, require considerable time, memory, and storage on large scale parallel/distributed/heterogeneous systems to compute, and require considerable skill and effort to distill useful information from the massive data sets which result. Expert knowledge is also required to quantitatively estimate solution accuracy and to estimate the time and effort required to achieve a desired accuracy. Data has become ubiquitous and is potentially very valuable in increasing solution accuracy and/or decreasing the effort required to solve, but mathematically sound methods for incorporating data into accurate simulations are incomplete. Simulations are not always timely, with results often not being available until after they are needed, for example in calculating failure of New Orleans levees during Katrina and in revising those estimates based on real time surge data. The emphasis in the Computational Mathematics program is on mathematical research directed towards developing capabilities in these and related areas.

For problems that are not time-limited, research areas of interest include but are not limited to the following:

Advances in Numerical Analysis. Novel methodologies are sought for solving currently intractable problems. New ways of taking advantage of symmetry, conservation, and recurrence are of interest, as are new ways of creating sparsity and new computational structures which can adapt to both the evolving solution and to the evolving run-time resource allocation of modern computer architectures. Rigorous analysis is sought for each in order to enable error bounds, error distribution, and error control.

Multiscale Methods. Problems of interest to the Army are increasingly characterized by the fact that behavior at microscopic scales has a large influence on performance of systems. To analyze these situations, algorithms are needed to deal with different mathematical models at different scales, interacting subsystems, and coupling between models and scales. The emphasis of this program is on mathematical methods which have some promise of wider application rather than methods limited only to specific application areas.

Fractional Order Methods. As an alternative to high order methods and other less-local operators, fractional operators are another nonlocal operator that have proven to work well in modeling and have the advantage of not enforcing dubious assumptions of smoothness, especially at discontinuities and interfaces. However, the nonlocality of fractional operators also typically introduces a significant increase in computational load. Advances in novel efficient computational methods for these operators are of interest

Army systems often operate under rapidly-changing unpredictable and adverse conditions. It is desirable for models to be computationally simulated and fast enough to drive decision making, exercise control, and to help avoid disaster. Such simulations need to be created, run, and interpreted in better than real time. Research directed towards making this goal achievable is of interest, such as:

Reduced Order Models. Full scale simulations are often not realizable in real time. In order to investigate the behavior of systems under a variety of possible scenarios, many runs are required. Reduced order models are one way to enable this. Possible methods to create these models include adaptive simplification methods based on singular value decompositions and reduced order numerics. To be useful, all such models should be equipped with reliable estimates of accuracy.

Problem Solving Environments. To enable rapid decision making that is driven by simulation, it is necessary to set up simulations very quickly and obtain results in an understandable format. Matlab is one current tool for such a problem solving environment. What are other approaches?

Embedded Simulation. As algorithms become more efficient and computational devices shrink, it will become increasingly possible to use real-time simulation to drive control systems. New methods which address this goal are welcome, especially those which permit user- controlled and/or adaptively-controlled tradeoffs between speed and accuracy.

Decision Making. One valid criticism of numerical simulation is that it takes so long to set up, run, and post-process the results that they cannot be used in a timely manner to guide decision making. Mathematical ideas that help address this problem are of interest.

TPOC: Dr. Joseph Myers, joseph.d.myers8.civ@mail.mil, (919) 549-4245

iii. Network Science

The objective of the Network Sciences Division is to discover mathematical principles to describe ever present networks in all walks of life (e.g., organic, social, electronic) and, in particular, the emergent properties of networks. Study of Network Science is necessarily multi-disciplinary drawing on tools and techniques from statistical mechanics, information theory, computer science, control theory and social sciences to studies interactions at large scale, be they in swarms of insects or ant colonies, human societies, or networked autonomous systems. The basic principles discovered should, in turn, lead to creation of algorithms and autonomous systems that can be used to reason across data generated from disparate sources, including, sensor networks, wireless networks, and adversarial human networks. Research in this Division has applications to a wide variety of developmental efforts and contributes to the solution of technology-related problems throughout the Army's Future Force operational goals engendered by principles such as the Net-Centric Warfare and Third Offset strategy.

Research in the Network Science Division, while primarily driven by discovery of foundational principles, will, however, be cognizant of and contribute to providing crucial underpinning support to ARL's Information Sciences Campaign. In particular, the following goals within ARL's Information Sciences Campaign are explicitly addressed including: (i) assessment and control of behavior goal by creating new methods in design and controllability of composite and multi-genre networks; (ii) social effects and human-machine interaction through the exploration of social and cognitive networks, and generation of intelligent actions in a mix of information agents and humans; (iii) unconventional communication networks and adaptive by making information available at the tactical edge while taking limited bandwidth and human-information interaction modalities into account, and (iv) taming flash-flood of information available at the tactical edge.

The Network Science Division hosts four main programs in Wireless and Hybrid Communication Networks, Social and Cognitive Networks, Intelligent Information Networks, Multi-Agent Network Control, and an international research program in Network Science and Intelligent Systems. The boundary between these programs is fluid and, thus, a research topic might fall in more than one program area. Furthermore, there are shared interests between the Social Sciences program in Physical Sciences Directorate and Social and Cognitive Networks (SCN) program in Network Science, with SCN paying special attention to the human dimension from a network science perspective, including study of connections between interdependent people (such as teams), between social systems and cognitive processing (such as collective learning and decision making), and between humans and machines, using tools and techniques from computer science to further the study of social and cognitive processes of humans embedded in large social, interconnected systems. It is perhaps worth emphasizing that research which elucidates and defines the common underpinning science cutting across different types of networks is particularly of interest to Network Science Division.

The Division's research areas are currently focused on five research areas that include one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in network science, are listed

in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Communications and Networks

This program is concerned with the investigation and advancing of network science applied to communication networks, in particular in wireless and tactical environments, with focus on Department of Defense and Army unique problems. These include, but not limited to, infrastructure-less wireless networks operating in congested and contested spectrum. Also of interest is the analysis of mutual interaction among the communications, social and information networks.

Wireless Network Theory. Research is required in the broad area of wireless network science including fundamental limits, performance characterization, novel architectures, and high fidelity simulation of multi-hop wireless networks with mobility, node loss, natural and man-made impairments and unpredictable, bursty traffic. Of particular importance is the extension of these findings in millimeter wave networks where spectrum is abundant, but connections are fragile and distances are short. Novel analytical tools and simulation techniques may be necessary to allow for the modeling of very large networking scenarios without losing the fidelity at the physical layer, which is critical in millimeter wave networks.

Emerging communications network paradigms of Software Defined Networking (SDN) and Network Function Virtualization (NFV) are also of interest as applied to wireless and hybrid networks. Concepts from SDN/NFV could be adapted for wireless ad hoc networks, using innovative methods. Complete centralization may not be desirable, but policy control and hierarchical control of semi-autonomous systems could be useful. Exploitation of SDN control architecture to tailor virtualized network resources according to the needs and objectives of the users is desired. Also, exposure of signaling traffic in wireless SDN creates significant security challenges which need to be resolved.

Mobile Ad Hoc and Sensor Networks. Networks serving Army needs operate in highly dynamic environments with limited or no infrastructure support. Available spectrum may be highly congested and contested, and mobile nodes may only have access to noisy local information with limited awareness of remote nodes in the network. Novel networking approaches may be needed to account for the lack of full network state information and reduce the penalty incurred due to coordination while sustaining acceptable performance.

Adaptive and specialized machine learning techniques are needed for dynamic allocation of network resources based on operation needs, traffic characteristics, mobility, natural and man-made spectrum interference conditions, and security considerations. Techniques to discover and capitalize on communication and networking opportunities. Networking and sensing architectures for cognitive mobile ad hoc networks needs to be developed with qualitative and quantitative performance measures, and the impacts of mobility, fading, and multi-user interference needs to be investigated. Concepts and constructs observed in networks encountered in nature could inspire adaptation strategies for ad hoc wireless networks.

Networking in combat operations may need to cope with the presence adversarial actions of various types, including strategically inserted spectral impediments. New signal processing, information theory, game theory and network science methodologies are needed to provide reliable and efficient communications in the presence of various adversarial actions. The analysis and characterization of fundamental tradeoffs among conflicting objectives such as Low Probability of Detection (LPD) vs. rate of communications vs. operating in a limited frequency spectrum are needed, along with novel techniques to achieve optimally located areas in the trade-off boundaries.

Providing energy efficient sensor networking under possibly hostile operating conditions presents considerable challenges. Such networks involve short packets and very large number of users, for which standard network access methods are known to be neither spectrum, nor energy efficient. Investigation of fundamental limits in network access methods which pertain to short packets, many users and hostile environments is desired, along with the discovery of protocols which could approximate these bounds.

Novel and Revolutionary Methods in Networking. The synergy among social networking and communication networking, particularly in a tactical mobile ad-hoc scenario, is a research area that could advance the design of new communication approaches. There are many social networking aspects that are common to mobile ad-hoc networking needs such as distributed decision making, robustness, cooperation, self-organization, cluster formation, search and exploration, to name a few. Social Networking Analysis concepts have been recently used in routing and storing of information for tactical wireless networks, with some encouraging results.

Distributed authentication methods, such as block-chain could be useful in tactical environments, but they may require excessive computation and storage burden. Rethinking of distributed authentication methods to fit tactical environments where links may be unreliable, energy and storage is limited is desired.

Among novel and revolutionary methods in networking, exploration of quantum information processing, teleportation and networked quantum information theory is of interest.

TPOC: Dr. Derya Cansever, derya.h.cansever.civ@army.mil, (919) 549-4330

(2) Social and Cognitive Networks

The goal of the Social and Cognitive Networks program is to understand human behaviors and cognitive processes leading to collective level phenomena particularly relevant in military settings with an emphasis on high performance teams and computational social science. Social networks are the underlying structure of interaction and exchanges between humans within both strategically designed and emergent or self-organized systems. Social networks allow for collective actions in which groups of people can communicate, collaborate, organize, mobilize, attack, and defend. The changing nature of DoD's missions

greatly increase the need for models that capture the cognitive, organizational, and cultural factors that drive activities of co-present, virtual, or distributed groups, teams, and populations. Better understanding the human dimension of complexity will provide critical insights about emerging phenomena, social diffusion and propagation, thresholds, and tipping points.

The Social and Cognitive Networks program supports projects that contribute substantive knowledge to theories about human behavior and interaction and make methodological advancements in modeling and analyzing social network structures. The U.S. Army is particularly interested in research that uses defense-relevant empirical data to feed into computational and mathematical models of human interaction. As such, this program funds projects successful in blending theories and methods from the social sciences with rigorous computational methods from computer science and mathematical modeling. Advances in this program are expected to lead to development of measures, theories, and models that capture behavioral and cognitive processes leading to emergent phenomena in teams, organizations, and populations.

Human Behavior and Interaction. This program supports research from disciplines such as communication, health and behavioral science, I/O and social psychology, library and information science, management science, and sociology that use a social networks lens to focus on the ways people think and interact whereby creating higher-order systems. Topics of interest include social influence, leadership, trust, team science, cooperation and competition, and crisis management. Such social influence and opinion dynamics research could focus on the formation and dissolution of civic-minded and violent ideological networks, mobilization of benign to hostile political movements, propagation of and enduring changes in attitudes leading to populations reaching consensus or contested states, and network-based interventions. Furthermore, topics of particular interest include social effects of human-machine teaming; multi-team systems and multilevel (nested) systems; and health topics related to education, healthcare behaviors, disease propagation, and wellness from a social networks perspective.

Information and Knowledge Management. This program supports social network centric research to study the ways people learn individually and collectively and how they utilize that information for decision making and goal attainment. Examples of relevant topics include transactive memories, public goods, collective action, information sharing, information fidelity, diffusion and propagation dynamics, and collective decision-making. Diffusion dynamics research will develop mechanistic understanding of opinion and behavior change associated with influence, contagion, and other social propagation processes. Collective decision-making research will contribute fundamental theories and models to predict, evaluate and simulate how teams organize, exchange information, build knowledge, influence, adapt, learn, and build consensus using cooperative strategies and emergent capabilities.

Social Network Analysis. In addition to the topical areas identified above, this program supports methodological advancements for social network analysis. Methodological research in this program will focus on important advances in exponential random graph

models (ERGMs or p^*), object oriented agent-based models, computational models, and dynamic simulations that resolve network modeling issues. Such research will focus on scalability of networks, hierarchical or multilevel (nested) systems, longitudinal networks, social influence models, network resilience, techniques to deal with missing, incomplete, or inaccurate network data, and techniques to deal with visualizing multilevel multimodal networks. Scalability and dimensionality research will identify overarching mechanisms that span scales and dimensions of human systems that will parameterize, model, and predict both small group and big data network models. Data accuracy research focuses on investigating effects of measurement error on metrics and inferences due to incomplete (missing or inaccurate) network data. These projects could include research examining small group dynamics within big data sets; multi-level models that account for nested cognitive, social, cultural, physical dimensions of systems; or link and subgroup estimation algorithms to deal with incomplete data and clandestine activities.

TPOC: Dr. Edward T. Palazzolo, edward.t.palazzolo.civ@mail.mil, (919) 549-4234

(3) Intelligent Information Networks

The overall objective of the Intelligent Information Networks program is to augment human decision makers (both commanders and soldiers) with enhanced-embedded battlefield intelligence that will provide them with the necessary situational awareness, reconnaissance, and decision making tools to decisively defeat any future adversarial threats which is in line with the DoD's adoption of net-centric warfare, variously defined as flattening the information space to interconnect soldiers and commanders to provide instantaneous access to information, knowledge, and situational awareness. Given this goal, it becomes necessary to understand (a) fundamentals of what intelligence means in the context of autonomous systems and how to build intelligent systems especially as it relates to interaction amongst a network of humans and machines, and (b) foundational algorithmic issues in representation and reasoning about networks inherent in societies and nature.

Integrated Intelligence, Theory of Mind, and Collective Intelligence. Intelligence emanates from several components acting in synergistic ways, be it human cognition that embodies cumulative effects of various separate components of the human brain or the collective intelligence of a network of agents (humans, birds, insects, etc.). Fundamental questions that need to be answered include: What is the least amount of knowledge necessary to bootstrap learning in autonomous systems (or in a network)? How can joint reasoning over various components be carried out (vision, knowledge representation, reasoning, planning, for instance) to obtain a sum that is more than its parts? Are there viable, computable theories of mind that can realistically implement reflection and meta-cognition? Can wisdom of crowds be harnessed to solve problems of importance to societies and problems that are deemed computationally hard? In particular, can a man in the middle of a man-machine ensemble, or, more appropriately, can a crowd and machine ensemble solve inherently hard problems? What exactly are the limitations of wisdom of crowd, when the crowd is made of non-experts? Is there a way for problems to be broken up so that a team of humans and machines can solve them together? Are there approaches to

mechanism design that teases out intelligence inherent in a crowd (or society) of interest in this thrust? These are some of the questions whose solution would likely address basic research problems that are of interest to the program.

Information Networks. In order to model network effects it is necessary to algorithmically represent large networks and reason about them. Unfortunately, information about networks is seldom complete – data available might be missing crucial pieces of information, might have contradictory pieces of information, or could be approximate (with associated notions of uncertainty). Representing and reasoning about these networks requires advances in knowledge representation, graph and data mining, natural language processing, algorithmic graph theory, machine learning, and uncertainty quantification and reasoning. Examples include the emerging area of Graphons which provide new tools for generating and reasoning about graphs that occur in practice (satisfying power law distributions), but also provide new tools for Machine Learning. In particular, a major goal of this thrust are tools and techniques that allow data driven approaches to capturing latent relationships with powers to both explain and predict. Advances in this thrust would not only lead to improved autonomous systems and algorithms, but also enhanced-embedded battlefield intelligence with tools for creating necessary situational awareness, reconnaissance, and decision making. Finally, it should be noted that algorithmic notions of approximations, tight performance bounds, probabilistic guarantees, etc., would be major concerns of the solution space. Large graphs and voluminous data characterize problems in Network Science.

Adversarial Reasoning. Development of appropriate mathematical tools to model and reason about societies and cultures, that brings together tools from Game Theory, Social Sciences and Knowledge Representation. Research of interest includes, but is not limited to, Game Theory for security applications while accounting for bounded rationality, development of Game Theory based on data regarding cultural and adversarial groups, and Behavioral Game Theory that can explain intelligence in groups and societies.

TPOC: Dr. Purush Iyer, s.p.iyer.civ@mail.mil, (919) 549-4204

(4) Multi-Agent Network Control

The objective of the Multi-Agent Network Control program is to establish the physical, mathematical and information processing foundations for the control of complex networks. The research program is concerned with developing novel mathematical abstractions and methods for the modeling and control of both individual agents as well as the collective behavior of large scale networks of heterogeneous multi-agent systems. In this regard, the term “agent” can span the biological, physical, and information and communication domain. Autonomy is central to program efforts as anticipated dynamics of the future battle space will require a greatly increased level of autonomy to enable the necessary mobility, sensor coverage, information flow, and responsiveness to support the military goals of information superiority, dominant maneuver, and precision engagement.

Distributed Control for Complex Networks. Distributed control techniques have played a major role in the study of networked systems. For example, they have been successfully used in robotics for replicating self-organized behaviors found in nature (e.g. bird flocking, fish schooling, and synchronization) and in developing applications such as formation control, rendezvous, robot coordination, and distributed estimation. A fundamental concept underlying these techniques is the notion of consensus. However, many control problems in complex networks cannot be framed as consensus problems. Hence, there is need for developing a new generation of distributed control methods for achieving more sophisticated control goals that are not amenable to a consensus-based formulation. In large-scale networks of interdependent dynamical systems this is likely to require hybrid control architectures that combine top-down and bottom-up design methods formally grounded in graph theory, dynamical systems theory, game theory, computational homology, and topology, amongst other disciplines. Research in this area should contribute to a better understanding of the tradeoffs between what can be achieved by a multi-agent system (e.g. controllability) versus (i) information processing requirements, network topology and computational overhead (ii) individual-agent control actuation capabilities, and (ii) degrees of autonomy and cognitive-behavioral issues arising from human-system interaction.

