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FY07 NRL DoD High Performance Computing Modernization Program Annual Reports

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Introduction

This book is a compilation of reports on all the work accomplished by NRL scientists and engineers and their collaborators using the DoD High Performance Computing Modernization Program's (HPCMP) resources for fiscal year 2007. The reports encompass work performed by researchers at all three NRL sites: Washington, DC; Stennis Space Center, Mississippi; and Monterey, California.

These reports are categorized according to the primary Computational Technology Area (CTA) as specified by the HPCMP, and include resources at the Major Shared Resources Centers as well as the Distributed Centers. This volume includes three indexes for ease of reference. These are an author index, a site index, and an NRL hierarchical index of reports from the Branches and Divisions in the Laboratory.

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Computational Chemistry and Materials Science (CCM)

Computational Electromagnetics and Acoustics (CEA)

Climate Weather Ocean Modeling (CWO)

CSM

Computational Structural Mechanics

- High-resolution, multidimensional modeling of materials and structures subjected to a broad range of impulsive loading that ranges from weak to intense.

- DoD application areas include conventional underwater explosion and ship response, structural acoustics, coupled field problems, space debris, propulsion systems, structural analysis, total weapon simulation, lethality/survivability of weapon systems (e.g., aircraft, ships, submarines, tanks), theater missile defense lethality analysis, optimization of techniques, and real-time, large-scale soldier and hardware-in-the-loop ground vehicle dynamic simulation.

Title: Geometric, Constitutive and Loading Complexities in Structural Materials
Author(s): A. B. Geltmacher[1], S. A. Wimmer[1], V. G. DeGiorgi[1], A. C. Leung[1], M. S. Quidwai[2], J. N. Baucom[1] and A. C. Lewis[1]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]SAIC, Washington, DC
CTA: CSM

Computer Resources: SGI Altix, HP XC Cluster and SGI Origin [ASC, OH]

Research Objectives: The research objective is developing a rational basis and mathematical description of complex material response for traditional structural materials and novel evolving materials. The technical approach is to utilize state of the art computational methods to model complex interactions both at and across scales. Scales of consideration include microscale, mesoscale and macroscale. Parameters of interest define material constitutive response (bulk and component), kinematics, nonlinearities, geometric complexities, loading path dependence, rate dependence, and interaction between loading types (electrical, thermal and mechanical). Work is not limited to structural performance of materials.

Methodology: The project uses finite element methods extensively, but the work is not limited to finite element methodologies. Other traditional, such as boundary element, and non-traditional, such as cellular automaton, techniques are explored and used as considered beneficial to the work. Nonlinear material mechanical constitutive response features are highlighted in much of work the performed. Implicit and explicit solutions methods are used as appropriate. The primary finite element codes used are ABAQUS and ANSYS. User subroutines are used for specialized material constitutive response. Coupled material responses, such as electrical-thermal for capacitor materials or electrical-mechanical for piezoelectric materials are exercised for evaluation of these effects. ABAQUS/Viewer, MSC PATRAN, and Tecplot are used for visualization of results, including animation. ABAQUS/CAE, CUBIT, MSC PATRAN and in-house software are used for model development.

Results: This project involves work in several topical areas. Work has been performed on the development of image-based microstructural models in 3D, strain and stress state visualization, material processing of multi-layer composites, prognostics modeling for material damage and fracture, and cellular automaton-based damage models. Representative results for one topic are presented here.

Biomechanics of Blunt Trauma: A device that can accurately describe the dynamic response of the human head would be a useful tool to understand traumatic brain injuries resulting from blast or blunt force trauma. A two dimensional transient finite element analysis was performed of a simplified brain model surrounded by cerebral spinal fluid and encased in PMMA. Viscoelastic material parameters of the brain tissue simulant were used. Low speed loading conditions were applied at different locations of this simple brain model structure. The von Mises stress and pressure contours at different times and displacement history plots are presented. The different loading conditions show distinct differences in the structural response of the brain. The inclusion of the brain ridges into the model influences the structural response of the models for these different types of loading conditions. Connecting the brain to the PMMA at the hippocampus has also shown to affect the dynamic response of the system.

Significance: The Naval Research Laboratory has developed a measurement device (GelMan-Brain) designed specifically to study the dynamic response of the brain from a variety of loading conditions to the human head. The transient analyses provided insight into key areas of interest and imparted insight on the optimal placement of sensors in a complex brain surrogate model.

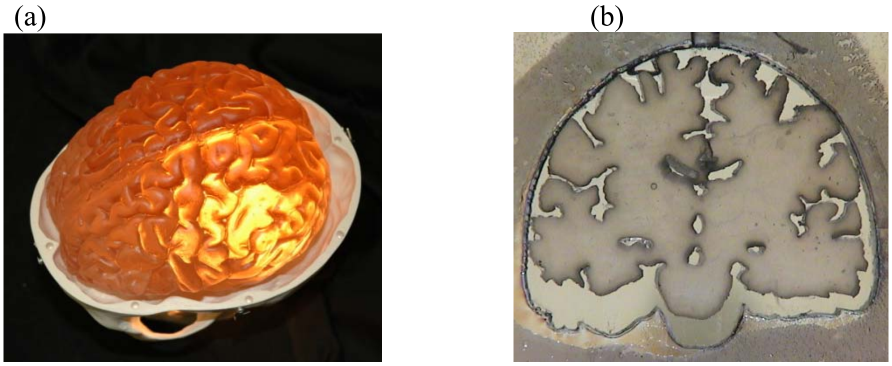


Figure 1: GelMan – Brain (a) three dimensional model (b) two dimensional model

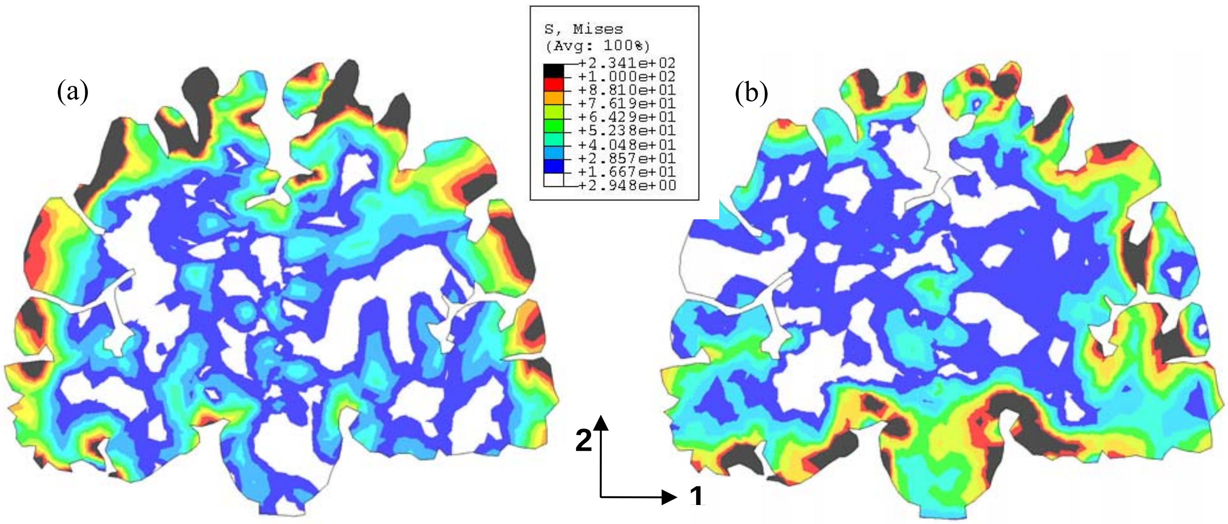


Figure 2. Von Mises stress contours at time = 0.0075 seconds for (a) Case 1: motion in the 2-direction (b) Case 2: motion in the 1-direction