Analysis of Complex Co-Evolving Networks. The high-dimensionality and complex, evolving topologies in complex networks of heterogeneous agents with possibly asymmetric interactions requires new mathematical techniques for characterizing out-of-equilibrium dynamics and the likely equilibrium outcomes that may emerge over different time spans. Due to random perturbations, transitions between equilibria are inevitable with some transitions occurring more readily than others. Thus for a complete understanding of the dynamics of interacting agents, one must understand how and when equilibrium is likely to unravel, and which new equilibrium, if any, is likely to arise in its place.

Information Structure, Causality, and Dynamics for Control. Understanding information processing within and for controlling complex networks requires new tools for causality and topological inference. Major programmatic interests center on formulating abstractions of cognitive processes and perception for fundamentally changing the way information is exploited to enable control and re-shaping the actions of multiple agents and complex networks. Further questions include: How does control as an objective effect communication and information processing in complex networks? What are the fundamental limits of causality? How do we infer causality and perform estimation in complex networks.

TPOC: Dr. Alfredo Garcia, alfredo.a.garcia31.civ@mail.mil, (919) 549-4282

(5) Network Science and Intelligent Systems (International Program)

As one of the ARO International Programs, the Network Science and Intelligent Systems Program is focused on supporting research at universities outside of the U.S., with the goal of providing key connections with world-class researchers outside the U.S. and supporting the most forward looking and promising research in network science.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

2. INTERNATIONAL RESEARCH INTERESTS

The U.S. Army Research Office has international research programs which are focused in specific research areas supporting the 10 scientific divisions. These research areas and information provided in the following are opportunities for foreign organizations and foreign public entities.

a. Energy Transport and Storage

As one of the ARO International Programs and part of the ARO Chemical Sciences Division portfolio, the Energy Transport and Storage Program is focused on supporting research at universities outside of the U.S., with the goal of building international partnerships and laying the foundational work upon which energy storage and power generation technologies depend. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

This program targets insightful and high-risk, fundamental research which addresses the core underlying limitations of energy transport/storage. Central to the mission of this program is the exploration of how materials and cell design can be tailored to enable targeted electrochemical reactions—while eliminating side reactions, hazards and other impediments, thereby surmounting hurdles and exploiting opportunities in chemical energy storage.

Energy Transport. This thrust supports research aimed at evaluation protocols for energy-relevant materials and the scrutiny of new solid ion conductors and liquid/slurry active materials. There is a tendency to focus upon the most favorable aspects of energy-relevant chemistries and materials, but such reports often either fail to identify or neglect the key limiting characteristics which researchers in general and the Army in particular require to overcome the constraints which restrict breakthroughs in a given energy technology. Projects which actively seek to obtain a global understanding of the underlying principles regarding how chemicals/materials impact the stability and performance of energy storage technologies are of Army interest. Advances in solid electrolytes hold the promise of revolutionizing energy storage technologies, but numerous factors such as limited ionic conductivity, poor ion selectivity, high reactivity, composition changes during processing or difficult processing methods, high contact resistance, unfavorable mechanical properties, defect propagation during cycling due to mechanical deformation, cost barriers, etc. remain major obstructions to the integration of solid electrolytes/separators into devices. Innovative approaches to propel these critical cell components forward are sought. The identification of promising, new liquid (or slurry) active materials (i.e., anolytes or catholytes) may potentially enable new cell designs which greatly simplify battery production, scalability and the tunable modularity of cells, thus enabling their assimilation into diverse Army-relevant energy storage applications. Other

innovative project themes are also welcome.

Thermal Energy Storage. This thrust's focus is on thermal energy storage phase change materials (PCMs). PCMs permit both passive and active heating/cooling that can significantly reduce or eliminate the necessity of conventional heating and cooling methods (for buildings, refrigeration, electronics, etc.). Many PCM applications, however, are restricted due to their high cost, low thermal conductivity, change in density, limited stability of thermal properties and tendency to subcool. The discovery and characterization of new PCMs (e.g., based upon solvates, eutectics, etc.) may overcome these challenges thereby enabling a path forward for their widespread implementation.

TPOC: Dr. Wesley Henderson, wesley.a.henderson4.civ@mail.mil, +81-46-407-9310 (Tokyo, Japan)

b. Synthetic Biology

As one of the ARO International Programs and part of the ARO Life Sciences Division portfolio, the Synthetic Biology Program is focused on supporting research at universities outside of the U.S., building international partnerships and laying the foundational work on which applications of synthetic biology will depend. Emphasis is on using synthetic biology techniques to understand basic biology and to design biological systems and processes with high reliability, scalability, and predictability. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

A major program thrust is investigation of the ways in which biological systems use and control evolutionary processes to become robust, complex, and adaptive. Investigations of interest include mutational hot spots, genetic rearrangement, horizontal gene flow, hyper stable DNA regions, recurrent editing, and maintenance through generations of "unused" adaptations, for example adaptations that allow resistance to dehydration maintained for generations in the absence of selective pressure. These naturally occurring processes may be combined with techniques that do not occur in nature, such as gene shuffling and directed editing, to create organisms that are both engineered and adapted. Combined with a systems biology approach, principles of encoding complexity and adaptivity can be derived. Sophisticated selective techniques are also sought, to drive evolutionary processes to desired ends and to create organisms with desired characteristics.

A second research thrust is the development of robust, predictable systems. Emphasis is not on what such a system does so much as how it can be created, maintained, and activated, to include consideration of the time course of reactions, energetics, methods of preservation and storage, methods of activation, stability, and reliability.

The third thrust of the program is on the creation and maintenance of hybrid prokaryotic-eukaryotic symbiotic systems. Such systems can potentially combine the relative ease of engineering of prokaryotes with the robustness and processing capability of eukaryotes. Areas of interest include the reliable formation of stable intracellular prokaryotic forms, release and

reformation of extracellular prokaryotic forms, transport of prokaryotic products into eukaryotic cytoplasm, membranes, and extracellular space, and eukaryotic processing of prokaryotic products. Studies of the innate immune system of both plants and animals are also of interest, as well as intracellular immune processes.

TPOC: Dr. Valerie Martindale, valerie.e.martindale.civ@mail.mil, +81-46-407-9309 (Tokyo, Japan)

c. Human Dimension

As one of the ARO International Programs and part of the ARO Life Sciences Division portfolio, the Human Dimension Program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal of identifying and modeling the co-evolutionary multiscale dynamics of human neural, cognitive, physical and social systems. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

The Human Dimension Program supports multidisciplinary basic research in areas that include neural and cognitive sciences, behavioral and social sciences and human factors and neural engineering with an emphasis on modeling, predicting and enhancing human perceptual, cognitive, affective, physical, and social performance in individuals, groups and societies. An overarching goal of the program is to provide foundational knowledge of neural, biophysiological and cognitive-based mechanisms underlying individual, group and societal cognition and performance across multiple time scales. In the long term, research in this area may enable new training tools to predict and optimize cognitive/physical performance and team intelligence, interfaces enabling humans to more efficiently control machines and psychophysiology-based predictive models of complex individual – societal dynamics. Basic research opportunities are sought in two primary research thrusts within this program: (i) Cognitive-Physical Interactions and (ii) Cognitive-Social Interactions.

Cognitive-Physical Interactions. The Cognitive-Physical Interactions thrust seeks to support high-risk seed projects that use multimodal approaches to uncover dynamic and multiscale interactions of neural-cognitive and physiological systems. The goal of this thrust area is to advance the experimental and analytical tools available to develop comprehensive understanding of the impact of group and individual state-trait variability on human performance, human-systems interfaces and team intelligence. Research topics are supported in diverse areas that can include the neurobiological mechanisms of expert skill learning, closed-loop brain-computer interfaces and novel mind-body interfaces such as the microbiome-gut-brain axis.

Cognitive-Social Interactions. The Cognitive-Social Interactions thrust seeks to develop new theories to understand the dynamic interrelationships between individual/group cognition, decision-making and the role that these influences play on interactions with large and small social systems. Multidisciplinary seed projects are supported that seek to advance the necessary analytical and experimental tools required to describe the underlying mechanistic interactions as they co-evolve in time and space. Research topics are supported in diverse areas that may

include modeling the impact of mindfulness on state transitions of human cognitive, physical and social systems and describing the longitudinal neural, cognitive and social mechanisms mediating development of leadership, expertise and intelligent teams.

TPOC: Dr. Frederick Gregory, frederick.d.gregory5.civ@mail.mil, +44 (0)1895-626517 (London, UK)

d. Quantum Scale Materials

As one of the ARO International Programs and part of the ARO Physics Division portfolio, the Quantum Scale Materials Program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal to accelerate new discoveries in quantum scale materials. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

Specific research topics of interest include, but are not limited to: topological states of matter and photons, matter and photons that can support anyon quasiparticles, quantum phase transitions, non-equilibrium quantum dynamics, novel materials for quantum information processing, quantum metrology with atoms, ions and photons, quantum networks, and novel quantum information effects, such as effect of free will (measurement independence) on quantum algorithms, such as teleportation, quantum communication and quantum computing.

Additionally, over time new areas of research in fundamental physics surface that provide previously unforeseen opportunities for accelerating scientific progress, and this BAA is intended to cover these cases.

TPOC: Thomas B. Bahder, thomas.b.bahder.civ@mail.mil, +81-46-407-9308 (Tokyo, Japan); (984) 209-0096 (U.S. cell)

e. Innovations in Materials

As one of the ARO International Programs and part of the ARO Materials Science Division, the Innovations in Materials Program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal of accelerating new discoveries in materials science. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

The Innovations in Materials program seeks to determine unique strategies and designs for optimizing materials with uncharacteristic or unexpected properties, architectures, and compositions. Research is focused on, but not limited to, areas such as: reconfigurable materials, predictive design of materials, multi-component materials incorporating hierarchical constructs, materials compositions and architectures for unprecedented property development, functional integration of materials, analytical techniques for interrogating multi-dimensional evolution of structures, properties and failure, and defect science and engineering.

Over time, new areas of research in fundamental materials science can develop that provide previously unforeseen opportunities for accelerating scientific progress, and this BAA is intended to cover these cases as well.

TPOC: Dr. Pani Varanasi, chakrapani.v.varanasi.civ@mail.mil, (919) 549-4325

f. Advanced Computing

As one of the ARO International Programs and part of the ARO Computing Science Division portfolio, the Advanced Computing program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal to accelerate new discoveries in advanced computing. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

The Advanced Computing program focuses on exploring new advances in computing design, algorithms, and techniques. The topic emphasizes large data science and analytics, visualization, security, algorithms for future cyber infrastructure, next-gen computing architectures and algorithms, and task specific computing architectures and algorithms. Specifically, novel computing capabilities are needed to support future Army data analysis needs with enhanced security and situational awareness built in from design. Further, these new advances must be solidly grounded in theory and scientific underpinnings and not incorporate ad hoc development, integration, or studies.

Large Data Science and Analytics. The Army has data analytic needs across many domains, with data originating from many disparate sources, resulting in "Big Data." Research is needed to create holistic solutions considering both the data analytic problem itself, through new computational and data analysis approaches, as well as the human element that must interact with and interpret the data, both in its raw and analyzed forms. Addressing the human component necessitates research that explores novel theories and approaches that accelerates our understanding of and ability to leverage complex and increasingly coupled relationships between humans and computing with the broad goal of advancing human capabilities, emphasizing perceptual and cognitive abilities. The goal must be a synergistic integration of the computational, mathematical, and statistical methods for data analysis as well as visualization theory for "making sense" of the data. Security and situational awareness must be incorporated as overriding principles.

Next-gen Computing Architectures and Algorithms. Research is needed to explore new ways of conceiving of and executing Army capabilities with greater reliability, performance, and scalability. Army data analysis needs continue to increase in terms of volume of data, source of data, and complexity of data. Yet typical compute capabilities, e.g., general purpose processors, are increasing in capability at much slower rates. How can Army compute needs continue to be met over the course of the next 20-30 years? Quantum computing, neuromorphic computing, and General Purpose Computation on Graphics Processing Unit (GPGPU) have shown promise but do not currently meet the needs and requirements of the Army. How can we adapt these capabilities to Army needs? These approaches themselves are new and have only become

viable in the last decade. What new approaches will evolve in the decades to come? The Army needs to necessitate that it be at the forefront of the development of such approaches.

Future architectures will require novel approaches to hardware, wired and wireless communications, and consideration of human-computer interactions. They will need to be reliable in hostile environments, adaptive to changing environments, fault tolerant, capable of supporting high-throughput applications and large-scale data storage and processing, and able to meet performance and energy objectives for applications ranging from very low-power sensors to high-performance computing systems. Architectures of the future will need to be designed from the ground up to ensure security and privacy.

There is an additional need to explore the ability for novel approaches to algorithms to assist the Army in meeting its needs. Such changes in approaches to algorithms may necessarily drive needed changes in architectures. Research must consider both the short term and long term prospects and needs of meeting Army challenges in the compute domain.

Task Specific Computing Architectures, Networks, and Algorithms. In contrast with the general purpose compute capabilities above, Army requirements in the tactical environment must become more restrictive, not less so. For instance, Soldiers in tactical environments are being asked to carry more gear, allocating less weight and power to existing capabilities. Thus the Army has a need for architectures and algorithms to fulfill specific tasks in which the use of general purpose capabilities specifically do not meet the task needs. For instance, general purpose capabilities will necessarily incorporate additional power, weight, and vulnerabilities. Meeting specific task needs of the Army in both fixed and tactical environments is becoming ever more critical as the Army becomes more integrated with compute, sensor, and network infrastructures. Research is needed across the spectrum of Army capabilities to develop architectures and algorithms that can execute existing capabilities with a smaller footprint or provide new needed capabilities with a minimal footprint. The critical footprint parameters will vary depending on the task, such as size, weight, energy, temperature, performance, security, etc.

Security and Algorithms for Future Cyber Infrastructure. Existing cyber infrastructures are saddled with limitations from long-standing protocols and algorithms. Legacy protocols and specifications that were originally designed for complete openness and security has had to be patched rather than integrated. Next generation cyber infrastructures need to be designed from the ground up without these limitations. Such a next-generation cyber infrastructure may be globally deployed or be Army specific. A future cyber infrastructure designed from the ground up can be envisioned to provide security (maintaining confidentiality, integrity, availability, non-repudiation), reliability, attribution, high performance, minimal resource utilization, minimal overhead, etc. Further, these characteristics would be scientifically and mathematically provable.

Also of interest under this topic are novel algorithms and security principles for future cyber infrastructures that enable novel capabilities, services, and operations not previously conceptualized or possible that could lead to improved Army capability and performance. The goal being to enhance cyber operations, situational awareness, data acquisition, position

reporting and to provide dynamic support for multiple mediums, failover, etc. One example of future cyber infrastructures is that of cyber-physical systems, especially the Internet of Things and Cloud Computing, and the need to secure many disparate interconnected devices. In an Army setting, supply is a critical component of mission success. Thus, a future Army can be envisioned with sensors associated with every resource (food, water, bullets, etc.) and providing unparalleled situational awareness. This situational awareness must be fostered, augmented, and secured.

TPOC: Dr. Robert F. Erbacher, robert.f.erbacher.civ@mail.mil, Sao Paulo, Brazil: +55 (11) 3250 5614

g. Network Science and Intelligent Systems

As one of the ARO International Programs and part of the ARO Network Science Division portfolio, the Network Science and Intelligent Systems program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal to accelerate new discoveries in network science and intelligent systems. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

Wireless Communications and Information Networks. Networks serving Army needs must operate in highly dynamic environments with limited infrastructure support. Networks will be disconnected, intermittent, and limited (DIL) environment, with limited state information and dynamic network connectivity and intermittent link connectivity as well as dynamic traffic load with various QoS constraints and priorities. Metrics, fundamental limits, and performance need to be characterized for tactical networks as well as new theory that will lead to reliable and efficient communications that meets QoS constraints. New algorithms and protocols that are more robust in the presence of various adversarial attacks are required.

One specific area of interest is SDN that can operate within tactical DIL networks. Standard SDN are centralized utilizing a reliable control plane, which are not available in this environment. Research is needed to investigate if SDN can be used in this environment and how architectures and control algorithms need to be modified to meet QoS requirements.

Social Network Analysis and Visualization. Mathematical models for dynamics of large social networks are of interest. Modeling of dynamics of the social network are of interest to include both (and possibly co-evolving) structure and content (e.g., opinion dynamics). Hierarchical, multi-level, and composite network models are of interest to model interactions between networks. Scalability issues should be investigated to understand when they are applicable and models should be vetted against established sociological concepts and, if possible, using experimental data. Multi-scale visualization of social network data is important for presenting results of analysis to users and assisting in manual analysis. Missing, incomplete, and inaccurate data are issues that should be considered in network analysis techniques.

Dynamics of Interdependent and Multilayer Networks. In the emerging field of networks science, the importance of research into interdependent and multilayer networks, such as

communications, social, and infrastructure networks, is becoming evident. The mathematics to understanding how to model, predict, and control such multi-layer and interdependent networks is an important research area.

Intelligent Systems. This part of the BAA invites proposals in the area of Network Inference, Data Mining, and Algorithmic Game Theory that supports aspects of Network Science, including understanding large groups, especially adversarial non-state actors. Work that advances Network Science by bringing new techniques from Game Theory, Machine Learning, Graph Algorithms, Reasoning under uncertainty, are welcome.

TPOC: Dr. Robert Ulman, robert.j.ulman.civ@mail.mil, (919) 549-4330

3. ARO SPECIAL PROGRAMS

a. Short-Term Innovative Research (STIR) Program

The objectives of the STIR program are to support rapid, short-term investigations to assess the merit of innovative new concepts in basic research. STIR program awards provide an excellent opportunity to showcase new concepts and explore new areas in basic research. Historically STIR program awards have helped shape new directions in research for the Army.

i. Eligibility. Proposals are sought from institutions of higher education, nonprofit organizations, state and local governments, foreign organizations, foreign public entities, and for-profit organizations (i.e. large and small businesses). Prospective applicants of a STIR proposal are encouraged to contact the appropriate TPOC/ Program Manager identified earlier in the research areas of this BAA, to ascertain the extent of interest in the specific research project.

ii. Research Sought. Proposals in the amount of \$60,000 or less are sought for research in the areas identified earlier in the research areas of this BAA.

iii. Proposal Preparation.