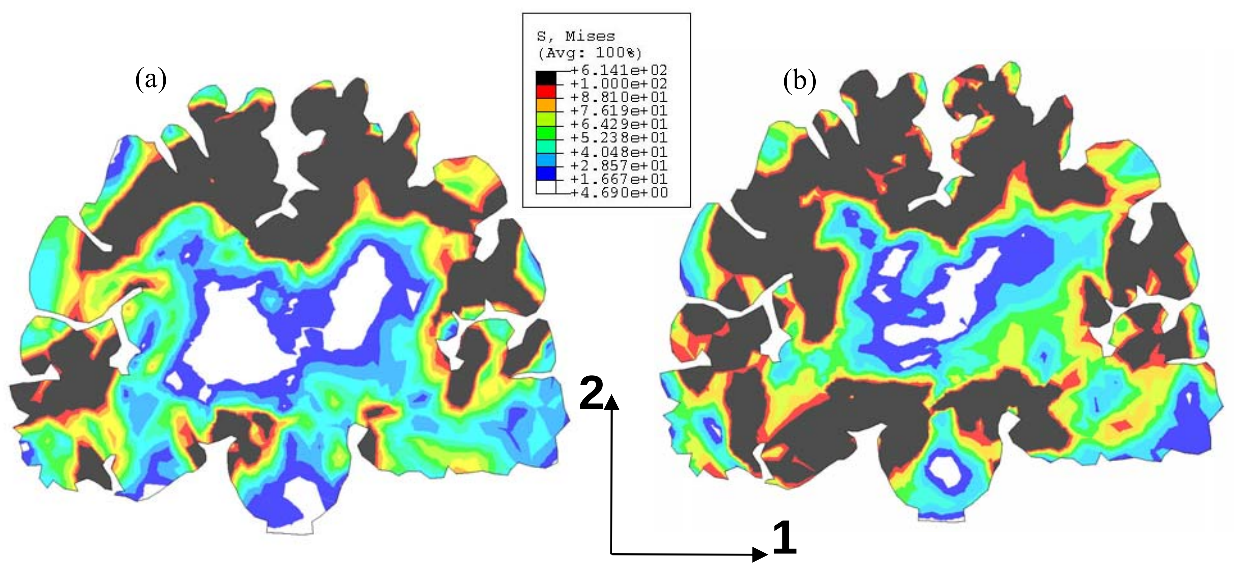


Figure 3. Von Mises stress contours at time = 0.00925 seconds for (a) Case 1: motion in the 2-direction (b) Case 2: motion in the 1-direction

Title: 2-D Arrays of Nanomechanical Resonators with Reduced Disorder
Author(s): Jeffrey W. Baldwin, Maxim K. Zalalutdinov, Michael J. Martin, and Brian H. Houston
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CSM

Computer Resources: Linux Cluster [ARL, MD]

Research Objectives: The fundamental research objective is to conduct advanced modeling of nanomechanical systems which augments our current fabrication and measurement capabilities. A computational model of nanomechanical arrays of coupled resonators has been made to support ongoing basic research where these systems are being studied experimentally. Specifically, we wish to quantify the 1-D and 2-D localization lengths associated with disorder.

Methodology: Specialized finite element software capable of millions of degrees of freedom and advanced matrix techniques are necessary for computation of the large, multi-element arrays modeled in these systems. In addition, with tens of thousands of eigenvalues needed in a system with two million degrees of freedom, the most sophisticated parallel eigenvalue analysis software is needed. Modal analysis is performed based on numerical simulations that employ finite elements methods (FEM) to predict the response of these arrays. Shell-type elements were used to model the resonators as plates, free on the outside and clamped on the pillars' edges. Counting the number of the normal modes of the array per frequency interval provides us with the density of states (DOS) for our "artificial crystals". The materials (silicon, for example) are generally anisotropic lending more difficulty and complexity to the problem. These systems have very high quality factors (Q) and low loss factors, which means a very high frequency refinement must be used over a large range of frequencies (kHz – GHz) to fully capture the structural response. This response is post-processed to obtain the mechanical energy broken down into its component forms. The analysis gives accurate frequency placement of the bandpass and stopbands in arrays of 2D nanomechanical resonators.

Results: Two-dimensional arrays of weakly coupled radio frequency (RF) nanomechanical resonators were designed using HPC computers and fabricated at the NRL Institute of Nanoscience using 50 nm thick nanocrystalline diamond films using electron beam lithography and dry etch techniques. Using finite element modeling allows us to create novel resonators with reduced disorder due to fabrication tolerances and to confine the frequency spread of individual resonators within ~ 0.6 % over the entire modal frequency range up to 100 MHz as shown in Table 1. Due to an optimized nanocrystalline diamond deposition process, high quality factors ($Q > 8{,}000$) have been demonstrated for particular modes of vibrations in single nanomechanical resonators. 2D arrays of coupled resonators exhibit an acoustic band, formed by the splitting of the individual resonant modes. The propagation of a wide-band signal within the array has been demonstrated using an optical imaging setup with two scanning lasers. The general trends that are observed both in computation and fabrication/testing show that there are modes of operation which are less prone to environmental losses and attachment losses. High quality factor individual resonators are generally required for the ultimate in sensing resolution, for example in a nanomechanical based chem-bio sensor. Modeling allows us to have a better understanding of the fundamental loss mechanisms and therefore mitigation of fabrication-induced disorder. This has already been shown to be the case as we have worked from beam-type structures to plate-type structures as shown in Figure 1.

Significance: The use of HPC computing time greatly decreases the fabrication-testing iteration time. Using the HPC computers, calculations run in minutes instead of days/weeks. There is significant cost savings to the development of nanomechanical resonator based systems. We believe this work will lead to mechanical-based high frequency (GHz) signal processing elements, ultra-fast single atomic mass unit mass detectors, and picoTesla magnetometers.

Table 1: FEM results of nanocrystalline diamond array unit cell

FEM Results (MHz)	Measured Frequency (MHz)	Percent Difference	Mode shape
37.006	39.71 +/- 0.7 %	7.3	(1,1) mode (asymmetric)
39.157	40.18 +/- 0.7 %	2.6	diagonal rocking degenerate
39.163	40.63 +/- 0.9 %	3.7	diagonal rocking degenerate
41.309	41.80 +/- 0.4 %	1.2	(1,1) mode (symmetric)
70.329	69.42 +/- 0.5 %	-1.3	diagonal asymmetric (1,1)
87.429	87.74 +/- 0.6 %	0.36	(2,0) mode
87.438	88.09 +/- 0.6 %	0.75	(2,0) mode

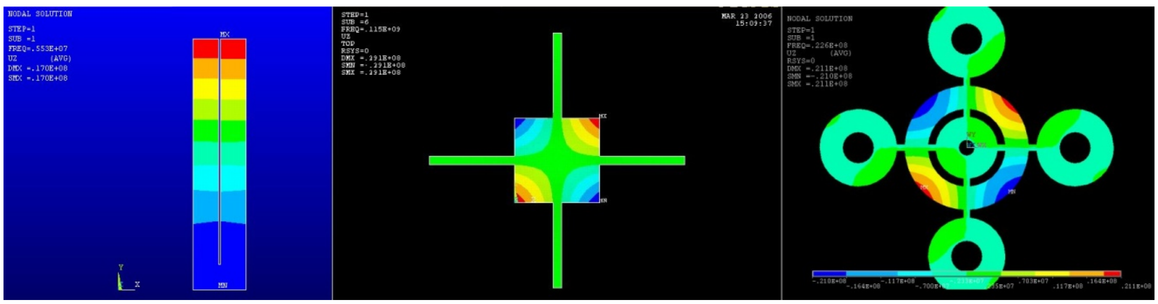


Figure 1. Progression of design of single array elements for the mitigation of fabrication-induced disorder using finite element code.

CFD

Computational Fluid Dynamics

- Accurate numerical solution of the equations describing fluid and gas motion and the related use of digital computers in fluid dynamics research.

- For basic studies of fluid dynamics, for engineering design of complex flow configurations, for predicting the interaction of chemistry with fluid flow for combustion and propulsions for interpreting and analyzing experimental data, and for extrapolating into regimes that are inaccessible or too costly to study.

- Encompasses all velocity regimes and scales of interest to the DoD without restrictions on the geometry and the motion of boundaries defining the flow.

- The physics to be considered may entail additional force fields, coupling surface physics and microphysics, changes of phase, change of chemical composition, and interactions among multiple phases in heterogeneous flows.

Title: Dispersed-Phase Structure in Magnetohydrodynamic Turbulence
Author(s): Damian W. I. Rouson[1], Xiaofeng Xu[2], Karla Morris[3] and S. C. Kassinos[4]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]General Motors Corp., Pontiac, MI; [3] City University of New York, New York, NY; [4]University of Cyprus, Nicosia, Cyprus
CTA: CFD

Computer Resources: SGI Altix [NRL, DC]

Research Objectives: This project studies how the structural morphology of magnetohydrodynamic (MHD) turbulence influences that of a discrete solid phase dispersed throughout the flow. We track the motion of rigid particles immersed in high-magnetic-diffusivity fluids, e.g., liquid metals and seawater, under the sudden application of external magnetic fields. Traditional turbulence models contain limited or no information about coherent structure in the turbulence. While structure-based models for single-phase flow have been developed over the past decade, no such models exist for multiphase flows. By defining and calculating a new set of dispersed-phase structure tensors, we seek to lay a foundation for structure-based, particle-laden flow models for conducting and non-conducting flows.

Methodology: MHD turbulence is governed by Maxwell's equations for electromagnetics coupled to the Navier-Stokes equations for fluid dynamics. The low magnetic Reynolds numbers characteristic of conducting liquids enable the Quasi-Static (QS) MHD approximation. In QS MHD, the magnetic induction equation can be solved analytically for the fluctuating magnetic field in terms of the fluid velocity. We solve the QS MHD equations with a hybrid explicit/implicit, third-order accurate Runge Kutta marching scheme and a Fourier-Galerkin spatial projection of all field variables. We simultaneously track passive, solid particles using the Stokes drag law. We post-process the simulation data to determine the evolution of the particle number density field and the associated dispersed-phase structure tensor statistics.

Results: The magnetic field damps velocity gradients aligned with the external magnetic field, inducing a two-dimensional, three-component (2D/3C) flow. Figure 1 shows the resulting structure in the particle spatial distribution when viewed along the magnetic field versus the lack of structure observed orthogonal to the magnetic field. Color coding the particles according to their instantaneous velocity demonstrates that particles clustered near each other in physical space also tend to be in close proximity in velocity. Figure 2 provides one example of the evolution of the dispersed-phase structure dimensionality tensor defined and measured for the first time in this work. The tensor's diagonal elements all start at zero, indicating that the initial particle distribution is uniform. All elements initially increase, after which the element corresponding to the magnetic field direction decreases as the structure in this direction is suppressed, while the elements corresponding to the two orthogonal directions continue to increase as the magnetic field induces increasingly strong clustering of the particles in those two directions.

Significance: Particle transport in MHD turbulence is of fundamental importance in several technologies of relevance to the Navy. For example, the Navy has patented a flow meter capable of measuring the velocity of conducting fluids. (U.S. Patent 5390548) This project is one step toward being able to determine the influence of the suspended particles likely to be encountered in natural environments. Particle-laden MHD also plays an important role in metallurgical processing, e.g., it describes the motion of nucleation sites in semi-solid, liquid-metal slurries undergoing magnetic stirring. Semi-solid processing is a promising metal forming technology.

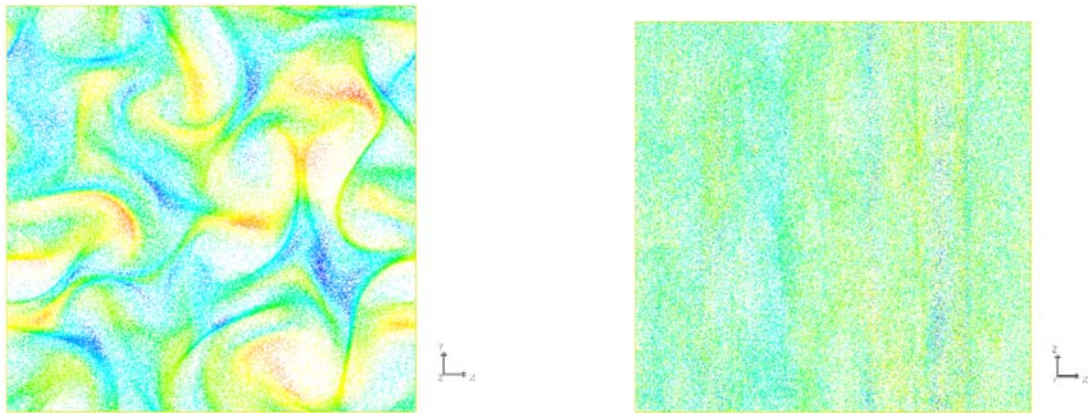


Figure 1. Particle positions color-coded for instantaneous velocity (red=fastest, blue=slowest): viewed along the direction of the magnetic field vector (left) and viewed orthogonal to the magnetic field vector (right).