(1) Eligible applicants should submit proposals that are no more than twenty (20) pages in length, inclusive of the budget, transmittal letter, and attachments. No brochures or explanatory material should be submitted with the proposal.

(2) Proposed research efforts must be "stand alone" and not predicated on the use of any facilities other than those under the direct control of the applicant. Research must be completed within nine (9) months of award of the agreement.

(3) The research proposal should follow the format set forth in Section II.D (Application and Submission Information) of this BAA. Limited rights in technical data and restricted rights in computer software should be identified as an attachment to the proposal. Otherwise, it will be concluded that the proposal does not contain any such limitations or restrictions

(4) No capital equipment may be purchased under a STIR Program award. Travel costs must not exceed \$500. Report preparation costs must not exceed \$100. Fee is not permitted under STIR Program awards. Due to the relatively small dollar amount and short-term nature of these awards, applicants are encouraged to maximize the benefit derived from this funding by prioritizing labor and employing other cost-saving measures in support of the STIR program effort. In particular, applicants are strongly encouraged to contribute as a cost-share or significantly reduce the indirect costs associated with proposed efforts.

(5) The principal investigator(s) (PI) should disclose and explain the relevance of the proposal to the research interests identified earlier in the research areas of this BAA.

(6) A brief, final technical report is required. Please note that your award document will reference Form 18, "Reporting Instructions," as found at <http://www.arl.army.mil/www/default.cfm?page=29>. You shall use these reporting instructions for format instructions only; the due date for receipt of a final technical report is thirty (30) days from completion of the award.

b. Young Investigator Program (YIP)

YIP awards are one of the most prestigious honors bestowed by the Army on outstanding scientists beginning their independent careers. The objective of the YIP is to attract outstanding young university faculty members to pursue fundamental research in areas relevant to the Army, to support their research in these areas, and to encourage their teaching and research careers. Young investigators meeting eligibility requirements may submit a YIP proposal. Outstanding YIP projects may be considered for a Presidential Early Career Award for Scientists and Engineers (PECASE).

i. Eligibility. This program is open to U.S. citizens, U.S. Nationals, and Permanent Resident Aliens holding tenure-track positions at U.S. institutions of higher education, who have held their graduate degrees (Ph.D. or equivalent) for fewer than five years at the time of application. Faculty at an institution of higher education which does not designate any faculty appointments as "tenure track" are eligible if that fact is so indicated in the proposal, and the supporting letter from the institute states that the faculty member submitting the proposal will be considered for a permanent appointment.

ii. Research Sought. Proposals are encouraged for research in areas described earlier in the research areas of this BAA. Proposals may be submitted at any time. As is the case for all other research programs, discussions with the cognizant TPOC/ Program Manager identified earlier in the research areas of this BAA is strongly recommended before submission of a formal proposal. An award in each topic area is not guaranteed. YIP awards will not exceed \$120,000 per year for three years.

iii. Proposal Preparation.

(1) An individual applying for a YIP award must submit a proposal and a supporting letter,

both through official channels in the institution of higher education where the individual is employed. Any resulting award will be made to the institution, not to the investigator. The proposal should follow the format set forth in Section II.D (Application and Submission Information) of this BAA.

TPOC: Contact the relevant Program Manager identified earlier in the research areas of this BAA.

(2) The supporting letter must be from the individual's Department Chairperson, Dean, or other official who speaks for the institution of higher education, and should address support for, and commitment to, the applicant. Strong university support for the applicant is essential. This support can include the applicant's nine-month academic salary, release time from administrative responsibilities, the purchase of equipment, support for the applicant's graduate students, waiver of indirect costs, departmental cost sharing, start-up funding, and so on. It must be clear that the institution of higher education views the individual as a truly outstanding, faculty member, and is making a long-term commitment to the proposal and the research.

iv. Evaluation Criteria. The evaluation criteria to be used in determining which proposals are selected for funding are described in Section II.E.1.a and Section II.E.1.b of this BAA. YIP proposals will be selected for award on a competitive basis after a peer scientific review.

v. Continued Support. Support under the YIP is limited to three years. Upon completion of the YIP award, a young investigator, through their institution, may apply and be considered for continued support in the research areas of this BAA.

c. Presidential Early Career Award for Scientists and Engineers (PECASE)

i. An individual may not directly apply for a PECASE award. Instead, once a year, ARO technical program managers will nominate PECASE candidates from among all ARO YIP and other proposals and whitepapers (if any) received. A technical program manager will make the PECASE nomination based on strong endorsement of the proposal by the external scientific reviewers and on the potential shown by the individual to contribute to science and to the mission of the Army.

ii. Following nomination of a PECASE candidate, a supplemental PECASE proposal will be requested in which the candidate will indicate how PECASE funding would augment the YIP award. PECASE awards are not to exceed \$200,000 per year for five years. The following supporting information at minimum is required in the PECASE proposal:

- (1) Letters (non-federal government) of recommendation;
- (2) Detailed scientific biographical information including a description of the candidate's leadership in the scientific community;
- (3) Description of the proposed candidate's publications (such as refereed journals, peer-reviewed conference papers, and books or book chapters; however, this is not an inclusive list);
- (4) Description of the candidate's presentations (such as invited talks and plenary presentations; however, this is not an inclusive list);

- (5) Summary of the candidate's past research accomplishments;
- (6) Summary of the candidate's community outreach efforts; and
- (7) Letters of commitment from institution(s) of higher education.

iii. Complete PECASE proposal packages will be evaluated by scientific reviewers. The proposals which demonstrate the greatest potential to contribute to science and to the mission of the Army will be rank ordered by an Army PECASE Evaluation Committee. The evaluation criteria to be used in determining which proposals are selected for funding are described in Section II.E.1.d of this BAA.

iv. Continued Support. Support under PECASE is limited to five years from date of award. Upon completion of the PECASE award, an individual, through their institution of higher education, may apply and be considered for continued support in the areas identified earlier in the research areas of this BAA.

TPOC: Contact the relevant Program Manager identified earlier in the research areas of this BAA.

d. Research Instrumentation (RI) Program

RI is designed to improve the capabilities of U.S. institutions of higher education to conduct research and educate scientists and engineers in areas important to national defense. Of the funds available to support ARO mission research described in this BAA, funds may be provided to purchase instrumentation in support of this research or in the development of new research capabilities.

i. Eligibility and Areas of Interest. It is highly recommended that potential applicants contact the appropriate TPOC/ Program Manager identified earlier in the research areas of this BAA for advice and assistance before preparation of an instrumentation proposal.

ii. Content of Request for Instrumentation. The request for instrumentation shall include:

- (1) A concise abstract (approximately 300 words but not to exceed 4,000 characters) that describes the instrumentation requested and the research to be supported by that instrumentation.
- (2) A budget that addresses the instrumentation to be purchased, cost per item, and total cost. Indicate the proposed source of the instrumentation and the name and telephone number of a contact at that source. The budget should indicate the amount of funds to be contributed by other sources toward the purchase of the instrumentation.
- (3) A description of how the proposed instrumentation will: (i) establish new research capabilities, (ii) contribute to research currently proposed to DoD, or (iii) enhance the quality of research currently being funded by ARO.
- (4) A description of how the proposed instrumentation will interface with or upgrade other

research facilities and instrumentation now available.

- (5) A description of the amounts and sources of ongoing or proposed support for the research to be supported by the instrumentation.

Note: Costs associated with equipment/facility modifications are generally considered unallowable and require the review and approval of the Grants Officer.

- iii. The evaluation criteria to be used in determining which proposals are selected for funding are described in Section II.E.1.a and II.E.1.c of this BAA.

e. Conference and Symposia Grants

- i. Introduction. The Army supports conferences and symposia (as defined in the DoD Travel Regulations) in areas of science that bring experts together to discuss recent research or educational findings or to expose other researchers or advanced graduate students to new research and educational techniques. The Army encourages the convening in the United States of major international conferences, symposia, and assemblies of international alliances.
- ii. Eligibility. Notwithstanding the Army's authority to provide grant support for such events, only non-commercial scientific, technical, or professional organizations that qualify for tax exemption may receive a conference grant/symposia grant. Those who meet this requirement should also be aware that the DoD does not permit "co-sponsorship" (as defined in DoD 5500.07-R) absent additional high level staffing and approval. In other words, the conference grant support identified in this BAA is NOT DoD sponsorship or co-sponsorship since ARL/ARO is neither an organizer, nor provider, of any substantial logistical support for the conferences addressed in this section.
- iii. Conference Support. Conference support proposals should be submitted a minimum of six (6) months prior to the date of the conference.
- iv. Technical Proposal Preparation. The technical portion of a proposal for support of a conference or symposium should include:
 - (1) A one page or less summary indicating the objectives of the project.
 - (2) The topics to be covered.
 - (3) The location and probable date(s) and why the conference is considered appropriate at the time specified.
 - (4) An explanation of how the conference will relate to the research interests of the Army and how it will contribute to the enhancement and improvement of scientific, engineering, and/or educational in general and activities as outlined earlier in the research areas of this BAA.
 - (5) The name of chairperson(s)/(PI)(s) and his/her biographical information.
 - (6) A list of proposed participants and the methods of announcement or invitation.
 - (7) A summary of how the results of the meeting will be disseminated.

(8) A signed cover page.

v. Cost Proposal Preparation. The cost portion of the proposal should show:

- (1) Total project conference costs by major cost elements.
- (2) Anticipated sources of conference income and amount from each.
- (3) Anticipated use of funds requested.
- (4) A signed budget.

vi. Participant Support. Funds provided cannot be used for payment to any federal government employee for support, subsistence, or services in connection with the proposed conference or symposium.

vii. Cognizant ARO TPOC/ Program Manager. It is highly recommended that potential applicants contact the appropriate TPOC/ Program Manager identified earlier in the research areas of this BAA for advice and assistance before preparation of a conference/symposia proposal.

f. High School Apprenticeship Program (HSAP)/Undergraduate Research Apprenticeship Program (URAP)

i. The HSAP funds the Science, Technology, Engineering, and Mathematics (STEM) apprenticeship of promising rising high school juniors and seniors to work in a university structured research environment under the direction of ARO sponsored PIs serving as mentors. The URAP provides similar opportunities for undergraduate students. HSAP and URAP participants must be U.S. citizens or have permanent resident status. Awards will be made as add-ons to research grants, Multidisciplinary University Research Initiative (MURIs), University-Affiliated Research Contracts (UARCs), and cooperative agreements that have at least 12 months period of performance remaining from the date of HSAP/URAP proposal submission.

ii. HSAP/URAP program goals are to:

- (1) Provide authentic science and engineering research experience to high school students interested in pursuing STEM, and undergraduate students pursuing science and engineering majors;
- (2) Introduce students to the Army's interest and investment in science and engineering research and the associated educational opportunities available to students through the Army's Educational Outreach Program (AEOP) and DoD;
- (3) Provide students with experience in developing and presenting scientific research;
- (4) Provide students with experience to develop an independent research program in preparation for research fellowships, graduate school, and careers in science and engineering research;
- (5) Benefit from the expertise of a scientist or engineer as a mentor for professional and academic development purposes; and

(6) Develop student's skills and background to prepare them for competitive entry to science and engineering undergraduate programs

iii. The HSAP/URAP is designed as an add-on to larger research projects and limited funding is available annually for PIs interested in participating. Due to the brief duration of the HSAP/URAP and limited funding we make every effort to maximize the number of student apprenticeship opportunities. PIs should submit a short proposal that clearly articulates the meaningful research that the student will conduct, along with the strategy for mentorship and facilitation of follow-on opportunities (e.g., university attendance, participation in other AEOP opportunities and other research experiences, etc.). PIs must determine what aspect(s) of their current research program the student will be working on, desired deliverables, and anticipated research outcomes (based on the HSAP/URAP program goals in f. ii. of this section). PIs should describe who within their organization will be responsible for day-to-day mentoring of the students (e.g. PI, research associate, graduate student, etc.). If direct supervision of students will be someone other than the PI, the mentor's resume must be provided. The proposal should identify the gains for the student and the organization for HSAP and URAP participation in terms of technical skills, scientific reasoning in specific domains, or publication opportunities. Follow-on opportunities and relationships for students within the organization are encouraged.

Proposals should include provisions to pay HSAP students a stipend equivalent to approximately \$10 per hour and URAP students a stipend equivalent to approximately \$15 per hour; not to exceed 300 hours total per student. Proposals should generally be limited to two students per PI, except for UARC and MURI awards on which up to 6 students are allowed. Student stipends must be listed under "participant support costs" on ARO Form 99 as described in Section II.H.2.e of this BAA.

If more than one student is proposed by a PI, there must be a near equal mix of HSAP and URAP (i.e. proposals should not be for multiple URAP students only unless approved by ARO). The institution of higher education must describe in its proposal how it will ensure the protection of minors through provision of a safe working environment.

(1) Evaluation Criteria. The evaluation criteria to be used in determining which proposals are selected for funding are described in Section II.E.1.e and II.E.2.c-d of this BAA.

(2) Describing an Outreach Strategy. A primary objective of the HSAP and URAP is to expose new students to research opportunities in a research laboratory. Thus, PIs must describe a plan to attract and engage students not related to the PI (family member) or already working with the PI, laboratory, or research project. The proposal shall also include a short description (3 to 5 sentences) of the project and specific student requirements (GPA, letters of recommendation, dates of the apprenticeship, etc.). For approved proposals, the description submitted by the PI will be marketed on the AEOP website and used in addition to the PIs outreach strategy to attract applicants. All student applications for the HSAP and URAP programs must be collected through the AEOP student application portal (www.usaeop.com).

PIs must include in the proposal a plan to conduct local outreach to promote awareness of the opportunity among students/schools, and then direct them to the AEOP website to apply. HSAP/URAP is a commuter program and PIs are encouraged to perform outreach to students who are able to commute daily. PIs and mentors must also complete a brief registration on the AEOP website if they have not done so previously. The PI will receive all of the applications and make the final decision about which students are invited to participate in the lab. At the conclusion of the apprenticeship student participants are required to develop a brief (one-page) abstract of their work to be included in an AEOP program booklet. PIs shall review and approve these abstracts before submission to ARO.

(3) **Timeline.** Consistent with the BAA, proposals are accepted on a rolling basis. PIs interested in receiving HSAP/URAP funding should submit proposals no later than (NLT) September 30 of the prior year to provide sufficient time for proposal review, award processing, and student outreach/recruitment. For example, to receive funding for use in summer 2019, proposals should be submitted by September 30, 2018.

vii. Proposals should not exceed three pages in length and must be submitted through www.grants.gov utilizing solicitation number W911NF-17-S-0002. Complete forms Standard Form (SF) 424, ARO Form 99 (clearly distinguishing high school students from undergraduates), and upload the proposal as an attachment. Please include the title of the research project, the grant number, and the specific number of HSAP and/or URAP opportunities requested on the first page of the proposal.

TPOC: Ms. Jennifer Ardouin, jennifer.r.ardouin.civ@mail.mil,

4. OTHER NON-ARO PROGRAM-RELATED INFORMATION

a. Visiting Scientist Program (VSP)

The VSP supports short-term travel opportunities for foreign/international scientists to the United States and to international conferences to socialize new S&T ideas or findings with the Army that support advancing basic research through collaboration. For additional information, contact the RDECOM International Technology Center at usarmy.blenheimcrescent.rdecom.mbx.rfec-atlantic@mail.mil.

b. DoD Programs

Each year the Army Research Office, along with the Office of Naval Research (ONR) and the Air Force Office of Scientific Research (AFOSR), participates in three programs sponsored by the Office of the Assistant Secretary of Defense for Research and Engineering. These three programs, titled the Defense University Research Instrumentation Program (DURIP), MURI, and the Research and Educational Program (REP) for HBCU/MIs are conducted under separate BAAs that are posted yearly on Grants.gov and the ARO website under “Funding Opportunities”. These BAAs have a definite closing date for proposal submission, and applicants are advised to review the BAAs for eligibility considerations.

For the purpose of Army funding under these three programs, the areas of interest for submitting proposals are limited to the research areas identified in this BAA.

(End of Section)

B. Federal Award Information

The ACC-APG RTP Division has the authority to award a variety of instruments on behalf of ARO. Anticipated awards will be made in the form of contracts, grants, cooperative agreements, technology investment agreements (TIAs), or other transactions for prototypes (OTAs). The ACC-APG RTP Division reserves the right to select the type of instrument most appropriate for the effort proposed. Applicants should familiarize themselves with these instrument types and the applicable regulations before submitting a proposal. Following are brief descriptions of the possible award instruments:

1. Procurement Contract. A legal instrument, consistent with 31 U.S.C. 6303, which reflects a relationship between the Federal Government and a state government, a local government, or other entity/contractor when the principal purpose of the instrument is to acquire property or services for the direct benefit or use of the Federal Government.

Contracts are primarily governed by the following regulations:

- a. Federal Acquisition Regulation (FAR)
- b. Defense Federal Acquisition Regulation Supplement (DFARS)
- c. Army Federal Acquisition Regulation Supplement (AFARS)

2. Grant. A legal instrument that, consistent with 31 U.S.C. 6304, is used to enter into a relationship:

- a. The principal purpose of which is to transfer a thing of value to the recipient to carry out a public purpose of support or stimulation authorized by a law or the United States, rather than to acquire property or services for the Federal Government's direct benefit or use.
- b. In which substantial involvement is not expected between the Federal Government and the recipient when carrying out the activity contemplated by the grant.
- c. No fee or profit is allowed.

3. Cooperative Agreement. A legal instrument which, consistent with 31 U.S.C. 6305, is used to enter into the same kind of relationship as a grant (see definition "grant"), except that substantial involvement is expected between the Federal Government and the recipient

when carrying out the activity contemplated by the cooperative agreement. The term does not include "cooperative research and development agreements" as defined in 15 U.S.C. 3710a. No fee or profit is allowed.