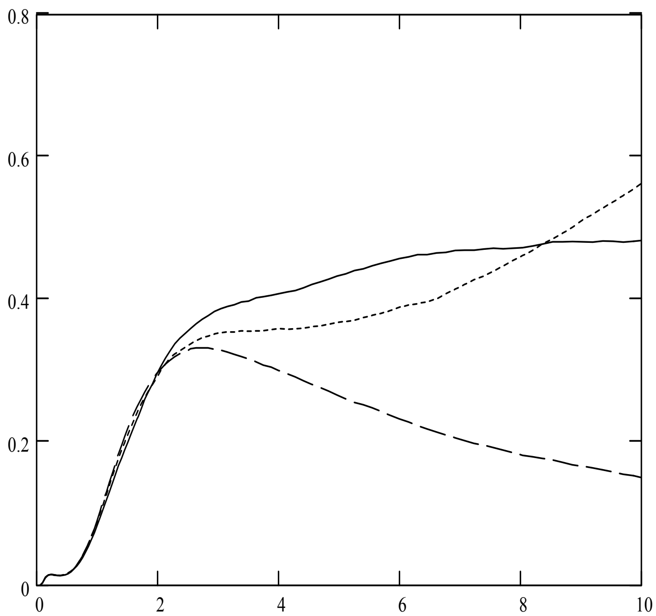


Figure 2. Dispersed phase structure dimensionality tensor diagonal elements: along the magnetic field (dashed line) and orthogonal to the magnetic field (solid and dotted lines).

Title: The Impact of Aerosol Dynamics on Fire, Explosion Safety and Suppression
Author(s): Ramagopal Ananth
Affliation(s): Naval Research Laboratory, Washington DC
CTA: CFD

Computer Resources: SGI Origin, SGI Altix [ASC, OH]

Research Objectives: Development of water mist technology is driven by the need to find replacement for the fire fighting agent Halon 1301. The halogen based agent is known to adversely affect the earth's ozone layer. Water can be a highly effective multi-phase fire suppression agent and has zero ozone depleting potential. However, water droplets cannot diffuse from the point of origin to the fire location unlike a gaseous agent. Therefore, the transport and distribution of water pose additional challenges and require considerable computational efforts.

Methodology: We used a commercial CFD software package FLUENT as well as developed in-house codes (user defined subroutines) to describe the multiphase flow dynamics with detailed chemistry. This is first model of its kind in combining the droplet physics through Lagrangian approach to track the droplets with GRI 3.0 chemistry for propane gas combustion. We have also used a larger University of California, San Diego's chemical mechanisms and showed that GRI 3.0 adequately describes the interactions between a physical agent (water) and a co-flow, diffusion flame.

Results: Before, introducing the water droplets, the model has been verified by the excellent agreement with the experimental data on flame extinction by nitrogen gas. With the droplets, the calculations show that the droplets entrained into the reaction kernel at the flame base are crucial for extinction. The reaction kernel detaches from the burner rim and blows-off when the droplet concentration is increased to the extinction concentration as shown in Figure 1. During the extinction, the maximum chain-branching reaction rate (H2+O=OH+H) in the reaction kernel was found to be reduced by a factor of 5 to a critical value (0.38 kgmol/m3sec). A large decrease in the reaction rate indicates that the maximum heat generations rates are too low to sustain the flame. The extinction concentrations predicted for 4 and 8 μm agree with the recent measurements [Fisher *et al.*, 31st Proc. Comb. Inst., 2731, 2006] with poly-disperse ultra-fine mist having Sauter mean diameter of 6.5 μm.

Significance: Navy vessels have many spaces containing obstructions, which prevent sprinklers and traditional water mist to reach behind obstructions. Extremely small droplets act as a pseudo gas and distribute better. Our computations describe the effects of drop size on the effectiveness in extinguishing the fires.

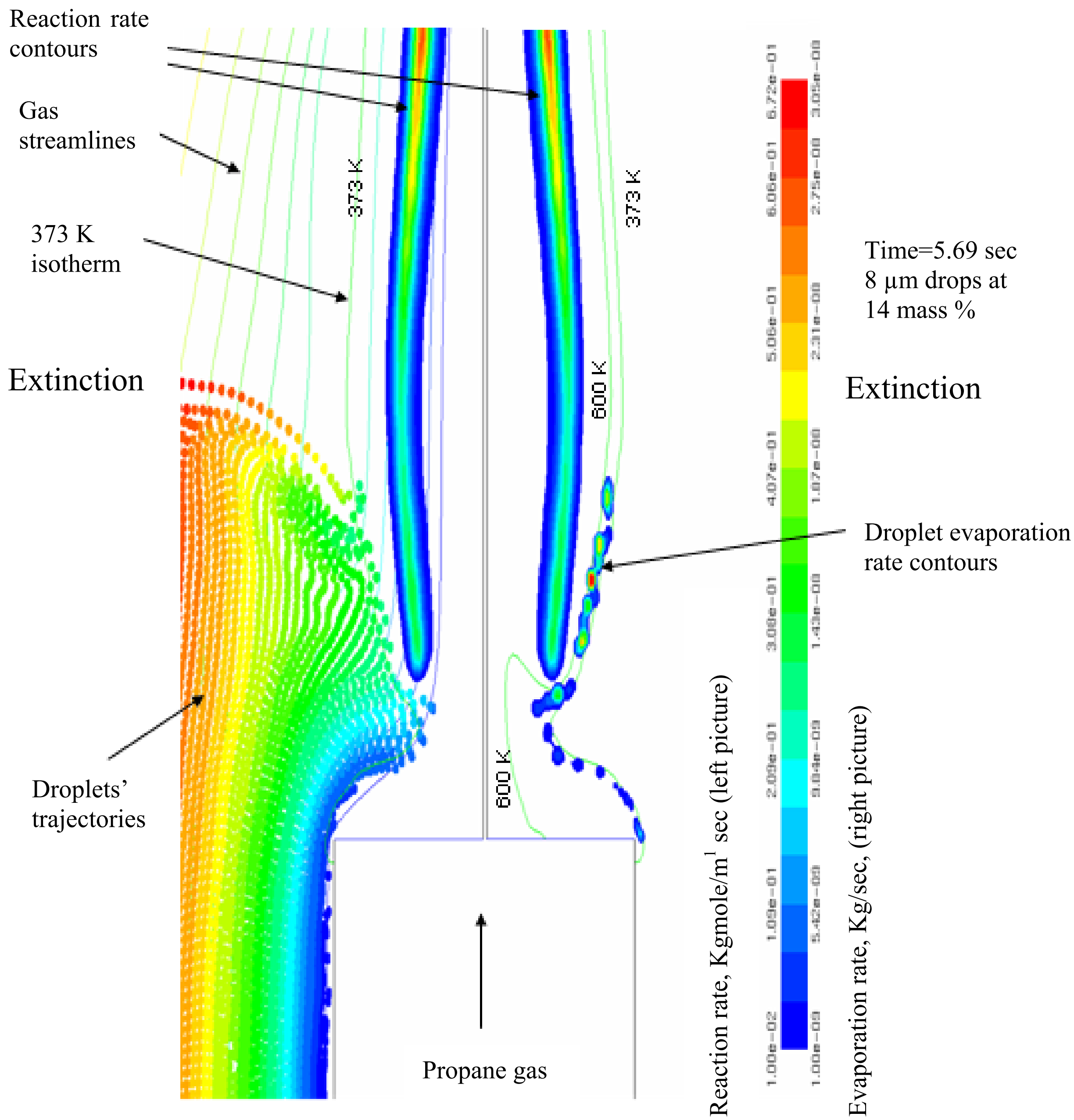


Figure 1. Lagrangian Computations of Water Drops Show Complete Evaporation at 600 K isotherm at 0.69 sec (time=5.69 sec) after Injection.
Left picture: Droplet trajectories (color lines) and 373 K isotherm (green line) superimposed on reaction rate contours.
Right picture: Evaporation rate contours superimposed on reaction rate contours and 373 K, 600 K isotherms (green lines)

Title: Simulations of the Ionosphere and Magnetosphere
Author(s): S. P. Slinker[1], J. D. Huba[1], P. Schuck[1], J. Krall[1] and G. Joyce[2]
Affiliation(s): [1]Naval Research Laboratory, Washington DC; [2]ICARUS, Washington, DC
CTA: CFD

Computer Resources: SGI Origin [ASC, OH]; SGI Altix [NRL, DC], [ASC, OH]; Linux Cluster [ARL, MD]

Research Objectives: Develop space weather forecasting capability. Simulate geomagnetic storms and other events of interest in order to understand the Earth's magnetosphere and ionosphere and to improve the model.

Methodology: The LFM model is a 3D magnetohydrodynamics model of the Earth's magnetosphere. Measured solar wind data are used as input conditions to drive the system. Currents in the inner boundary are closed in the ionosphere where an elliptic potential equation is solved. Both OpenMP and MPI versions are used. SAMI3 is a 3D simulation model of the Earth's ionosphere covering all latitudes.

Results: The major effort this year was the successful coupling of LFM and SAMI3. The resulting model is driven by the solar wind and solar radiation. The magnetosphere model produces the high latitude electric field which drives the ionosphere model. It also estimates the flux and energy of precipitating auroral electrons which produce ionization in the polar atmosphere. In return SAMI3 provides the conductances needed by LFM to find the electric fields which drive the plasma at the inner boundary of the magnetosphere. The coupled code employs MPI. Two geomagnetic storms occurring on 24 August 2005 and 14 January 1988 were simulated with the combined model.

A version of the stand-alone SAMI3 ionosphere model was installed and benchmarked. This version was used in a study of the effects of solar flares on the ionosphere.

A simulation of the magnetosphere was done for the 22 November 2003 events. This was a period of northward interplanetary magnetic field (IMF) and unusual auroral arcs in the polar cap were observed.

Several geomagnetic storm studies were undertaken with LFM. New runs were performed for the events of 24 August 2005, 08 November 2004, and 15 May 2005, while the simulations of the storms of 28 October and 20 November 2003 were extended. These events were the focus of a Living with a Star Coordinated Data Analysis Workshop (LWS-CDAW).

Significance: Potential protection of communication satellites and the power grid. Support of ongoing experiments in remote sensing of the space environment. Provide input to ionospheric and thermospheric models.

Title: 3D Simulations of Thermonuclear Supernovae
Author(s): Vadim N. Gamezo and Elaine S. Oran
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Cray XD1, SGI Altix [NRL, DC]; SGI Altix [ASC, OH]

Research Objectives: Model and understand three-dimensional (3D) phenomena involved in Type Ia supernova (SN Ia) explosions, including propagation of turbulent thermonuclear flames, formation of detonation waves, and propagation of the detonation through the partially burned expanding star.

Methodology: We focus at the deflagration-to-detonation transition (DDT), which is a critical unsolved problem in Type Ia supernova models. The physics of this phenomenon in Type Ia supernovae and terrestrial chemical systems is similar, but still not well understood. This similarity allows us to use similar methods to study DDT in astrophysical and terrestrial systems, and validate our numerical models using terrestrial combustion experiments. The numerical model is based on reactive Navier-Stokes equations coupled with the ideal-gas equation of state and a one-step Arrhenuis kinetics of energy release. The equations are solved using the explicit, second-order, Godunov-type numerical scheme incorporating a Riemann solver, and a structured adaptive mesh based on the fully threaded tree data structure.

Results: We successfully model the flame acceleration and DDT in channels with obstacles filled with hydrogen-air mixture, reproduce main experimental results, and analyze underlying physical mechanisms and the stochastic nature of DDT. Basic mechanisms for the flame and flow acceleration involve thermal expansion of combustion products, shock-flame and flame-vortex interactions, and Rayleigh-Taylor, Richtmyer-Meshkov, and Kelvin-Helmholtz instabilities. The accelerating flow generates strong shocks that reflect from channel walls and obstacles and eventually create hot spots that produce detonations through Zeldovich's gradient mechanism.

In supernovae, we observe an additional mechanism for shock acceleration related to different length scales of carbon and oxygen burning in a white dwarf. The slow oxygen burning can release almost as much energy as the fast carbon burning, and occurs in a hot material where carbon is already depleted. Shocks that propagate through the hot and relatively thick oxygen burning zone can pick up energy and even produce detonations driven only by the oxygen burning. When this oxygen detonation enters the cold unburned material, it can ignite it and produce a regular carbon-oxygen detonation.

Significance: Type Ia supernovae play an important, fundamental role in astronomy, cosmology, and particle physics. Due to their extreme brightness, these supernovae are used as "standard candles" to measure distances, curvature, and the rate of expansion of the universe. Observations of distant SN Ia indicate that there exists an unknown "repulsive force" (dark energy) which acts against "normal" gravity and leads to an accelerating expansion of the universe. This poses fundamental challenges and also provides important clues to theories of matter. Understanding the physics of SN Ia explosions, and DDT phenomena in particular, is a crucial ingredient in calibrating SN Ia as distance indicators and in separating the effects of stellar evolution and supernova environment from global cosmological effects.

DDT phenomena also play an important role in terrestrial combustion. This study is relevant for a number of practical applications, including hydrogen safety and pulse-detonation engines (PDE). For example, the results summarizing the effect of obstacle spacing on flame acceleration and DDT can be directly used to design detonation initiation devices for PDE.

Title: Unsteady Air-wakes for Ship Topside Design

Author(s): J. Geder[1], W. C. Sandberg[1] and F. Camelli[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]George Mason University, Fairfax, VA
CTA: CFD

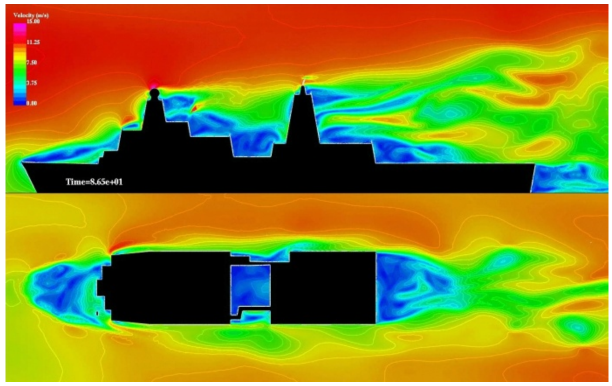
Computer Resources: SGI Altix [NRL, DC]

Research Objectives: The project involves the analysis of air-wake and stack gas temperature for the LPD17. The overall goal of these computations is to understand the impact of the air-wake in the landing process. Extending the air-wake knowledge to include prediction of dangerous velocity bursting events for landing and coupling this information into a landing period designator, will lead to improved safety in the landing process.