4. Technology Investment Agreement (TIA). Assistance Transaction other than a Grant or Cooperative Agreement (see 32 CFR Part 37). A legal instrument, consistent with 10 U.S.C. 2371, which may be used when the use of a contract, grant, or cooperative agreement is not feasible or appropriate for basic, applied, and advanced research projects. The research covered under a TIA shall not be duplicative of research being conducted under an existing DoD program. To the maximum extent practicable, TIAs shall provide for a 50/50 cost share between the Government and the applicant. An applicant's cost share may take the form of cash, independent research and development (IR&D), foregone intellectual property rights, equipment, access to unique facilities, and/or other means. Due to the extent of cost share, and the fact that a TIA does not qualify as a "funding agreement" as defined at 37 CFR 401.2(a), the intellectual property provisions of a TIA can be negotiated to provide expanded protection to an applicant's intellectual property. No fee or profit is allowed on TIAs.

5. Other Transaction for Prototype (OTA). A legal instrument, consistent with 10 U.S.C. 2371b, which may be used when the use of a contract, grant, or cooperative agreement is not feasible or appropriate for prototype projects directly relevant to enhancing the mission effectiveness of military personnel and the supporting platforms, systems, components, or materials proposed to be acquired or developed by the Department of Defense, or to improvement of platforms, systems, components, or materials in use by the armed forces. The effort covered under an OTA shall not be duplicative of effort being conducted under an existing DoD program (please refer to the "Other Transactions" OT Guide for Prototype Projects dated January 2017 (Version 1.2.0)). This document, along with other OTA resources, may be accessed at the following link:

<http://www.acq.osd.mil/dpap/cpic/cp/10USC2371bOTs.html>.

6. Grants and cooperative agreements for institutions of higher education, nonprofit organizations, foreign organizations, and foreign public entities are primarily governed by the following:

- a. Federal statutes
- b. Federal regulations
- c. 2 CFR Part 200, as modified and supplemented by DoD's interim implementation found at 2 CFR Part 1103
- d. 32 CFR Parts 21, 22, 26, and 28
- e. DoD Research and Development General Terms and Conditions
- f. Agency-specific Research Terms and Conditions

7. Grants and cooperative agreements for for-profit and nonprofit organizations exempted from Subpart E—Cost Principles of 2 CFR Part 200, are primarily governed by the following:

- a. Federal statutes
- b. Federal regulations
- c. 32 CFR Part 34 - Administrative Requirements for Grants and Agreements with

For-Profit Organizations

- d. 32 CFR Parts 21, 22, 26, and 28
- e. DoD Research and Development General Terms and Conditions
- f. Agency-specific Research Terms and Conditions

8. TIAs are primarily governed by the following:

- a. Federal statutes
- b. Federal regulations
- c. 32 CFR Part 37 – Technology Investment Agreements
- d. DoD Research and Development General Terms and Conditions
- e. Agency-specific Research Terms and Conditions

9. OTAs are primarily governed by the following:

- a. Federal statutes
- b. Federal regulations
- c. Office of Secretary of Defense implementation guidance titled Other Transactions (OT) Guide for Prototype Projects

10. The following websites may be accessed to obtain an electronic copy of the governing regulations and terms and conditions:

- a. FAR, DFARS, and AFARS: <http://farsite.hill.af.mil/>
- b. Code of Federal Regulations (CFR): <http://www.ecfr.gov>
- c. DoD Research and Development General Terms and Conditions: <https://www.onr.navy.mil/Contracts-Grants/submit-proposal/grants-proposal/grants-terms-conditions.aspx>
- d. Agency-specific Research Terms and Conditions: <http://www.arl.army.mil/www/default.cfm?page=8>

(End of Section)

C. Eligibility Information

1. Eligible Applicants

Eligible applicants under this BAA include institutions of higher education, nonprofit organizations, state and local governments, foreign organizations, foreign public entities, and for-profit organizations (i.e. large and small businesses) for scientific research in mechanical sciences, mathematical sciences, electronics, computing science, physics, chemistry, life sciences, materials science, network science, and environmental sciences. Whitepapers and proposals will be evaluated only if they are for fundamental scientific study and

experimentation directed toward advancing the scientific state of the art or increasing basic knowledge and understanding. Whitepapers and proposals focused on specific devices or components are beyond the scope of this BAA.

2. Cost Sharing or Matching

Generally, there is no requirement for cost sharing, matching, or cost participation to be eligible for award under this BAA. Cost sharing and matching is not an evaluation factor used under this BAA. Exceptions may exist if the applicant is proposing the use of a TIA or an OTA as an award instrument. Cost-sharing requirements may be found at 32 CFR 37 for TIAs. Cost-sharing requirements for OTAs may be found at Section C2.16 COST SHARING in the January 2017 document titled “Other Transactions” OT Guide for Prototype Projects.

In addition, if cost sharing is proposed on a grant or cooperative agreement proposal submitted by a nonprofit or institution of higher education, the award will be subject to the restrictions at 2 CFR 200.306. If cost sharing is proposed on a contract proposal, the award will be subject to the restrictions at FAR 35.003.

3. Other

Pursuant to the policy of FAR 35.017 and supplements, selected Federally Funded Research and Development Centers (FFRDC) may propose under this BAA as allowed by their sponsoring agency and in accordance with their sponsoring agency policy.

(End of Section)

D. Application and Submission Information

1. Address to View Broad Agency Announcement

This BAA may be accessed via the following websites:

- a. Grants.gov (www.grants.gov)
- b. Federal Business Opportunities (www.fbo.gov)
- c. ARL website <http://www.arl.army.mil/www/default.cfm?Action=6&Page=8>.

Amendments to this BAA, if any, will be posted to these websites when they occur. Interested parties are encouraged to periodically check these websites for updates and amendments.

The following information is for those wishing to respond to the BAA:

2. Content and Form of Application Submission

a. General Information

i. Preliminary Inquiries: The ARO receives several hundred research proposals annually. Because of financial constraints, we are able to provide support for only a limited number of the proposals received. We realize the preparation of a research proposal often represents a substantial investment of time and effort by the applicant. Therefore, in an attempt to minimize this burden, we strongly encourage applicants interested in submitting proposals to make preliminary inquiries as to the general need for the type of research effort contemplated, before expending extensive effort in preparing a whitepaper and/or detailed proposal or submitting proprietary information. The TPOC names, telephone numbers, and email addresses are listed immediately after each research area of interest and they should be contacted, as appropriate, prior to the submission of whitepapers or proposals.

*NOTE: The Government will not be obligated by any discussion that arises out of preliminary inquiries.

ii. Classified Submissions: Classified proposals are not accepted under this BAA.

iii. Use of Color in Proposals: All proposals received will be stored as electronic images. Electronic color images require a significantly larger amount of storage space than black-and-white images. As a result, applicants' use of color in proposals should be minimal and used only when necessary for details. Do not use color if it is not necessary.

iv. Post-Employment Conflict of Interest: There are certain post-employment restrictions on former federal employees, including special government employees (18 U.S.C. 207). If a

prospective applicant believes a conflict of interest may exist, the situation should be discussed with the TPOC listed in the BAA for their area of scientific research who will then coordinate with appropriate ARO legal counsel prior to the applicant expending time and effort in preparing a proposal.

v. Statement of Disclosure Preference: In accordance with Section II.D.2.e.iii of this BAA, Form 52 or 52A shall be completed stating your preference for release of information contained in your proposal. Copies of these forms may be downloaded from the ARO web site at <http://www.arl.army.mil/www/default.cfm?page=29> under "For the Researcher" (Forms, ARO BAA Forms).

NOTE: Proposals may be handled for administrative purposes by support contractors. These support contractors are prohibited from submitting proposals under this BAA and are bound by non-disclosure and/or conflict of interest requirements as deemed appropriate.

vi. Equipment (see instrument-specific regulations provided in Section II.B of this BAA): Normally, title to equipment or other tangible property purchased with Government funds vests with nonprofit institutions of higher education or with nonprofit organizations whose primary purpose is conducting scientific research if vesting will facilitate scientific research performed for the Government. For-profit organizations are expected to possess the necessary plant and equipment to conduct the proposed research. Deviations may be made on a case-by-case basis to allow for-profit organizations to purchase equipment but regulatory disposition instructions must be followed.

b. The Application Process

The application process is in three stages as follows:

i. Stage 1- Verify the accuracy of your Unique Entity Identifier (formerly DUNS) at the Dun and Bradstreet (D&B) website <http://fedgov.dnb.com/webform> before registering with the System for Award Management System (SAM) at <https://www.sam.gov>. Prospective applicants must be registered in SAM prior to submitting an application or plan. The SAM obtains Legal Business Name, Doing Business Name (DBA), Physical Address, and Postal Code/ Zip+4 data fields from D&B. If corrections are required, registrants will not be able to enter/modify these fields in SAM; they will be pre-populated using D&B Unique Entity Identifier record data. When D&B confirms the correction has been made, the registrant must then re-visit sam.gov and click a "yes" to D&B's changes. Only at this point will the D&B data be accepted into the SAM record. Allow a minimum of two (2) business days for D&B to send the modified data to SAM.

ii. Stage 2 - Prospective proposers are requested to submit whitepapers prior to the submission of a complete, more detailed proposal. The purpose of whitepapers is to minimize the labor and cost associated with the production of detailed proposals that have very little chance of being selected for funding. Based on assessment of the whitepapers, feedback will be provided to the proposers to encourage or discourage them from submitting proposals. Whitepapers should present the effort in sufficient detail to allow evaluation of the concept's

scientific merit and its potential contributions of the effort to the Army mission.

iii. Stage 3 - Interested applicants are required to submit proposals. All proposals submitted under the terms and conditions cited in this BAA will be reviewed regardless of the feedback on, or lack of submission of, a whitepaper. If applicants have not submitted whitepapers, proposals may still be submitted for funding consideration. Proposals must be submitted in order for the applicant to be considered for funding.

All proposals for Assistance Instruments must be submitted electronically through Grants.gov using Workspace. Proposals for Contracts may be submitted via either Grants.gov or email to: usarmy.rtp.aro.mbx.baa@mail.mil. See Section II.D.f of this BAA for information on the proposal submission process.

Requests for waiver of electronic submission requirements may be submitted via email to: usarmy.rtp.aro.mbx.baa@mail.mil or regular mail:

Army Research Office
ATTN: RDRL-RO (Proposal Processing)
P.O. Box 12211
RTP, NC 27709-2211

All required forms for proposals may be downloaded from the ARO web site at <http://www.arl.army.mil/www/default.cfm?page=29> under "For the Researcher" (Forms, ARO BAA Forms).

c. Whitepaper Preparation

i. Whitepapers should focus on describing details of the proposed research, including how it is innovative, how it could substantially increase the scientific state of the art, Army relevance, and potential impact.

ii. Whitepapers are limited to seven (7) total pages; five (5) pages for whitepaper technical content, one (1) cover page and a one (1) page addendum as discussed below. Evaluators will only review the whitepaper cover page, up to five whitepaper technical content pages, and the one-page addendum.

Whitepapers must be in the following format but do not require any special forms:

- Page Size: 8 ½ x 11 inches
- Margins – 1 inch
- Spacing – single
- Font – Times New Roman, 12 point

iii. Combine all files and forms into a single PDF before submitting.

iv. Format and content of whitepapers:

(1) COVER PAGE (not to exceed one page):

The whitepaper cover page shall include at a minimum: Title of the whitepaper, name of the individual and organization submitting the whitepaper, the research area and number against which the whitepaper is submitted, and the TPOC name.

(2) TECHNICAL CONTENT (not to exceed five pages):

(a) A detailed discussion of the effort's scientific research objective, approach, relationship to similar research, and level of effort shall be submitted. Also include the nature and extent of the anticipated results and, if known, the manner in which the work will contribute to the accomplishment of the Army's mission and how this contribution would be demonstrated.

(b) The type of support, if any, the applicant requests of the Government, such as facilities, equipment, demonstration sites, test ranges, software, personnel or materials, shall be identified as Government Furnished Equipment (GFE), Government Furnished Information (GFI), Government Furnished Property (GFP), or Government Furnished Data (GFD). Applicants shall indicate any Government coordination that may be required for obtaining equipment or facilities necessary to perform any simulations or exercises that would demonstrate the proposed capability.

(c) The cost portion of the whitepaper shall contain a brief cost estimate revealing all the component parts of the proposal, including research hours, burden, material costs, travel, etc.

(3) ADDENDUM (not to exceed one page):

Include biographical sketches of the key personnel who will perform the research, highlighting their qualifications and experience.

v. RESTRICTIVE MARKINGS ON WHITEPAPERS:

(1) Any proprietary data that the applicant intends to be used only by the Government for evaluation purposes must be clearly marked. The applicant must also identify any technical data or computer software contained in the whitepaper that is to be treated by the Government as limited rights in technical data and restricted rights in computer software. In the absence of such identification, the Government will conclude there are no limitations or restrictions on technical data or computer software included in the whitepaper. Records or data bearing a restrictive legend may be included in the whitepaper. It is the intent of the Army to treat all whitepapers as procurement sensitive before award and to disclose their contents only for the purpose of evaluation.

Care must be exercised to ensure that classified, sensitive, and critical technologies are not included in a whitepaper. If such information is required, appropriate restrictive markings and procedures should be applied prior to submission of the whitepaper.

(2) Applicants are cautioned, however, that portions of the whitepapers may be subject to

release under terms of the Freedom of Information Act, 5 U.S.C. 552, as amended.

vi. EVALUATION AND DISPOSITION OF WHITEPAPERS:

(1) Evaluation Process: Applicants are advised that invitations for proposals will be made based on the whitepaper submission and the availability of funding. The whitepaper will be evaluated for the concept's scientific merit and potential contributions of the effort to the Army mission. Applicants whose whitepapers are evaluated as having significant scientific merit may be invited to submit a proposal. However, an applicant may submit a proposal despite not submitting a whitepaper or receiving a proposal invite from the Government.

(2) Disposition Process: The applicant will be notified in writing after completion of the evaluation. Whitepapers will not be returned to applicants.

d. Whitepaper Submission

All whitepapers must be emailed directly to the TPOC. In the email subject line, include the phrase "Whitepaper Submission," the BAA number W911NF-17-S-0002, and the research topic number from Section II.A of this BAA. Whitepapers submitted via email must be in a single PDF formatted file as an email attachment.

e. Preparation of Proposals

i. COVER PAGE:

(1) A Cover Page is required. For contract proposals submitted by email, use ARO Form 51. For all Assistance instruments and contract proposals submitted via Grants.gov, use the SF 424 (R&R) Form. Proposals will not be processed without either: (1) a signed Cover Page, ARO Form 51, or (2) a SF 424 (R&R) Form.

(2) Should the project be carried out at a branch campus or other component of the applicant, that branch campus or component should be identified in the space provided (Block 11 on the ARO Form 51 and Block 12 on the SF 424 (R&R) Form).

(3) The title of the proposed project should be brief, scientifically representative, intelligible to a scientifically-literate reader, and suitable for use in the public domain.

(4) The proposed duration for which support is requested should be consistent with the nature and complexity of the proposed activity. For research areas listed at Sections II.A.1 through II.A.3 of this BAA applicants shall discuss the preferred performance period with the TPOC.

(5) Specification of a desired starting date for the project is important and helpful; however, requested effective dates cannot be guaranteed.

(6) Pursuant to 31 U.S.C. 7701, as amended by the Debt Collection Improvement Act of 1996 [Section 31001(I)(1), Public Law 104-134] and implemented by 32 CFR 22.420(d), federal agencies shall obtain each awardees' Taxpayer Identification Number (TIN). The TIN is being obtained for purposes of collecting and reporting on any delinquent amounts that may arise out of an awardees' relationship with the Government.

(7) Applicants shall provide their organization's Unique Entity Identifier (formerly DUNS). This number is a nine-digit number assigned by D&B Information Services. See Section II.D.3 of this BAA for requirements pertaining to the Unique Entity Identifier.

(8) Applicants shall provide their assigned Commercial and Government Entity (CAGE) Code. The CAGE Code is a 5-character code assigned and maintained by the Defense Logistics Service Center (DLSC) to identify a commercial plant or establishment.

ii. TABLE OF CONTENTS:

Use the following format for the Table of Contents. Forms are available at <http://www.arl.army.mil/www/default.cfm?page=29> under "For the Researcher" (Forms, ARO BAA Forms).

SECTION	PAGE NUMBER
Table of Contents	A-1
Statement of Disclosure Preference (Form 52 or 52A)	B-1
Research and Related Other Project Information	B-2
Project Abstract	C-1
Project Description (Technical Proposal)	D-1 - D-□
Biographical Sketch	E-1 - E-□
Bibliography	F-1 - F-□
Current and Pending Support	G-1 - G-□
Facilities, Equipment, and Other Resources	H-1 - H-□
Proposal Budget	I-1 - I-□
Contract Facilities Capital Cost of Money (DD Form 1861)	J-1
Appendices	K-□
List Appendix Items: _____	

This format applies to all proposals submitted via email and via Grants.gov. Applicants' should show the location of each section of the proposal, as well as major subdivisions of the project description.

iii. STATEMENT OF DISCLOSURE PREFERENCE (FORM 52 OR 52A): Complete and sign ARO Form 52 (Industrial Contractors) or ARO Form 52A (Educational and Nonprofit Organizations).

iv. RESEARCH AND RELATED OTHER PROJECT INFORMATION: Must be completed and signed by all applicants.

v. PROJECT ABSTRACT:

(1) The project abstract shall be completed on the form entitled “Publicly Releasable Project Abstract” found at the following website:

<http://www.arl.army.mil/www/default.cfm?page=218>.

(2) Unless otherwise instructed in this BAA, the project abstract shall include a concise statement of work and basic approaches to be used in the proposed effort. The abstract should include a statement of scientific objectives, methods to be employed, and the significance of the proposed effort to the advancement of scientific knowledge.

(3) The abstract should be no longer than one (1) page (maximum 4,000 characters).

(4) The project abstract shall be marked by the applicant as publically releasable. By submission of the project abstract, the applicant confirms that the abstract is releasable to the public. For a proposal that results in a grant award, the project abstract will be posted to a searchable website available to the general public to meet the requirements of Section 8123 of the DoD Appropriations Act, 2015. The website address is

<https://dodgrantawards.dtic.mil/grants>.

vi. PROJECT DESCRIPTION (TECHNICAL PROPOSAL): The technical portion of the proposal shall contain the following:

(1) A complete discussion stating the background and objectives of the proposed work, the scientific approaches to be considered, the relationship to competing or related research, and the level of effort to be employed. Include also the nature and extent of the anticipated results and how they will significantly advance the scientific state-of-the-art. Also, if known, include the manner in which the work will contribute to the accomplishment of the Army's mission. Ensure the proposal identifies any scientific uncertainties and describes specific approaches for the resolution or mitigation of the uncertainties.

(2) A brief description of your organization. If the applicant has extensive government contracting experience and has previously provided the information to the ARL, the information need not be provided again. A statement setting forth this condition should be made.

(3) The names of other federal, state, local agencies, or other parties receiving the proposal and/or funding the proposed effort. If none, state so. Concurrent or later submission of the proposal to other organizations will not prejudice its review by the ARO if we are kept informed of the situation.

(4) A statement regarding possible impact, if any, of the proposed effort on the environment, considering as a minimum its effect upon water, atmosphere, natural resources, human resources, and any other values.

(5) A statement regarding the use of Class I and Class II ozone- depleting substances. Ozone- depleting substances are any substance designated as Class I by EPA, including but not limited to chlorofluorocarbons, halons, carbon tetrachloride, and methyl chloroform, and any substance designated as Class II by EPA, including but not limited to hydrochlorofluorocarbons. See 40 CFR Part 82 for detailed information. If Class I or II substances are to be utilized, a list shall be provided as part of the applicant's proposal. If none, state so.

(6) The type of support, if any, requested by the applicant (e.g., facilities, equipment, and materials).

vii. BIOGRAPHICAL SKETCH:

(1) This section shall contain the biographical sketches for key personnel only.

(a) Primary PI: The Primary PI provides a single or initial point of communication between the ARO and the awardee organization(s) about scientific matters. If not otherwise designated, the first PI listed will serve as the Primary PI. This individual can be changed with notification to ARO. ARO does not infer any additional scientific stature to this role among collaborating investigators.

(b) Co-PIs: The individual(s) a research organization designates as having an appropriate level of authority and responsibility for the proper conduct of the research and submission of required reports to ARO. When an organization designates more than one PI, it identifies them as individuals who share the authority and responsibility for leading and directing the research, intellectually and logistically. ARO does not infer any distinction among multiple PIs.

(2) The following information is required:

(a) Relevant experience and employment history including a description of any prior Federal employment within one year preceding the date of proposal submission.

(b) List of up to five publications most closely related to the proposed project and up to five other significant publications, including those being printed. Patents, copyrights, or software systems developed may be substituted for publications.

(c) List of persons, other than those cited in the publications list, who have collaborated on a project or a book, article, report or paper within the last four years. Include pending publications and submissions. Otherwise, state "None."

(d) Names of each investigator's own graduate or post-graduate advisors and advisees.

NOTE: The information provided in (c) and (d) is used to help identify potential conflicts or bias in the selection of reviewers.

(3) For the personnel categories of postdoctoral associates, other professionals, and students

(research assistants), the proposal may include information on exceptional qualifications of these individuals that merit consideration in the evaluation of the proposal.

(4) The biographical sketches are limited to three (3) pages per investigator and other individuals that merit consideration.

viii. BIBLIOGRAPHY: A bibliography of pertinent literature is required. Citations must be complete (including full name of author(s), title, and location in the literature).

ix. CURRENT AND PENDING SUPPORT:

(1) All project support from whatever source must be listed. The list must include all projects requiring a portion of the PI's and other key personnel's time, even if they receive no salary support from the project(s).

(2) The information should include, as a minimum: (i) the project/proposal title and brief description, (ii) the name and location of the organization or agency presently funding the work or requested to fund such work, (iii) the award amount or annual dollar volume of the effort, (iv) the period of performance, and (v) a breakdown of the time required of the PI and/or other key personnel.

x. FACILITIES, EQUIPMENT, AND OTHER RESOURCES: The applicant should include in the proposal a listing of facilities, equipment, and other resources already available to perform the research proposed.

xi. PROPOSAL BUDGET (including DD Form 1861):

(1) Each proposal must contain a budget for each year of support requested and a cumulative budget for the full term of requested support. Each budget year and the cumulative budget for the full term must be documented on ARO Form 99. ARO Form 99 may be reproduced, but you may not make substitutions in prescribed budget categories nor alter or rearrange the cost categories as they appear on the form. The proposal may request funds under any of the categories listed so long as the item is considered necessary to perform the proposed work and is not precluded by applicable cost principles. In addition to the forms, the budget proposal should include budget justification for each year.

(2) A signed summary budget page must be included. The documentation pages should be titled "Budget Explanation Page" and numbered chronologically starting with the budget form. The need for each item should be explained clearly.

(3) All cost data must be current and complete. Costs proposed must conform to the following principles and procedures:

Institutions of Higher Education: 2 CFR Part 200

Nonprofit Organizations: 2 CFR Part 200

For-Profit/Commercial Organizations: FAR Part 31, DFARS Part 231, FAR Subsection 15.403-5, and DFARS Subsection 215.403-5.

* For those nonprofit organizations specifically exempt from the provisions of Subpart E of 2 CFR Part 200 (see 2 CFR 200.401(c)), FAR Part 31 and DFARS Part 231 shall apply.

(4) Sample itemized budgets and the information they must include for a contract and for grants and cooperative agreements can be found at Section II.H of this BAA (Other Information). Before award of a cost-type contract or assistance instrument it must be established that an approved accounting system and financial management system exist.

xii. APPENDICES: Some situations require that special information and supporting documents be included in the proposal before funding can be approved. Such information and documentation should be included by appendix to the proposal.

- (1) To evaluate compliance with Title IX of the Education Amendments of 1972 (20 U.S.C. A Section 1681 Et. Seq.), the Department of Defense is collecting certain demographic and career information to be able to assess the success rates of women who are proposed for key roles in applications in STEM disciplines. To enable this assessment, each application must include the following forms completed as indicated.

(A) Research and Related Senior/Key Person Profile (Expanded) form:

The Degree Type and Degree Year fields on the Research and Related Senior/Key Person Profile (Expanded) form will be used by DoD as the source for career information. In addition to the required fields on the form, applicants must complete these two fields for all individuals that are identified as having the project role of PD/PI or Co-PD/PI on the form. Additional senior/key persons can be added by selecting the “Next Person” button.

(B) Research and Related Personal Data form:

This form will be used by DoD as the source of demographic information, such as gender, race, ethnicity, and disability information for the Project Director/Principal Investigator and all other persons identified as Co-Project Director(s)/Co-Principal Investigator(s). Each application must include this form with the name fields of the Project Director/Principal Investigator or any Co-Project Director(s)/Co-Principal Investigator(s) completed; however, provision of the demographic information in the form is voluntary. If completing the form for multiple individuals, each Co-Project Director/Co-Principal Investigator can be added by selecting the “Next Person” button. The demographic information, if provided, will be used for statistical purposes only and will not be made available to merit reviewers. Applicants who do not wish to provide some or all of the information should check or select the “Do not wish to provide” option.

f. Submission of Proposals

Proposals must be submitted by email (only when a contract is requested) or through Grants.gov. Proposals must be submitted through the applicant’s organizational office having responsibility for Government business relations. All signatures must be that of an

official authorized to commit the organization in business and financial affairs.

Proposal content requirements remain the same for both email and Grants.gov submission.

i. EMAIL SUBMISSION (only when a **Contract is the requested form of agreement**):

- (1) Proposals requesting a Contract may be emailed directly to usarmy.rtp.aro.mbx.baa@mail.mil. Do not email full proposals to the TPOC. All emailed proposals must adhere to the format requirements and contain the information outlined in Section II.D.2.e of this BAA.
- (2) The applicant must include with its proposal submission the representations required by Section II.F.2.a.i of this BAA. The representations must include applicant POC information and be signed by an authorized representative. Note: If the applicant's SAM Representations and Certifications include its response to the representations a hard copy representation is not required with proposal submission.
- (3) All forms requiring signature must be completed, printed, signed, and scanned into a PDF document. All documents must be combined into a single PDF formatted file to be attached to the email.
- (4) Proposal documents (excluding required forms) must use the following format:
 - Page Size – 8 ½ x 11 inches
 - Margins – 1 inch
 - Spacing – single
 - Font – Times New Roman, 12 point, single-sided pages

ii. GRANTS.GOV SUBMISSION (For **all proposals requesting Assistance agreements**.)

Proposals requesting a Contract may be submitted either via Grants.gov or email:

- (1) Grants.gov Registration (See Section II.D.2.g below) must be accomplished prior to application submission in Grants.gov.

NOTE: All web links referenced in this section are subject to change by Grants.gov and may not be updated here.

- (2) Specific forms are required for submission of a proposal. The forms are contained in the Application Package available through the Grants.gov application process. To access these materials, go to <http://www.grants.gov>, select "Apply for Grants," and then select "Get Application Package." A Grant Application Package and Application Instructions are available through the Grants.Gov Apply portal under CFDA Number 12.431/Funding Opportunity Number W911NF-17-S-0002. Select "Apply" and then "Apply Now Using Workspace."

*NOTE: Effective 31 December 2017, the legacy PDF application package on Grants.gov will be retired and applicants must apply online at Grants.gov using the application Workspace. For access to complete instructions on how to apply for opportunities using Workspace refer to <https://www.grants.gov/web/grants/applicants/workspace-overview.html>.

The following documents are mandatory: (1) Application for Federal Assistance (R&R) (SF 424 (R&R)), and (4) Attachments form.

(3) The SF 424 (R&R) form is to be used as the cover page for all proposals submitted via Grants.gov. The SF 424 (R&R) must be fully completed. Authorized Organization Representative (AOR) usernames and passwords serve as “electronic signatures” when your organization submits applications through Grants.gov. By using the SF 424 (R&R), proposers are providing the certification required by 32 CFR Part 28 regarding lobbying (see Section II.F.2.a.ii of this BAA). Block 11, “Descriptive Title of Applicant’s Project,” must reference the research topic area being addressed in the effort by identifying the specific paragraph from Section II.A of this BAA.

(4) The Attachments form must contain the documents outlined in Section II.D.2.e.ii entitled “Table of Contents”. All documents must be combined into separate and single PDF formatted files using the Table of Contents names. Include “W911NF-17-S-0002” in the title so the proposal will be distinguished from other BAA submissions and upload each document to the mandatory Attachments form.

(5) The applicant must include with its proposal submission the representations required by Section II.F.2.a.ii of this BAA. The representations must include applicant POC information and be signed by an authorized representative. Attach the representations document to an available field within the Attachments form. Note: If the applicant’s SAM Representations and Certifications include its response to the representations a hard copy representation is not required with proposal submission.

(6) The Grants.gov User Guide at: http://www.grants.gov/help/html/help/index.htm?callingApp=custom#t=Get_Started%2FGet_Started.htm will assist AORs in the application process. Remember that you must open and complete the Application for Federal Assistance (R&R) (SF 424 (R&R)) first, as this form will automatically populate data fields in other forms. If you encounter any problems, contact customer support at 1-800-518-4726 or at support@grants.gov. If you forget your user name or password, follow the instructions provided in the Credential Provider tutorial. Tutorials may be printed by right-clicking on the tutorial and selecting “Print”.

(7) As it is possible for Grants.gov to reject the proposal during this process, it is strongly recommended that proposals be uploaded at least two days before any established deadline in the BAA so that they will not be received late and be ineligible for award consideration. It is also recommended to start uploading proposals at least two days before the deadline to plan ahead for any potential technical and/or input problems involving the applicant’s own equipment.

g. Grants.gov Registration

i. Each organization that desires to submit applications via Grants.Gov must complete a one-time registration. There are several one-time actions your organization must complete in order to submit applications through Grants.gov (e.g., obtain a Unique Entity Identifier, register with the SAM, register with the credential provider, register with Grants.gov and obtain approval for an

AOR to submit applications on behalf of the organization). To register please see <http://www.grants.gov/web/grants/applicants/organization-registration.html>

- ii. Please note the registration process for an Organization or an Individual can take between three to five business days or as long as four weeks if all steps are not completed in a timely manner.
- iii. Questions relating to the registration process, system requirements, how an application form works, or the submittal process should be directed to Grants.gov at 1-800-518-4726 or support@grants.gov.

3. Unique Entity Identifier and System for Award Management (SAM)

- a. Each applicant (unless the applicant is an individual or Federal awarding agency that is exempt from those requirements under 2 CFR 25.110(b) or (c), or has an exemption approved by the Federal awarding agency under 2 CFR 25.110(d)) is required to:
 - i. Be registered in SAM prior to submitting its application;
 - ii. Provide a valid unique entity identifier (formerly DUNS) in its application; and
 - iii. Maintain an active SAM registration with current information at all times during which it has an active Federal award or an application or plan under consideration by a Federal awarding agency.
- b. The Federal awarding agency may not make a Federal award to an applicant until the applicant has complied with all applicable unique entity identifier and SAM requirements. If an applicant has not fully complied with the requirements by the time the Federal awarding agency is ready to make a Federal award, the Federal awarding agency may determine that the applicant is not qualified to receive a Federal award and use that determination as a basis for making a Federal award to another applicant.

4. Submission Dates and Times

a. Proposals

Proposals will be considered until and including the closing date of this announcement (see cover page of this announcement for opening/closing dates), except for special programs identified in this BAA that may announce specific opening/closing dates. Proposals submitted after the closing date will not be considered by the Government.

b. Proposal Receipt Notices

- i. Grants.gov: After a proposal is submitted to Grants.gov, the AOR will receive a series of three emails from Grants.gov. The first two emails will be received within 24 to 48 hours after submission. The first email will confirm time of receipt of the proposal by the Grants.gov system and the second will indicate that the proposal has either been successfully validated by the system prior to transmission to the grantor agency or has been rejected due to errors. A third email will be received once the grantor agency has confirmed receipt of the proposal. Reference the Grants.gov User Guide at

http://www.grants.gov/help/html/help/index.htm?callingApp=custom#t=Get_Started%2FGet_Star ted.htm for information on how to track your application package.

For the purposes of this BAA, an applicant's proposal is not considered received by ARO until the AOR receives email #3.

ii. Email Submission: After a proposal is submitted to usarmy.rtp.aro.mbx.baa@mail.mil, the AOR will receive an email confirming time of receipt of the proposal by the grantor agency. For the purposes of this BAA, an applicant's proposal is not considered received by the grantor agency until the AOR receives the email confirming receipt of the proposal.

5. Intergovernmental Review

Not Applicable

6. Funding Restrictions

There are no specific funding restrictions associated with this BAA (e.g. direct costs, indirect costs, etc.).

7. Other Submission Requirements

a. Information to Be Requested from Successful Applicants: Applicants whose proposals are accepted for funding will be contacted before award to provide additional information required for award. The required information may include requests to clarifying budget explanations, representations, certifications, and some technical aspects.

b. For Contracts Only: Performance Work Statements (PWS). Prior to award the Contracting Officer may request that the contractor submit a PWS for the effort to be performed, which will be incorporated into the contract at the time of award.

(End of Section)

E. Proposal Review Information

1. Criteria

a. Except for the PECASE and HSAP/URAP programs, proposals submitted in response to this BAA will be evaluated using the criteria listed below (in descending order of importance):

- i. The overall scientific and/or technical merits of the proposal.
- ii. The potential contributions of the effort to the Army mission and the extent to which the research effort will contribute to balancing the overall ARO research program.
- iii. The qualifications, capabilities, and experience of the proposed PI, team leader, or other key personnel who are critical to achievement of the proposed objectives.
- iv. The applicant's record of past performance.

b. The following criterion will be evaluated, in addition to the criteria listed in Section II.E.1.a, in the evaluation of proposals submitted against the YIP. This criterion is of least importance:

Long-term commitment by the institution of higher education to the young investigator and the proposed research.

c. The following criterion will be evaluated, in addition to the criteria listed in Section II.E.1.a, in the evaluation of proposals submitted against the RI Program. This criterion is of least importance.

The applicant's capabilities, related experience, facilities, techniques, or unique combinations of these, which are integral factors for achieving the proposed objectives.

d. Proposals submitted in response to the PECASE program will be evaluated using the criteria listed below. The criteria are listed in descending order of importance (NOTE: Criteria i, ii, and iii are of equal importance):

- i. The overall scientific and/or technical merits of the proposal.
- ii. Scientific leadership.
- iii. Publications.
- iv. The potential contributions of the effort to the Army mission and the extent to which the research effort will contribute to balancing the overall ARO research program.
- v. Presentations.
- vi. Commitment letters from institution of higher education.
- vii. Community outreach.

e. Proposals submitted in response to the HSAP/URAP program will be evaluated using the criteria listed below (in descending order of importance):

- i. The overall scientific and/or technical merits of the proposal.
- ii. The potential contributions of the effort to the Army mission.
- iii. Educational merit to include the proposed student research, mentorship strategy, anticipated outcomes for the student and applicant, student qualifications, and number of proposed students.

****NOTE:** Cost sharing will not be a consideration in proposal evaluation.

2. Review and Selection Process

- a. Upon receipt of a proposal, the ARO staff will perform an initial review of its scientific merit and potential contribution to the Army mission, and also determine if funds are expected to be available for the effort. Proposals not considered having sufficient scientific merit or relevance to the Army's needs, or those in areas for which funds are not expected to be available, may not receive further review.
- b. All proposals are treated as procurement sensitive and are disclosed only for the purpose of evaluation. Proposals not declined as a result of an initial review will be subject to a peer review by highly qualified scientists. While the applicant may restrict the evaluation to scientists from within the Government, to do so may prevent review of the proposal by those most qualified in the field of research covered by the proposal. The applicant must indicate on the appropriate proposal form (Form 52 or 52A) any limitation to be placed on disclosure of information contained in the proposal.
- c. Each proposal will be evaluated based on the evaluation criteria in Section II.E.1 of this BAA rather than against other proposals for research in the same general area.
- d. Upon completion of an evaluation against the criteria in Section II.E.1, a proposal selected for possible award will be analyzed for the realism and reasonableness of costs. Proposal costs must be determined reasonable and realistic before the Government can make an award.