Methodology: The steps in any of these simulations are: geometry reconstruction from CAD or blue print information, tessellation of the computational domain, solution of the partial differential equations with their boundary conditions, and visualization and analysis of the solution. The solution step is one of the most consuming in the whole process, e.g., this step took in the order of months in the LPD-17 and T-AKE-1 studies. An unstructured-grid based LES solver was used to compute the unsteady aerodynamics about the ship superstructure due to the combined effects from the ship forward speed and the incident wind, including variable wind gusting.

Results: The unsteady air-wake for the LPD17 has been extensively studied. We have analyzed real time histories for 0, 15, 30, 45 and 60 degrees wind from port and from 15 degrees starboard. All these runs have been carried out at the NRL facilities, using the two ALTIX systems, niobe and morpheus. We have identified very high velocity gradient zones which could be hazardous for both manned air vehicles such as helos and UAV launch and recovery operations. An example of this is shown below.

Significance: The capability to compute the unsteady air wake time history a vehicle may encounter enables one to investigate many launch and recovery scenarios the results from which can lead to improved safety guidance by alerting pilots to unsafe conditions before they encounter them.



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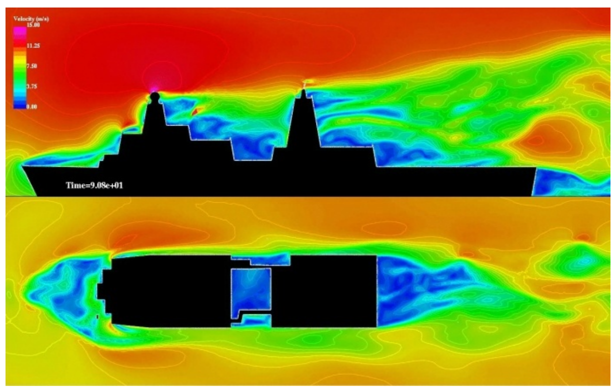

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Figure 1. Vertical and horizontal planes indicating zones of high velocity gradients evolving in time to create dangerous vertical and lateral gust bursts aft of the transom that can be hazardous for air vehicle operations aboard the LPD-17 Class ships

Title: Adaptive Re-meshing for Unsteady Flight in Insects and Fishes
Author(s): W. C. Sandberg[1], R. Ramamurti[1], J. Geder[1] and R. Löhner[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2] George Mason University, Fairfax, VA
CTA: CFD

Computer Resources: SGI Altix [NRL, DC]

Research Objectives: Develop adaptive re-meshing strategies and computational technology for unsteady incompressible flows past flapping and deforming surfaces. Utilize these methods to investigate the mechanisms of lift and thrust production in very large amplitude non-linear wing and fin motions in insects and fish.

Methodology: An implicit finite element solver, FEFLOIC, for 3-D incompressible flows based on unstructured grids was used as the primary flow solver. This model is one of the DoD HPC benchmark codes. The flow solver was combined with adaptive re-meshing techniques for these transient problems with moving grids and was also integrated with the rigid body motion in a self-consistent manner which allowed the simulation of fully coupled fluid-rigid body interaction problem of arbitrary geometric complexity in three dimensions. New re-meshing routines were incorporated into this code.

Results: 3-D unsteady CFD simulations were successfully carried out to model the dynamic behavior of multiple compliant elements of a deformable flapping pectoral fin. The unsteady force production time-histories obtained from the flapping computations were used in the design of a two-fin vehicle. The unsteady force time histories were also incorporated into a new hybrid vehicle control development methodology.

Significance: Flapping control surfaces which are capable of generating high lift or thrust at low speeds are of immense value to the Navy. Underwater research vessels operate at low speeds where the effectiveness of conventional control surfaces is often unsatisfactory. Improved position control and thrust control is extremely important for carrying out missions, particularly when operating in close proximity to the bottom. A computational capability to design low speed, high thrust devices and low speed high lift vehicles is quite important in developing innovative autonomous underwater vehicles.

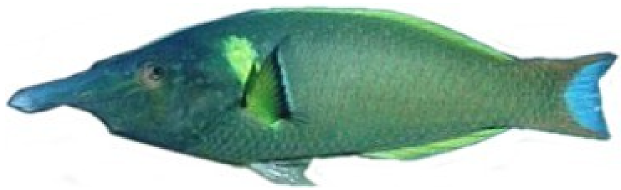


Figure 1. Gomphosus varius (Bird wrasse) with pectoral fins

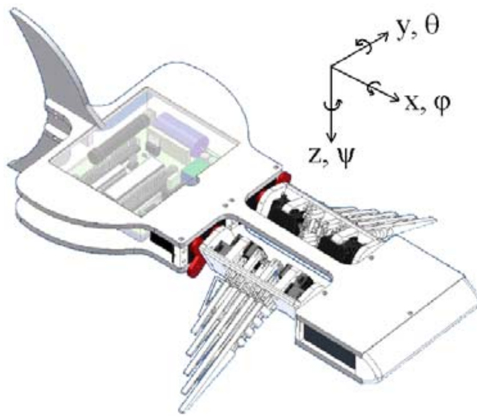


Figure 2. Vehicle with pectoral fins for which hybrid unsteady force controller was developed

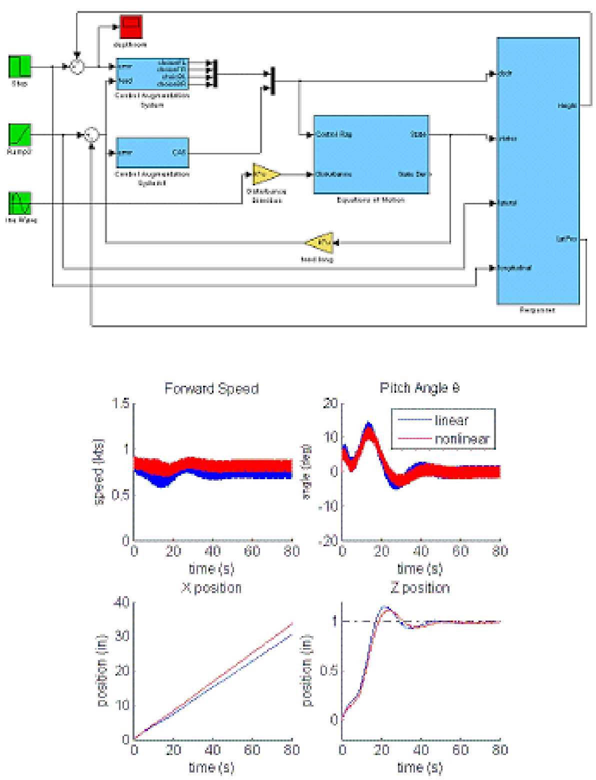


Figure 3. Vertical plane vehicle response from hybrid unsteady force controller

Title: Contaminant Transport and Source Simulations for Urban and Environmental Hazard Assessment
Author(s): Adam Moses, Keith Obenschain, Gopal Patnaik, Jay Boris and Theodore Young
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Linux Cluster [ARL, MD]; SGI Altix [NRL, DC]

Research Objectives: Perform high-resolution detailed 3D CFD simulations for urban areas of specific interest to construct the underlying Dispersion Nomograf™ databases for fast and accurate plume predictions by CT-Analyst® and to develop methods to incorporate these physics based plume predictions into existing military Modeling and Simulation (M&S) tools.