3. Recipient Qualification

a. Grant, Cooperative Agreement, and TIA Proposals:

- i. The Grants Officer is responsible for determining a recipient's qualification prior to award. In general, a Grants Officer will award grants or cooperative agreements only to qualified recipients that meet the standards at 32 CFR 22.415. To be qualified, a potential recipient must:
 - (1) Have the management capability and adequate financial and technical resources, given those that would be made available through the grant or cooperative agreement, to execute the program of activities envisioned under the grant or cooperative agreement;

- (2) Have a satisfactory record of executing such programs or activities (if a prior recipient of an award);
- (3) Have a satisfactory record of integrity and business ethics; and
- (4) Be otherwise qualified and eligible to receive a grant or cooperative agreement under applicable laws and regulations.

Applicants are requested to provide information with proposal submissions to assist the Grants Officer's evaluation of recipient qualification.

ii. In accordance with Office of Management and Budget (OMB) guidance in parts 180 and 200 of Title 2, CFR, it is DoD policy that DoD Components must report and use integrity and performance information in the Federal Awardee Performance and Integrity Information System (FAPIIS), or any successor system designated by OMB, concerning grants, cooperative agreements, and TIAs as follows:

If the total Federal share will be greater than the simplified acquisition threshold on any Federal award under a notice of funding opportunity (see 2 CFR 200.88 Simplified Acquisition Threshold):

- (1) The Federal awarding agency, prior to making a Federal award with a total amount of Federal share greater than the simplified acquisition threshold, will review and consider any information about the applicant that is in the designated integrity and performance system accessible through SAM (currently FAPIIS) (see 41 U.S.C. 2313);
- (2) An applicant, at its option, may review information in the designated integrity and performance systems accessible through SAM and comment on any information about itself that a Federal awarding agency previously entered and is currently in the designated integrity and performance system accessible through SAM;
- (3) The Federal awarding agency will consider any comments by the applicant, in addition to the other information in the designated integrity and performance system, in making a judgment about the applicant's integrity, business ethics, and record of performance under Federal awards when completing the review of risk posed by applicants as described in 2 CFR 200.205 Federal awarding agency review of risk posed by applicants.

b. Contract Proposals:

i. Contracts shall be awarded to responsible prospective contractors only. See FAR 9.104-1 for a listing of the general standards against which an applicant will be assessed to determine responsibility.

Applicants are requested to provide information with proposal submission to assist the Contracting Officer's evaluation of responsibility.

ii. FAPIIS will be checked prior to making an award. The web address is:

<https://www.fapiis.gov/fapiis/index.action>. The applicant representing the entity may comment in this system on any information about the entity that a federal government official entered. The information in FAPIIS will be used in making a judgment about the entity's integrity, business ethics, and record of performance under Federal awards that may affect the official's determination that the applicant is qualified to receive an award.

(End of Section)

F. Award Administration Information

1. Award Notices

Applicants whose proposals are recommended for award may be contacted by a Contract/Grant Specialist to discuss additional information required for award. This may include representations and certifications, revised budgets or budget explanations, certificate of current cost or pricing data, subcontracting plan for small businesses, and/or other information as applicable to the proposed award. The anticipated start date will be determined at that time.

The notification email must not be regarded as an authorization to commit or expend funds. The Government is not obligated to provide any funding until a Government Contracting/Grants Officer signs the award document.

The award document signed by the Government Contracting/Grants Officer is the official and authorizing award instrument. The authorizing award instrument, signed by the Contracting/Grants Officer, will be emailed to the PI and AOR.

2. Administrative and National Policy Requirements

a. Required Representations and Certifications:

i. Contract Proposals:

(1) Representations and certifications shall be completed by successful applicants prior to award. FAR Online Representations and Certifications are to be completed through SAM at <https://www.SAM.gov>. As appropriate, DFARS and contract-specific certification packages will be provided to the contractor for completion prior to award.

(2) FAR 52.203-18, PROHIBITION ON CONTRACTING WITH ENTITIES THAT REQUIRE CERTAIN CONFIDENTIALITY AGREEMENTS OR STATEMENTS—REPRESENTATION (JAN 2017)

(a) Definition. As used in this provision--

“Internal confidentiality agreement or statement”, “subcontract”, and “subcontractor”, are defined in the clause at 52.203-19, Prohibition on Requiring Certain Internal Confidentiality Agreements or Statements.

(b) In accordance with section 743 of Division E, Title VII, of the Consolidated and Further Continuing Appropriations Act, 2015 (Pub. L. 113-235) and its successor provisions in subsequent appropriations acts (and as extended in continuing resolutions), Government agencies are not permitted to use funds appropriated (or otherwise made available) for contracts with an entity that requires employees or subcontractors of such entity seeking to report waste, fraud, or abuse to sign internal confidentiality agreements or statements prohibiting or otherwise restricting such employees or subcontractors from lawfully reporting such waste, fraud, or abuse to a designated investigative or law enforcement

representative of a Federal department or agency authorized to receive such information.

(c) The prohibition in paragraph (b) of this provision does not contravene requirements applicable to SF 312, (Classified Information Nondisclosure Agreement), Form 4414 (Sensitive Compartmented Information Nondisclosure Agreement), or any other form issued by a Federal department or agency governing the nondisclosure of classified information.

(d) Representation. By submission of its offer, the applicant represents that it will not require its employees or subcontractors to sign or comply with internal confidentiality agreements or statements prohibiting or otherwise restricting such employees or subcontractors from lawfully reporting waste, fraud, or abuse related to the performance of a Government contract to a designated investigative or law enforcement representative of a Federal department or agency authorized to receive such information (e.g., agency Office of the Inspector General).

(3) FAR 52.209-11, REPRESENTATION BY CORPORATIONS REGARDING DELINQUENT TAX LIABILITY OR A FELONY CONVICTION UNDER FEDERAL LAW (FEB 2016)

As required by sections 744 and 745 of Division E of the Consolidated and Further Continuing Appropriations Act, 2015 (Pub. L 113-235), and similar provisions, if contained in subsequent appropriations acts, the Government will not enter into a contract with any corporation that--

Has any unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or have lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability, where the awarding agency is aware of the unpaid tax liability, unless an agency has considered suspension or debarment of the corporation and made a determination that suspension or debarment is not necessary to protect the interests of the Government; or

Was convicted of a felony criminal violation under any Federal law within the preceding 24 months, where the awarding agency is aware of the conviction, unless an agency has considered suspension or debarment of the corporation and made a determination that this action is not necessary to protect the interests of the Government.

The applicant represents that—

It is is not a corporation that has any unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or have lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability; and

It is is not a corporation that was convicted of a felony criminal violation

under a Federal law within the preceding 24 months.

ii. Grant and Cooperative Agreement Proposals:

(1) Grant awards greater than \$100,000 require a certification of compliance with a national policy mandate concerning lobbying. Statutes and Government-wide regulations require the certification to be submitted prior to award. When submitting your grant through Grants.gov, by completing blocks 18 and 19 of the SF 424 (R&R) Form, the grant applicant is providing the certification on lobbying required by 32 CFR Part 28; otherwise a copy signed by the AOR must be provided. Below is the required certification:

CERTIFICATION AT APPENDIX A TO 32 CFR PART 28 REGARDING LOBBYING: Certification for Contracts, Grants, Loans, and Cooperative Agreements the undersigned certifies, to the best of his or her knowledge and belief, that:

(1) No Federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of an agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any Federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.

(2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit SF-LLL, "Disclosure Form to Report Lobbying," in accordance with its instructions.

(3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers (including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements) and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by 31 U.S.C. 1352. Any person who fails to file the required certification shall be subject to a civil penalty of not less than \$10,000 and not more than \$100,000 for each such failure.

(2) In accordance with Continuing Appropriations Act, 2017 (Pub. L. 114-223), or any other Act that extends to fiscal year (FY) 2017 funds the same prohibitions as contained in section 743, division E, title VII, of the Consolidated Appropriations Act, 2016 (Pub. L. 114-113), none of the funds appropriated or otherwise made available by that or any other Act may be made available for a grant or cooperative agreement with an entity that requires its employees or contractors

seeking to report fraud, waste, or abuse to sign internal confidentiality agreements or statements prohibiting or otherwise restricting those employees or contractors from lawfully reporting that waste, fraud, or abuse to a designated investigative or law enforcement representative of a Federal department or agency authorized to receive the information.

PROHIBITION ON CONTRACTING WITH ENTITIES THAT REQUIRED CERTAIN INTERNAL CONFIDENTIALITY AGREEMENTS – REPRESENTATION

Agreement with the representation below will be affirmed by checking the “I agree” box in block 17 of the SF424 (R&R) as part of the electronic proposal submitted via Grants.gov. The representation reads as follows:

By submission of its proposal or application, the applicant represents that it does not require any of its employees, contractors, or subrecipients seeking to report fraud, waste, or abuse to sign or comply with internal confidentiality agreements or statements prohibiting or otherwise restricting those employees, contractors, subrecipients from lawfully reporting that waste, fraud, or abuse to a designated investigative or law enforcement representative of a Federal department or agency authorized to receive such information.

*Note that: Section 743 states that it does not contravene requirements applicable to SF 312, Form 4414, or any other form issued by a Federal department or agency governing the nondisclosure of classified information.

(3) Recipients are required to submit the following representation with the application package IAW the instructions at Section II.D.2.f.ii of this BAA:

REPRESENTATIONS UNDER DOD ASSISTANCE AGREEMENTS: APPROPRIATIONS PROVISIONS ON TAX DELINQUENCY AND FELONY CONVICTIONS

The applicant is () is not () a “Corporation” meaning any entity, including any institution of higher education, other nonprofit organization, or for-profit entity that has filed articles of incorporation.

If the applicant is a “Corporation” please complete the following representations:

(a) The applicant represents that it is () is not () a corporation that has any unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or have lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability.

(b) The applicant represents that it is () is not () is not a corporation that was convicted of a criminal violation under any Federal law within the preceding 24 months.

NOTE: If an applicant responds in the affirmative to either of the above representations, the applicant is ineligible to receive an award unless the agency suspension and debarment official (SDO) has considered suspension or debarment and determined that further action is not required to protect the Government's interests. The applicant therefore should provide information about its tax liability or conviction to the agency's SDO as soon as it can do so, to facilitate completion of the required considerations before award decisions are made.

b. Policy Requirements:

The following list provides notable national policy requirements that may be applicable to an award. NOTE: The following is not an all-inclusive list of policy requirements. For assistance awards, refer to the DoD Research and Development General Terms and Conditions at <http://www.onr.navy.mil/Contracts-Grants/submit-proposal/grants-proposal/grants-terms-conditions.aspx> for additional national policy requirements that may apply. For contract awards, appropriate clauses will be added to award documents.

i. PROTECTION OF HUMAN SUBJECTS:

(1) Assistance Instruments:

(a) The recipient must protect the rights and welfare of individuals who participate as human subjects in research under this award and comply with the requirements at 32 CFR part 219, Department of Defense Instruction (DoDI) 3216.02, 10 U.S.C. 980, and when applicable, Food and Drug Administration (FDA) regulations.

(b) The recipient must not begin performance of research involving human subjects, also known as human subjects research (HSR), that is covered under 32 CFR part 219, or that meets exemption criteria under 32 CFR 219.101(b), until you receive a formal notification of approval from a DoD Human Research Protection Official (HRPO). Approval to perform HSR under this award is received after the HRPO has performed a review of the recipient's documentation of planned HSR activities and has officially furnished a concurrence with the recipient's determination as presented in the documentation.

(c) In order for the HRPO to accomplish this concurrence review, the recipient must provide sufficient documentation to enable his or her assessment as follows:

(i) If the HSR meets an exemption criteria under 32 CFR 219.101(b), the documentation must include a citation of the exemption category under 32 CFR 219.101(b) and a rationale statement.

(ii) If the recipient's activity is determined as "non-exempt research involving human subjects", the documentation must include:

- Assurance of Compliance (i.e., Department of Health and Human Services Office for Human Research Protections (OHRP) Federal Wide Assurance (FWA)) appropriate for the scope of work or program plan; and

- Institutional Review Board (IRB) approval, as well as all documentation reviewed by the IRB to make their determination.

(d) The HRPO retains final judgment on what activities constitute HSR, whether an exempt category applies, whether the risk determination is appropriate, and whether the planned HSR activities comply with the requirements in paragraph (a) of this section.

(e) The recipient must notify the HRPO immediately of any suspensions or terminations of the Assurance of Compliance.

(f) DoD staff, consultants, and advisory groups may independently review and inspect the recipient's research and research procedures involving human subjects and, based on such findings, DoD may prohibit research that presents unacceptable hazards or otherwise fails to comply with DoD requirements.

(g) Definitions for terms used in this article are found in DoDI 3216.02.

(2) Contracts: The appropriate clauses shall be added to the award.

ii. ANIMAL USE:

(1) Assistance Instruments:

(a) Prior to initiating any animal work under the award, the recipient must:

(i) Register the recipient's research, development, test, and evaluation or training facility with the Secretary of Agriculture in accordance with 7 U.S.C. 2136 and 9 CFR section 2.30, unless otherwise exempt from this requirement by meeting the conditions in 7 U.S.C. 2136 and 9 CFR parts 1-4 for the duration of the activity.

(ii) Have the recipient's proposed animal use approved in accordance with DoDI 3216.01, Use of Animals in DoD Programs by a DoD Component Headquarters Oversight Office.

(iii) Furnish evidence of such registration and approval to the grants officer.

(b) The recipient must make the animals on which the research is being conducted, and all premises, facilities, vehicles, equipment, and records that support animal care and use available during business hours and at other times mutually agreeable to the recipient, the United States Department of Agriculture Office of Animal and Plant Health Inspection Service (USDA/APHIS) representative, personnel representing the DoD component oversight offices, as well as the grants officer, to ascertain that the recipient is compliant with 7 U.S.C. 2131 et seq., 9 CFR parts 1-4, and DoDI 3216.01.

(c) The recipient's care and use of animals must conform with the pertinent laws of the United States, regulations of the Department of Agriculture, and regulations, policies, and procedures of the DoD (see 7 U.S.C. 2131 et seq., 9 CFR parts 1-4, and DoDI 3216.01).

(d) The recipient must acquire animals in accordance with DoDI 3216.01.

(2) Contracts: The appropriate clauses shall be added to the award.

iii. BIOLOGICAL SAFETY PROGRAM REQUIREMENTS:

(1) Assistance Instruments and Contracts: Awards may be subject to biological safety program requirements IAW:

(a) Army Regulation (AR) 385-10, Chapter 20

http://armypubs.army.mil/epubs/DR_pubs/DR_a/pdf/web/r385_10.pdf

(b) Department of Army (DA) Pamphlet (PAM) 385-69

http://armypubs.army.mil/epubs/DR_pubs/DR_a/pdf/web/p385_69.pdf

(c) DoD Manual 6055.18-M, Enclosure 4, Section 13

<http://www.dtic.mil/whs/directives/corres/pdf/605518m.pdf>

(d) DoD Executive Agent List (see item 3)

http://www.oaa.army.mil/aea_functions.aspx

iv. MILITARY RECRUITING:

(1) Assistance Instruments: This is to notify potential applicants that each grant or cooperative agreement awarded under this announcement to an institution of higher education must include the following term and condition:

(a) As a condition for receiving funds available to the DoD under this award, you agree that you are not an institution of higher education (as defined in 32 CFR part 216) that has a policy or practice that either prohibits, or in effect prevents:

(i) The Secretary of a Military Department from maintaining, establishing, or operating a unit of the Senior Reserve Officers Training Corps (ROTC)—in accordance with 10 U.S.C. 654 and other applicable Federal laws—at that institution (or any sub-element of that institution);

(ii) Any student at that institution (or any sub-element of that institution) from enrolling in a unit of the Senior ROTC at another institution of higher education.

(iii) The Secretary of a Military Department or Secretary of Homeland Security from gaining access to campuses, or access to students (who are 17 years of age or older) on campuses, for purposes of military recruiting in a manner that is at least equal in quality and scope to the access to campuses and to students that is provided to any other employer; or

(iv) Access by military recruiters for purposes of military recruiting to the names of students (who are 17 years of age or older and enrolled at that institution or any sub-element of that institution); their addresses, telephone listings, dates and places of birth, levels of education, academic majors, and degrees received; and the most recent educational institutions in which

they were enrolled.

(b) If you are determined, using the procedures in 32 CFR part 216, to be such an institution of higher education during the period of performance of this award, we:

(i) Will cease all payments to you of DoD funds under this award and all other DoD grants and cooperative agreements; and

(ii) May suspend or terminate those awards unilaterally for material failure to comply with the award terms and conditions.

(2) Contracts: Each contract awarded under this announcement to an institution of higher education shall include the following clause: DFARS 252.209-7005, Military Recruiting on Campus.

v. SUBCONTRACTING:

(1) Assistance Instruments: N/A

(2) Contracts: Pursuant to Section 8(d) of the Small Business Act (15 U.S.C. § 637(d)), it is the policy of the Government to enable small business and small disadvantaged business (SDB) concerns to be considered fairly as subcontractors. All other than U.S. small businesses proposing contracts expected to exceed \$700,000 and that have subcontracting possibilities are required to submit a subcontracting plan IAW FAR 19.702(a), and shall do so with their proposal.

Subcontracting plans are determined to be acceptable or unacceptable based on the criteria established at FAR 19.705-4, DFARS 219.705-4, and AFARS 5119.705-4. Goals are established on an individual contract basis and should result in realistic, challenging and attainable goals that, to the greatest extent possible, maximize small business participation in subcontracting for Small Business, SDB, Woman-Owned Small Business (WOSB), Economically-Disadvantaged Women-Owned Small Business (EDWOSB), Service-Disabled Veteran-Owned Small Business (SDVOSB), Veteran-Owned Small Business (VOSB), and Historically Underutilized Business Zone (HUBZone) Small Business consistent with applicants' make-or-buy policy, the pool of and availability of qualified and capable small business subcontractors, their performance on subcontracts, and existing relationships with suppliers.

Subcontracting goals should result in efficient contract performance in terms of cost, schedule, and performance and should not result in increased costs to the Government or undue administrative burden to the prime contractor. For reference, DoD Small Business Subcontracting Goals may be found at:

<http://www.acq.osd.mil/osbp/statistics/sbProgramGoals.shtml>.

vi. EXPORT CONTROL LAWS:

(1) Assistance Instruments: N/A

(2) Contracts: Applicants should be aware of current export control laws and are responsible for ensuring compliance with all International Traffic in Arms Regulation (ITAR) (22 CFR 120 et. Seq.) requirements, as applicable. In some cases, developmental items funded by the Department of Defense are now included on the United States Munition List (USML) and are therefore subject to ITAR jurisdiction. Applicants should address in their proposals whether ITAR restrictions apply or do not apply, such as in the case when research products would have both civil and military application, to the work they are proposing to perform for the Department of Defense. The USML is available online at <http://www.ecfr.gov/cgi-bin/text-idx?node=pt22.1.121>. Additional information regarding the President's Export Control Reform Initiative can be found at <http://export.gov/ecr/index.asp>.

vii. DRUG-FREE WORKPLACE:

(1) Assistance Instruments: The recipient must comply with drug-free workplace requirements in Subpart B of 2 CFR part 26, which is the DoD implementation of 41 U.S.C. chapter 81, "Drug-Free Workplace."

(2) Contracts: The appropriate clause(s) shall be added to the award.

viii. DEBARMENT AND SUSPENSION:

(1) Assistance Instruments: The recipient must comply with requirements regarding debarment and suspension in Subpart C of 2 CFR part 180, as adopted by DoD at 2 CFR part 1125. This includes requirements concerning the recipient's principals under an award, as well as requirements concerning the recipient's procurement transactions and subawards that are implemented in DoD Research and Development General Terms and Conditions PROC Articles I through III and SUB Article II.

(2) Contracts: The appropriate clause(s) shall be added to the award.

ix. REPORTING SUBAWARDS AND EXECUTIVE COMPENSATION:

(1) Assistance Instruments: The recipient must report information about subawards and executive compensation as specified in the award term in Appendix A to 2 CFR part 170, "Reporting subaward and executive compensation information," modified as follows:

(a) To accommodate any future designation of a different Government wide Web site for reporting subaward information, the Web site "http://www.fsrs.gov" cited in paragraphs a.2.i. and a.3 of the award provision is replaced by the phrase "http://www.fsrs.gov or successor OMB-designated Web site for reporting subaward information";

(b) To accommodate any future designation of a different Government wide Web site for reporting executive compensation information, the Web site "http://www.sam.gov" cited in paragraph b.2.i. of the award provision is replaced by the phrase "https://www.sam.gov or successor OMB-designated Web site for reporting information on total compensation"; and

(c) The reference to “Sec. ____ .210 of the attachment to OMB Circular A-133, “Audits of States, Local Governments, and Non-Profit Organizations” in paragraph e.3.ii of the award term is replaced by “2 CFR 200.330, as implemented in DoD Research and Development General Terms and Conditions SUB Article I of this award.”

(2) Contracts: The appropriate clause(s) shall be added to the award.

3. Reporting

a. Additional reports including number and types will be specified in the award document, but will include as a minimum monthly financial status reports. The reports shall be prepared and submitted in accordance with the procedures contained in the award document and mutually agreed upon before award. Reports and briefing material will also be required as appropriate to document progress in accomplishing program metrics. A final report that summarizes the project and tasks will be required at the conclusion of the performance period for the award.

b. ARMY MANPOWER CONTRACTOR REPORTING: For Contracts Only. The Office of the Assistant Secretary of the Army (Manpower & Reserve Affairs) operates and maintains a secure Army data collection site where the contractor will report ALL contractor manpower (including subcontractor⁶ manpower) required for performance of this contract. The contractor is required to completely fill in all the information in the format using the following web address: <https://cmra.army.mil/>. The required information includes:

- (1) Contracting Office, Contracting Officer, Contracting Officer’s Technical Representative;
- (2) Contract number, including task and delivery order number;
- (3) Beginning and ending dates covered by reporting period;
- (4) Contractor name, address, phone number, email address, identity of contractor employee entering data;
- (5) Estimated direct labor hours (including sub-contractors);
- (6) Estimated direct labor dollars paid this reporting period (including sub-contractors);
- (7) Total payments (including sub-contractors);
- (8) Predominate Federal Service Code (FSC) reflecting services provided by contractor (and separate predominant FSC for each sub-contractor if different);
- (9) Estimated data collection cost;
- (10) Organizational title associated with the Unit Identification Code (UIC) for the Army Requiring Activity (the Army Requiring Activity is responsible for providing the contractor with its UIC for the purposes of reporting this information);
- (11) Locations where contractor and sub-contractors perform the work (specified by zip code in the United States and nearest city, country, when in an overseas location, using standardized nomenclature provided on website);
- (12) Presence of deployment or contingency contract language; and
- (13) Number of contractor and sub-contractor employees deployed in theater this reporting period (by country).

As part of its submission, the contractor will also provide the estimated total cost (if any) incurred to comply with this reporting requirement. Reporting period will be the period of

performance not to exceed 12 months ending 30 September of each Government FY and must be reported by 31 October of each calendar year. Contractors may use a direct XML data transfer to the database server or fill in the fields on the website. The XML direct transfer is a format for transferring files from a contractor's systems to the secure web site without the need for separate data entries for each required data element at the web site. The specific formats for the XML direct transfer may be downloaded from the web site.

c. If the total Federal share exceeds \$500,000 on any Federal award under a notice of funding opportunity, the post-award reporting requirements reflected in Appendix XII to 2 CFR 200 will be included in the award document. This requirement also applies to modifications of awards that: 1) increase the scope of the award, 2) are issued on or after January 1, 2016, and 3) increase the federal share of the award's total value to an amount that exceeds \$500,000.

(End of Section)

G. Agency Contacts

1. Questions of a technical or programmatic nature shall be directed to the TPOC for each research area of interest. The TPOC information may be found in the description of each research area of interest in Section II.A of this BAA.
2. Questions of a business or administrative nature are to be directed to the following email: usarmy.rtp.aro.mbx.baa@mail.mil
3. Comments or questions submitted should be concise and to the point, eliminating any unnecessary verbiage. In addition, the relevant part and paragraph of the announcement should be referenced.
4. Requests to withdraw a proposal shall be directed to usarmy.rtp.aro.mbx.baa@mail.mil.

(End of Section)

H. Other Information

Below are two separate outlines of the informational requirements for a sample cost proposal. Section H.1 is for a procurement contract and Section H.2 is for grants and cooperative agreements.

1. CONTRACT Proposals

Cost Proposal – {No Page Limit}

Cover sheet to include:

1	BAA number
2	Technical area
3	Lead organization submitting proposal
4	Type of business, selected among the following categories: “LARGE BUSINESS”, “SDB”, “OTHER SMALL BUSINESS”, “HBCU”, “MI”, “OTHER EDUCATIONAL”, OR “OTHER NONPROFIT”
5	Contractor’s reference number (if any)
6	Other team members (if applicable) and type of business for each
7	Proposal title
8	TPOC to include: salutation, last name, first name, street address, city, state, zip code, telephone, fax (if available), electronic mail (if available)
9	Administrative point of contact to include: salutation, last name, first name, street address, city, state, zip code, telephone, fax (if available), and electronic mail (if available)
10	Award instrument requested: cost plus fixed fee (CPFF), cost-contract—no fee, cost sharing contract – no fee, or other type of procurement contract (specify)
11	Place(s) and period(s) of performance
12	Total proposed cost separated by basic award and option(s) (if any)
13	Name, address, and telephone number of the proposer’s cognizant Defense Contract Management Agency (DCMA) administration office (if known)
14	Name, address, and telephone number of the proposer’s cognizant Defense Contract Audit Agency (DCAA) audit office (if known)
15	Date proposal was prepared
16	DUNS number
17	TIN number
18	CAGE code
19	Subcontractor information
20	Proposal validity period
21	Any Forward Pricing Rate Agreement, other such approved rate information, or such other documentation that may assist in expediting negotiations (if available)

a. Reasoning for Submitting a Strong Cost Proposal

The ultimate responsibility of the Contracting Officer is to ensure that all prices offered in a proposal are fair and reasonable before contract award. To establish the reasonableness of the offered prices, the Contracting Officer may ask the applicant to provide supporting documentation that assists in this determination. The applicant's ability to be responsive to the Contracting Officer's requests can expedite contract award. As specified in Section 808 of Public Law 105-261, an applicant who does not comply with a requirement to submit information for a contract or subcontract in accordance with paragraph (a)(1) of FAR 15.403-3 may be ineligible for award.

b. DCAA-Accepted Accounting System

i. Before a cost-type contract can be awarded, the Contracting Officer must confirm that the applicant has a DCAA-accepted accounting system in place for accumulating and billing costs under Government contracts [FAR 53.209-1(f)]. If the applicant has DCAA correspondence, which documents the acceptance of its accounting system, this should be provided to the Contracting Officer (i.e. attached or referenced in the proposal). Otherwise, the Contracting Officer will submit an inquiry directly to the appropriate DCAA office and request a review of the applicant's accounting system.

ii. If an applicant does not have a DCAA-accepted accounting system in place, the DCAA review process can take several months depending upon the availability of the DCAA auditors and the applicant's internal processes. This will delay contract award.

iii. For more information about cost proposals and accounting standards, view the link titled "Information for Contractors" on the main menu of the DCAA website.

c. Field Pricing Assistance

During the pre-award cost audit process, the Contracting Officer may solicit support from DCAA to determine commerciality and price reasonableness of the proposal [FAR 15.404-2]. Any proprietary information or reports obtained from DCAA field audits will be appropriately identified and protected within the Government.

d. Sample Cost Proposal – "Piece by Piece"

To help guide applicants through the pre-award cost audit process, a sample cost proposal is detailed below. This sample allows the applicant to see exactly what the Government is looking for so that all cost and pricing back-up data can be provided to the Government in the first cost proposal submission. Review each cost element within the proposal, and take note of the types of documentation that the Contracting Officer will require from the applicant.

i. Direct Labor: The first cost element included in the cost proposal is Direct Labor. Each proposed employee must be listed by name and labor category.

Below is the Direct Labor as proposed by our sample applicant:

DIRECT LABOR		YEAR 1			YEAR 2		
Employee Name	Labor Category	Direct Hourly Rate	Hours	Total Direct Labor	Direct Hourly Rate	Hours	Total Direct Labor
Andy Smith	Program Manager	\$55.00	720.00	\$39,600.00	\$56.65	720.00	\$40,788.00
Bryan Andrews	Senior Engineer	\$40.00	672.00	\$26,880.00	\$41.20	672.00	\$27,686.40
Cindy Thomas	Principal Engineer	\$50.00	512.00	\$25,600.00	\$51.50	512.00	\$26,368.00
David Porter	Entry Level Engineer	\$10.00	400.00	\$4,000.00	\$10.30	400.00	\$4,120.00
Edward Bean	Project Administrator	\$25.00	48.00	\$1,200.00	\$25.75	48.00	\$1,236.00
Subtotal Direct Labor (DL)				\$97,280.00			\$100,198.40

(1) For this cost element, the Contracting Officer requires the applicant to provide adequate documentation in order to determine that the labor rate for each employee/labor category is fair and reasonable. The documentation must explain how these labor rates were derived. For example, if the rates are DCAA-approved labor rates, provide the Contracting Officer with copies of the DCAA documents stating the approval. This is the most acceptable means of documentation to determine the rates fair and reasonable. Other types of supporting documentation may include General Service Administration (GSA) contract price lists, actual payroll journals, or Salary.com research. If an employee listed in a cost proposal is not a current employee (maybe a new employee, or one contingent upon the award of this contract), a copy of the offer letter stating the hourly rate, signed and accepted by the employee, may be provided as adequate documentation.

Sometimes the hourly rates listed in a proposal are derived through subjective processes, i.e., blending of multiple employees in one labor category, or averaged over the course of the year to include scheduled payroll increases, etc. These situations should be clearly documented for the Contracting Officer.

(2) Another cost element in Direct Labor is labor escalation, or the increase in labor rates from year to year. In the example above, the proposed labor escalation is 3% (ex., Andy Smith's direct labor rate increased by 3% from \$55.00/hour in Year 1 to \$56.65/hour in Year 2). Often times, an applicant may not propose escalation on labor rates during a 24-month period. Whatever the proposed escalation rate is, please be prepared to explain why it is fair and reasonable. For example, a sufficient explanation for our sample escalation rate would be "The Government's General Schedule Increase and Locality Pay for the same time period (name FY) in the same location (name location) was published as 3.5%; therefore a 3% increase is fair and reasonable".

ii. *Other Direct Costs (ODCs)*: This section of the cost proposal includes all other directly-related costs required in support of the effort (i.e., materials, subcontractors, consultants, travel, etc.). Any cost element that includes various items must be detailed in a cost breakdown.

(1) **Direct Material Costs**: This subsection of the cost proposal will include any special tooling, test equipment, and material costs necessary to perform the project. Items included in this section must be carefully reviewed relative to need and appropriateness for the work proposed, and must, in the opinion of the Contracting Officer, be advantageous to the Government and directly related to the specific topic.

The Contracting Officer will require adequate documentation from the applicant to determine the cost reasonableness for each material cost proposed. The following methods are ways in which the Contracting Officer can determine this [FAR 15.403-1]:

(a) **Adequate Price Competition**. A price is based on adequate price competition when the applicant solicits and receives quotes from two or more responsible vendors for the same or similar items or services. Based on these quotes, the applicant selects the vendor who represents the best value to the Government. The applicant will be required to provide to the Contracting Officer copies of all vendor quotes received.

*NOTE: Price competition is not required for items at or below the micropurchase threshold (\$3,000) [FAR 15.403-1]. If an item’s unit cost is less than or equal to \$3,000, price competition is not necessary. However, if an item’s total cost over the period of performance (unit cost x quantity) is higher than \$3,000, two or more quotes must be obtained by the applicant.

(b) **Commercial Prices**. Commercial prices are those published on current price lists, catalogs, or market prices. This includes vendors who have prices published on a GSA-schedule contract. The applicant will be required to provide copies of such price lists to the Contracting Officer.

(c) **Prices set by law or regulation**. If a price is mandated by the Government (i.e. pronouncements in the form of periodic rulings, reviews, or similar actions of a governmental body, or embodied in the laws) that is sufficient to set a price.

Below is the list of Direct Material costs included in our sample proposal:

DIRECT MATERIAL COSTS	YEAR 1	YEAR 2
Raw Materials	\$35,000.00	\$12,000.00
Computer for experiments	\$4,215.00	\$0.00
Cable (item #12-3657, 300 ft)	\$1,275.00	\$0.00
Software	\$1,825.00	\$1,825.00
Subtotal Direct Materials Costs	\$42,315.00	\$13,825.00

“Raw Materials”: This is a generic label used to group many material items into one cost item within the proposal. The Contracting Officer will require a detailed breakout of all the items that

make up this cost. For each separate item over \$3,000 (total for Year 1 + Year 2), the applicant must be able to provide either competitive quotes received, or show that published pricing was used.

“Computer for experiments”: This item is most likely a grouping of several components that make up one system. The Contracting Officer will require a detailed breakout of all the items that make up this cost. For each separate item over \$3,000 (total for Year 1 + Year 2), the applicant must be able to provide either competitive quotes received, or show that published pricing was used.

“Cable”: Since this item is under the simplified acquisition threshold of \$3,000, competitive quotes or published pricing are not required. Simply provide documentation to show the Contracting Officer where this price came from.

“Software”: This cost item could include either one software product, or multiple products. If this includes a price for multiple items, please provide the detailed cost breakdown. Note: The price for Year 1 (\$1,825) is below the simplified acquisition threshold; however, in total (Year 1 + Year 2) the price is over \$3,000, so competitive quotes or published pricing documentation must be provided.

Due to the specialized types of products and services necessary to perform these projects, it may not always be possible to obtain competitive quotes from more than one reliable source. Each cost element over the simplified acquisition threshold (\$3,000) must be substantiated. There is always an explanation for how the cost of an item was derived; document how you came up with that price.

When it is not possible for an applicant to obtain a vendor price through competitive quotes or published price lists, the Contracting Officer may accept other methods to determine cost reasonableness. Below are some examples of other documentation, which the Contracting Officer may accept to substantiate costs:

- (a) Evidence that a vendor/supplier charged another applicant a similar price for similar services. Has the vendor charged someone else for the same product? Two (2) to three (3) invoices from that vendor to different customers may be used as evidence.
- (b) Previous contract prices. Has the applicant charged the Government a similar price under another Government contract for similar services? If the Government has already paid a certain price for services, then that price may already be considered fair and reasonable. Provide the contract number, and billing rates for reference.
- (c) DCAA approved. Has DCAA already accepted or verified specific cost items included in your proposal? Provide a copy of DCAA correspondence that addressed these costs.

(2) ODCs: Below is the remaining ODC portion of our proposal including equipment, subcontractors, consultants, and travel. Assume in this scenario that competitive quotes or catalog prices were not available for these items:

ODCs	YEAR 1	YEAR 2
Equipment Rental for Analysis	\$5,500.00	\$5,600.00
Subcontractor – Widget, Inc.	\$25,000.00	\$0.00
Consultant: John Bowers	\$0.00	\$12,000.00
Travel	\$1,250.00	\$1,250.00
Subtotal: ODCs	\$31,750.00	\$18,850.00

“Equipment Rental for Analysis”: The applicant explains that the Year 1 cost of \$5,500 is based upon 250 hours of equipment rental at an hourly rate of \$22.00/hr. One (1) invoice from the vendor charging another vendor the same price for the same service is provided to the Contracting Officer as evidence. Since this cost is over the simplified acquisition threshold, further documentation to determine cost reasonableness is required. The applicant is able to furnish another invoice charging a second vendor the same price for the same service.

“Subcontractor – Widget, Inc.”: The applicant provides a copy of the subcontractor quote to the Contracting Officer in support of the \$25,000 cost. This subcontractor quote must include sufficient detailed information (equivalent to the data included in the prime’s proposal to the Government), so that the Contracting Officer can make a determination of cost reasonableness.

(a) As stated in Section 3.5(c)(6) of the DoD Cost Proposal guidance, “All subcontractor costs and consultant costs must be detailed at the same level as prime contractor costs in regards to labor, travel, equipment, etc. Provide detailed substantiation of subcontractor costs in your cost proposal.”