Methodology: Use the model, FAST3D-CT, perform the time-accurate, high-resolution 3D CFD, as an offline detailed urban contaminant transport scenario generator. Data from the detailed simulations is then be distilled into a compact data set called "Dispersion Nomografs" that can be later utilized by CT-Analyst to render instantaneous plume predictions, sensor fusion and placement for a variety of urban and metrological parameters and conditions. Develop needed Application Programmers Interface (API) and synchronization software to interface with and incorporate this leading edge technology into existing military M&S systems.

Results: The extensive CFD simulations, which incorporated the high-resolution building and terrain geometry, were performed for the metropolitan area of Baghdad Iraq and the "Dispersion Nomograf" data set built for CT-Analyst. A Java enhanced API was developed and incorporated into CT-Analyst to facilitate plume rendering use in the M&S application OneSAF.

Significance: Immediately upon deployment of these advancements, users of OneSAF will find greater fidelity in the plume models and as a result far more accurate and realistic scenarios that can be realized. OneSAF can now utilize the CT-Analyst API to determine the time dependent plume locations and concentrations in areas of interest within the simulation, and determine the attenuation of visibility along a line of sight. This will therefore be beneficial to all current and future operators of the M&S.

Productivity Measures: A fifty square kilometer area of metropolitan Baghdad, Iraq was completed and a full Dispersion Nomograf data set built for released to the proper authorities for ongoing operations. To date this is the largest contiguous area we've carried out the complete set of CFD simulations on and, which subsequently led to the high resolution Dispersion Nomograf data set capability for a much larger area of this sensitive location.

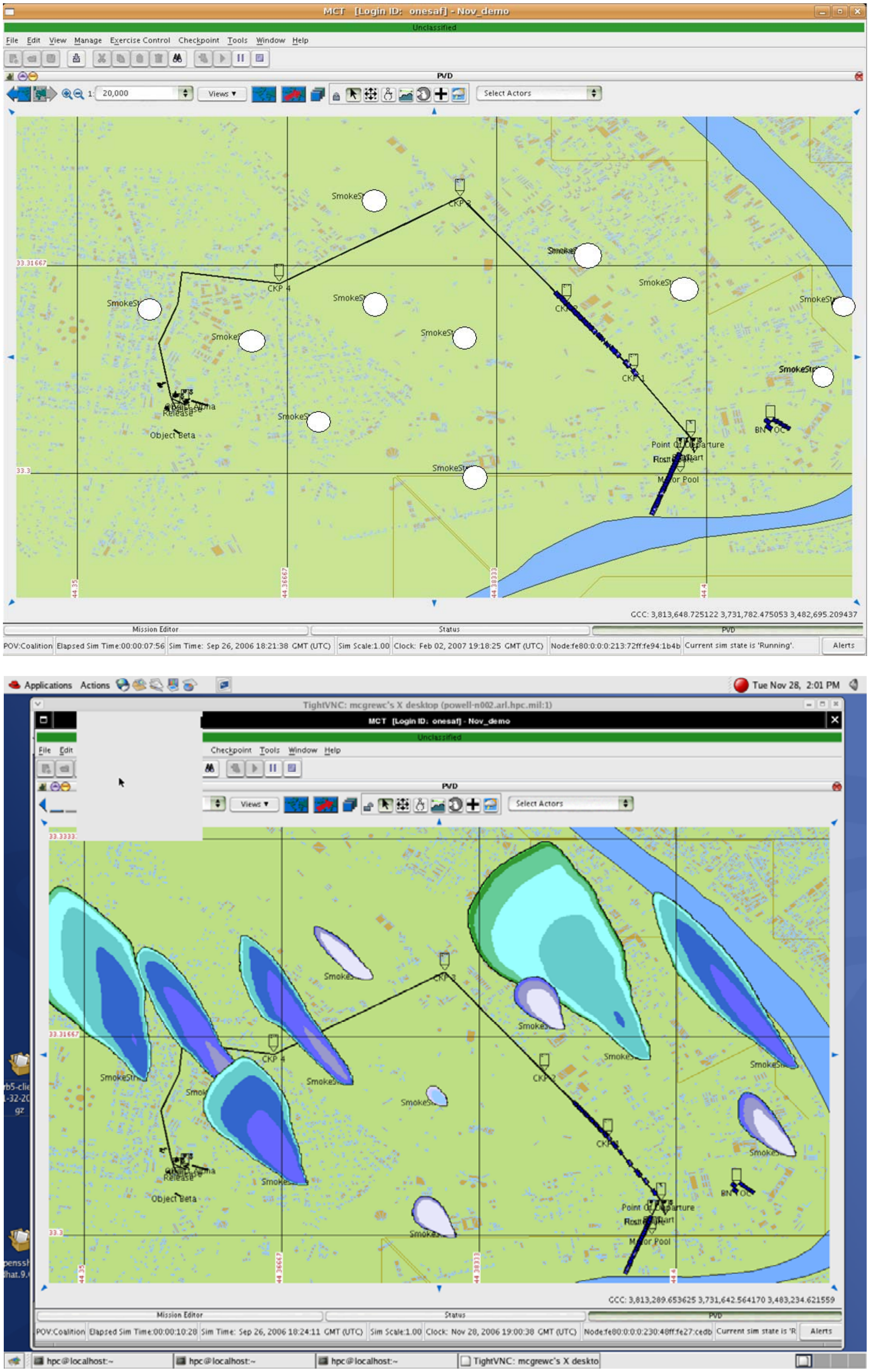


Figure : OneSAF depiction of plumes using their standard plume model (Top) vs. CT-Analyst Plumes (Bottom)

Title: Applications of FEFLO Incompressible Flow Solver
Author(s): R. Ramamurti
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

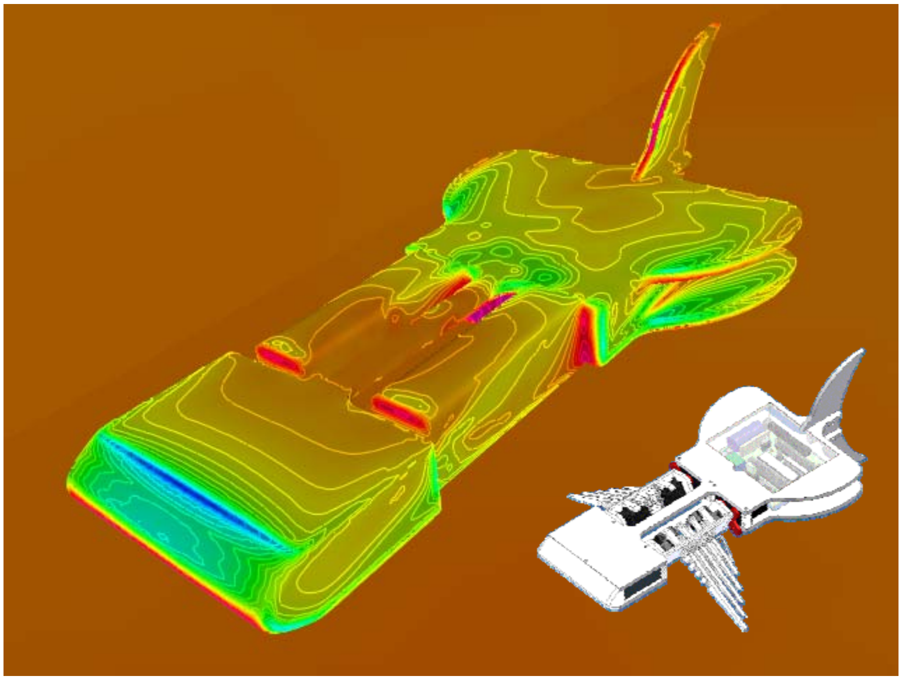
Computer Resources: SGI Altix [NRL, DC]

Research Objective: Perform three-dimensional (3-D) numerical simulations of flow past complex configurations. The proposed studies will investigate the mechanism for the thrust and lift generation and enhancement flapping wings/fins in insects and fishes and apply it UUVs.