(b) In accordance with FAR 15.404-3, “the Contracting Officer is responsible for the determination of price reasonableness for the prime contract, including subcontracting costs”. This means that the subcontractor’s quote/proposal may be subject to the same scrutiny by the Contracting Officer as the cost proposal submitted by the prime. The Contracting Officer will need to determine whether the subcontractor has an accepted purchasing system in place and/or conduct appropriate cost or price analyses to establish the reasonableness of proposed subcontract prices. Due to the proprietary nature of cost data, the subcontractor may choose to submit their pricing information directly to the Contracting Officer and not through the prime. This is understood and encouraged.

(c) When a subcontractor is selected to provide support under the prime contract due to its specialized experience, the Contracting Officer may request sole source justification from the applicant.

“Consultant – John Bowers”: The applicant shall provide a copy of the consultant’s quote to the Contracting Officer as evidence. In this example, the consultant will be charging an hourly rate of \$125 an hour for 96 hours of support. The applicant indicates to the Contracting Officer that this particular consultant was used on a previous contract with the Government (provide contract number), and will be charging the same rate. A copy of the consultant’s invoice to the applicant under the prior contract is available as supporting evidence. Since the Government has paid this price for the same services in the past, determination has already been made that the price is fair.

“Travel”: The Contracting Officer will require a detailed cost breakdown for travel expenses to determine whether the total cost is reasonable based on Government per diem and mileage rates. This breakdown shall include the number of trips, the destinations, and the number of travelers. It will also need to include the estimated airfare per round trip, estimated car rental, lodging rate per trip, tax on lodging, and per diem rate per trip. The lodging and per diem rates must comply with the Joint Travel Regulations. Please see the following website to determine the appropriate lodging and per diem rates: <http://www.defensetravel.dod.mil>. Additionally, the applicant must provide why the airfare is fair and reasonable as well. Sufficient back up for both airfare and car rental would include print outs of online research at the various travel search engines (Expedia, Travelocity, etc.), documenting the prices for airfare and car rentals are fair and reasonable.

Below is a sample of the travel portion:

TRAVEL	Unit	Trips	Travelers	Nights	Days	Unit Cost	Total Travel
Airfare	roundtrip	1	1			\$996.00	\$996.00
Lodging	day	1	1	1		\$75.00	\$75.00
Tax on Lodging (12%)	day	1	1	1		\$9.00	\$9.00
Per Diem	day	1	1		2	\$44.00	\$88.00
Automobile Rental	day	1	1		2	\$41.00	\$82.00
Subtotal Travel							\$1,250.00

iii. *Indirect Costs*: Indirect costs include elements such as fringe benefits, general and administrative (G&A), overhead, and material handling costs. The applicant shall indicate in the cost proposal both the indirect rates (as a percentage) as well as how those rates are allocated to the costs in the proposal.

Below is the indirect portion of our sample proposal:

INDIRECTS	YEAR 1	YEAR 2
Subtotal Direct Labor (DL):	\$97,280.00	\$100,198.40
Fringe Benefits, if not included in Overhead, rate (15.0000 %) X DL =	\$14,592.00	\$15,029.76
Labor Overhead (rate 45.0000 %) X (DL + Fringe) =	\$50,342.40	\$51,852.67
Total Direct Labor (TDL):	\$162,214.40	\$167,080.83

In this example, the applicant includes a fringe benefit rate of 15.00% that it allocated to the direct labor costs. The applicant also proposes a labor overhead rate of 45.00% that is allocated to the direct labor costs plus the fringe benefits.

All indirect rates and the allocation methods of those rates must be verified by the Contracting Officer. In most cases, DCAA documentation supporting the indirect rates and allocation methods can be obtained through a DCAA field audit or proposal review. Many applicants have already completed such reviews and have this documentation readily available. If an applicant is unable to participate in a DCAA review to substantiate indirect rates, the Contracting Officer may request other accounting data from the applicant to make a determination.

iv. *Facilities Capital Cost of Money (FCCM)*: Cost of money is an imputed cost that is not a form of interest on borrowings (see FAR 31.205-20). FCCM is an “incurred cost” for cost-reimbursement purposes under applicable cost-reimbursement contracts and for progress payment purposes under fixed-price contracts. It refers to (1) FCCM (48 CFR 9904.414) and (2) cost of money as an element of the cost of capital assets under construction (48 CFR 9904.417). If cost of money is proposed in accordance with FAR 31.205-10, a DD Form 1861 is required to be completed and submitted with the applicant’s proposal.

v. *Fee/Profit*: The proposed fee percentage will be analyzed in accordance with DFARS 215.404, the Weighted Guidelines Method.

vi. *Subcontracting Plan*: If the total amount of the proposal exceeds \$700,000 and the applicant is a large business or an institute of higher education (other than HBCU/MI) and the resultant award is a contract, the applicant shall be prepared to submit a subcontracting plan for small business and SDB concerns. A mutually agreeable plan will be included in and made a part of the contract (see Section II.F.2.b.v).

2. GRANT and COOPERATIVE AGREEMENT Proposals

Before award it must be established that an approved accounting system and financial management system exist.

a. *Direct Labor*: Show the current and projected salary amounts in terms of man-hours, man-months, or annual salary to be charged by the PI(s), faculty, research associates, postdoctoral associates, graduate and undergraduate students, secretarial, clerical, and other technical personnel either by personnel or position. State the number of man-hours used to calculate a man-month or man-year. For proposals from universities, research during the academic term is deemed part of regular academic duties, not an extra function for which additional compensation or compensation at a higher rate is warranted. Consequently, academic term salaries shall not be augmented either in rate or in total amount for research performed during the academic term. Rates of compensation for research conducted during non-academic (summer) terms shall not exceed the rate for the academic terms. When part or all of a person's services are to be charged as project costs, it is expected that the person will be relieved of an equal part or all of his or her

regular teaching or other obligations. For each person or position, provide the following information:

- i. The basis for the direct labor hours or percentage of effort (e.g., historical hours or estimates);
- ii. The basis for the direct labor rates or salaries. Labor costs should be predicted upon current labor rates or salaries. These rates may be adjusted upward for forecast salary or wage cost-of-living increases that will occur during the agreement period. The cost proposal should separately identify the rationale applied to base salary/wage for cost-of-living adjustments and merit increases. Each must be fully explained;
- iii. The portion of time to be devoted to the proposed research, divided between academic and non-academic (summer) terms, when applicable;
- iv. The total annual salary charged to the research project; and
- v. Any details that may affect the salary during the project, such as plans for leave and/or remuneration while on leave.

Note: There is no page limitation for budget proposals or budget justifications.

b. Fringe Benefits and Indirect Costs (Overhead, G&A, and Other): The most recent rates, dates of negotiation, the base(s) and periods to which the rates apply must be disclosed and a statement included identifying whether the proposed rates are provisional or fixed. If the rates have been negotiated by a Government agency, state when and by which agency. A copy of the negotiation memorandum should be provided. If negotiated forecast rates do not exist, applicants must provide sufficient detail to enable a determination to be made that the costs included in the forecast rate are allocable according to applicable cost provisions. Applicants' disclosure should be sufficient to permit a full understanding of the content of the rate(s) and how it was established. As a minimum, the submission should identify:

- i. All individual cost elements included in the forecast rate(s);
- ii. Basis used to prorate indirect expenses to cost pools, if any;
- iii. How the rate(s) was calculated;
- iv. Distribution basis of the developed rate(s);
- v. Basis on which the overhead rate is calculated, such as "salaries and wages" or "total costs;" and
- vi. The period of the applicant's FY.

c. Permanent Equipment: If facilities or equipment are required, a justification why this property should be furnished by the Government must be submitted. State the organization's inability or

unwillingness to furnish the facilities or equipment. Applicants must provide an itemized list of permanent equipment showing the cost for each item. Permanent equipment is any article or tangible nonexpendable property having a useful life of more than one year and an acquisition cost of \$5,000 or more per unit. The basis for the cost of each item of permanent equipment included in the budget must be disclosed, such as:

- i. Vendor Quote: Show name of vendor, number of quotes received and justification, if intended award is to other than lowest bidder.
- ii. Historical Cost: Identify vendor, date of purchase, and whether or not cost represents lowest bid. Include reason(s) for not soliciting current quotes.
- iii. Engineering Estimate: Include rationale for quote and reason for not soliciting current quotes.

If applicable, the following additional information shall be disclosed in the applicant's cost proposal:

- iv. Special test equipment to be fabricated by the awardee for specific research purposes and its cost.
- v. Standard equipment to be acquired and modified to meet specific requirements, including acquisition and modification costs, listed separately.
- vi. Existing equipment to be modified to meet specific research requirements, including modification costs. Do not include equipment the organization will purchase with its funds if the equipment will be capitalized for Federal income tax purposes. Proposed permanent equipment purchases during the final year of an award shall be limited and fully justified.
- vii. Grants and cooperative agreements may convey title to an institution for equipment purchased with project funds. At the discretion of the Contracting/Grants Officer, the agreement may provide for retention of the title by the Government or may impose conditions governing the equipment conveyed to the organization per the governing laws and regulations.

d. *Travel*: Forecasts of travel expenditures (domestic and foreign) that identify the destination and the various cost elements (airfare, mileage, per diem rates, etc.) must be submitted. The costs should be in sufficient detail to determine the reasonableness of such costs. Allowance for air travel normally will not exceed the cost of round-trip, economy air accommodations. Specify the type of travel and its relationship to the research project. Requests for domestic travel must not exceed \$3,000 per year per PI. Separate, prior approval by the ARL is required for all foreign travel (i.e., travel outside the continental U.S., its possessions and Canada). Foreign travel requests must not exceed \$1,800 each per year per PI. Special justification will be required for travel requests in excess of the amounts stated above and for travel by individuals other than the PI(s). Individuals other than the PI(s) are considered postdoctoral associates, research associates, graduate and undergraduate students, secretarial, clerical, and other technical personnel.

Additional travel may be requested for travel to Army laboratories and facilities to enhance agreement objectives and to achieve technology transfer.

(1) *Participant Support Costs*: This budget category refers to costs of transportation, per diem, stipends, and other related costs for participants or trainees (but not employees) in connection with ARO-sponsored conferences, meetings, symposia, training activities, apprenticeships and workshops (see the “Other Programs” section as described earlier in this BAA). Generally, indirect costs are not allowed on participant support costs. The number of participants to be supported should be entered in the parentheses on the budget form. These costs should also be justified in the budget justification page(s) attached to the cost proposal.

(2) *Materials, Supplies, and Consumables*: A general description and total estimated cost of expendable equipment and supplies are required. The basis for developing the cost estimate (vendor quotes, invoice prices, engineering estimate, purchase order history, etc.) must be included. If possible, provide a material list.

(3) *Publication, Documentation, and Dissemination*: The budget may request funds for the costs of preparing, publishing, or otherwise making available to others the findings and products of the work conducted under an agreement, including costs of reports, reprints, page charges, or other journal costs (except costs for prior or early publication); necessary illustrations, cleanup, documentation, storage, and indexing of data and databases; and development, documentation, and debugging of software.

(4) *Consultant Costs*: Applicants normally are expected to utilize the services of their own staff to the maximum extent possible in managing and performing the project's effort. If the need for consultant services is anticipated, the nature of proposed consultant services should be justified and included in the technical proposal narrative. The cost proposal should include the names of consultant(s), primary organizational affiliation, each individual's expertise, daily compensation rate, number of days of expected service, and estimated travel and per diem costs.

(5) *Computer Services*: The cost of computer services, including computer-based retrieval of scientific, technical, and educational information, may be requested. A justification/explanation based on the established computer service rates at the proposing organization should be included. The budget also may request costs, which must be shown to be reasonable, for leasing automatic data processing equipment. The purchase of computers or associated hardware and software should be requested as items of equipment.

(6) *Subawards (Subcontracts or Subgrants)*: A precise description of services or materials that are to be awarded by a subaward must be provided. For subawards totaling \$10,000 or more, provide the following specific information:

- A clear description of the work to be performed;
- If known, the identification of the proposed subawardee and an explanation of why and how the subawardee was selected or will be selected;

iii. The identification of the type of award to be used (cost reimbursement, fixed price, etc.);

iv. Whether or not the award will be competitive and, if noncompetitive, rationale to justify the absence of competition; and

v. A detailed cost summary.

k. ODCs: Itemize and provide the basis for proposed costs for other anticipated direct costs such as communications, transportation, insurance, and rental of equipment other than computer related items. Unusual or expensive items must be fully explained and justified.

l. Profit/Fee: Profit/fee is not allowed for the recipient of or subaward to an assistance instrument, where the principal purpose of the activity to be carried out is to stimulate or support a public purpose (i.e., to provide assistance), rather than acquisition (i.e., to acquire goods and services for the direct benefit of the Government). A subaward is an award of financial assistance in the form of money, or property in lieu of money, made under a DoD grant or cooperative agreement by a recipient to an eligible subrecipient. The term includes financial assistance for substantive program performance by the subrecipient of a portion of the program for which the DoD grant or cooperative agreement was made. It does not include the recipient's procurement of goods and services needed to carry out the program.

m. Subcontracting Plan: Subcontracting plans do not apply to assistance instruments.

n. FCCM: If cost of money is proposed, a completed FCCM (DD Form 1861) is required.

(End of Section)

APPENDIX 1: TABLE OF ACRONYMS

ACC	Army Contracting Command
AEOP	Army Educational Outreach Program
AFARS	Army Federal Acquisition Regulation Supplement
AFOSR	Air Force Office of Scientific Research
AMO	Atomic, Molecular, and Optical
AMP	Atomic and Molecular Physics
AOR	Authorized Organization Representative
APG	Aberdeen Proving Ground
AR	Army Regulation
ARL	Army Research Laboratory
ARO	Army Research Office
BAA	Broad Agency Announcement
CAGE	Commercial and Government Entity
CCE	Core Campaign Enablers
CFR	Code of Federal Regulations
C4ISR	Command, Control, Communications, Computers, Intelligence, Surveillance, and Reconnaissance
CFDA	Catalog of Federal Domestic Assistance
CMP	Condensed Matter Physics
CPFF	Cost Plus Fixed Fee
DA	Department of Army
D&B	Dun and Bradstreet
DBA	Doing Business Name
DCAA	Defense Contract Audit Agency
DCMA	Defense Contract Management Agency
DFARS	Defense Federal Acquisition Regulation Supplement
DLSC	Defense Logistics Service Center
DoD	Department of Defense
DoDI	Department of Defense Instruction
DTN	Disruption (or Delay) Tolerant Networks
DURIP	Defense University Research Instrumentation Program
EDWOSB	Economically-Disadvantaged Woman-Owned Small Business
ERGM	Exponential Random Graph Model
FAPIIS	Federal Awardee Performance and Integrity Information System
FAR	Federal Acquisition Regulation
FCCM	Facilities Capital Cost of Money
FFRDC	Federally Funded Research and Development Center
FQP	Foundational Quantum Physics
FSC	Federal Service Code
FWA	Federal Wide Assurance
FY	Fiscal Year
G&A	General and Administrative
GFD	Government Furnished Data

GFE	Government Furnished Equipment
GFI	Government Furnished Information
GFP	Government Furnished Property
GPGPU	General Purpose Computation on Graphics Processing Unit
GSA	General Service Administration
HBCU/MI	Historically Black Colleges and Universities and Minority-Serving Institutions
HSAP	High School Apprenticeship Program
HRPO	Human Research Protection Official
HSR	Human Subjects Research
HUBZone	Historically Underutilized Business Zone
IED	Improvised Explosive Device
IoT	Internet of Things
IR&D	Independent Research and Development
IRB	Institutional Review Board
ITAR	International Traffic in Arms Regulation
MURI	Multidisciplinary University Research Initiative
NFV	Network Function Virtualization
ODC	Other Direct Cost
OMB	Office of Management and Budget
OHRP	Office for Human Research Protections
ONR	Office of Naval Research
OTA	Other Transaction for Prototype
PAM	Pamphlet
PCM	Phase Change Material
PDE	Partial Differential Equation
PDF	Portable Document Format
PECASE	Presidential Early Career Award for Scientists and Engineers
PI	Principal Investigator
POC	Point of Contact
PWS	Performance Work Statement
QCON	Quantum Computation and Quantum Networking
QoI	Quality of Information
QoS	Quality of Service
QSIM	Quantum Sensing, Imaging, and Metrology
RDECOM	Research, Development, and Engineering Command
RDX	Royal Demolition eXplosive
REP	Research and Educational Program
ROTC	Reserve Officer Training Corps
R&R	Research and Related
RTP	Research Triangle Park
SAM	System for Award Management
SCN	Social and Cognitive Networks
SDB	Small Disadvantaged Business
SDO	Suspension and Debarment Official

SDN	Software Defined Networking
SDVOSB	Service-Disabled Veteran-Owned Small Business
SF	Standard Form
SLV	Survivability, Lethality, and Vulnerability
SO	Supersymmetric Optics
S&T	Science & Technology
STEM	Science, Technology, Engineering, and Mathematics
STIR	Short-Term Innovative Research
TIA	Technology Investment Agreement
TIN	Taxpayer Identification Number
TPOC	Technical Point of Contact
UARC	University-Affiliated Research Contract
UAV	Unmanned Aerial Vehicle
UGA	Unmanned Ground Vehicle
UIC	Unit Identification Code
URAP	Undergraduate Research Apprenticeship Program
U.S.C.	United States Code
USDA/APHIS	Department of Agriculture Office of Animal and Plant Health Inspection Service
USML	United States Munition List
VOSB	Veteran-Owned Small Business
VSP	Visiting Scientist Program
WOSB	Woman-Owned Small Business
YIP	Young Investigator Program

(End Section)

APPENDIX 2: SCHEDULE OF AMENDMENTS

Amendments to this BAA will be issued according to the following schedule to incorporate programmatic or administrative changes to this document, if necessary.

NOTE: Amendments may be issued more frequently at the discretion of the Government.

Estimated Date of Issuance
November 1, 2017
March 1, 2018
June 1, 2018
November 1, 2018
March 1, 2019
June 1, 2019
November 1, 2019
March 1, 2020
June 1, 2020
November 1, 2020
March 1, 2021
June 1, 2021

(End Section)