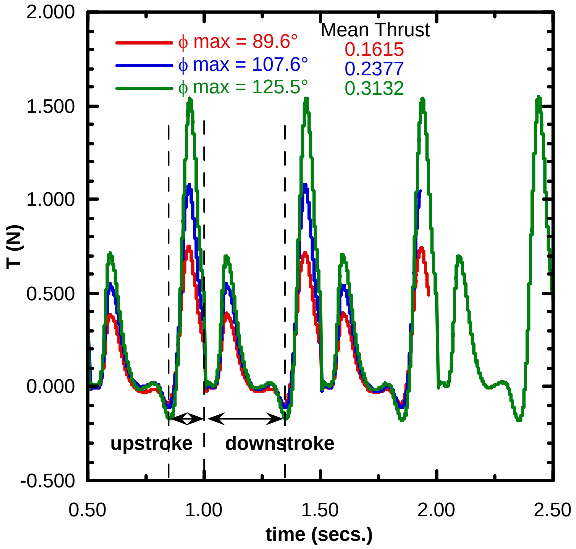
Methodology: An implicit finite element solver, called FEFLOIC, for 3-D incompressible flows based on unstructured grids is used. The flow solver is combined with adaptive remeshing techniques for transient problems with moving grids and is also integrated with the rigid body motion in a self-consistent manner which allows the simulation of fully coupled fluid-rigid body interaction problems of arbitrary geometric complexity in three dimensions. The motion of the wing/fin is prescribed from experimental observations.

Results: An application of flapping foils propulsion that was studied extensively last year is for a notional UUV with the deforming fin. The lift, drag characteristics of a UUV under development were mapped out for several angles of attack and side-slip conditions. In order to develop the controller for the notional UUV we need positive lift generating kinematics. To achieve this, several computations were performed on a notional vehicle at 1kt with a flapping fin at 2Hz, varying the amplitude, starting location of the fin and the flexibility of the fin.

Significance: Simulations have enabled characterization of the thrust and lift generation mechanisms in flapping foil propulsion for unmanned underwater vehicles. The flapping foil propulsion has many applications, such as submersible propulsion, maneuvering and flow control and aerodynamics of unconventional MAVs.



Pressure distribution on NRL UUV moving at 2 kts, $\alpha = 20°$.



Effect of amplitude on thrust production of a flapping fin, $f = 2$Hz.

Title: Aerosol Release Experiment
Author(s): Carolyn R. Kaplan
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

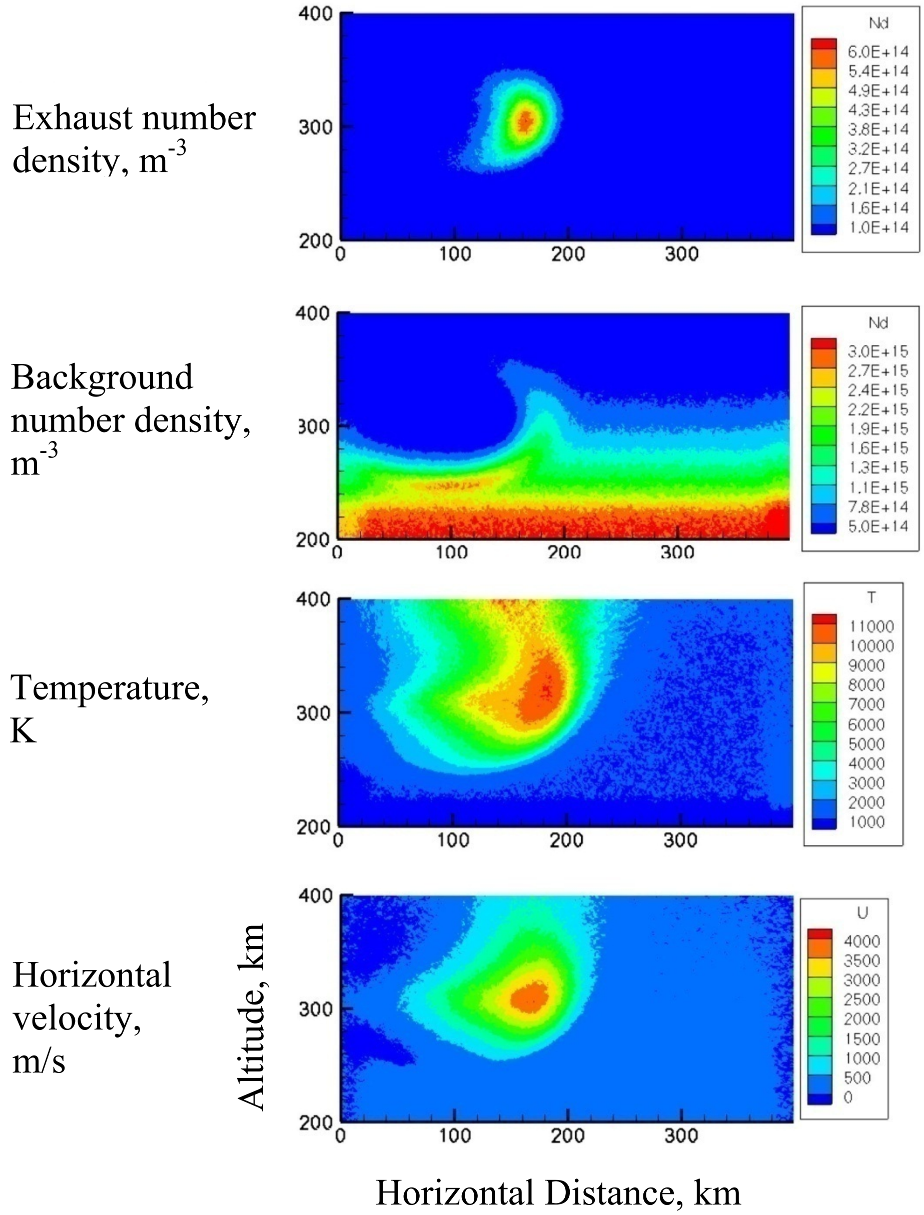
Computer Resources: SGI Altix [NRL, DC]

Research Objectives: Simulations are conducted in support of the NRL Shuttle Ionospheric Modification with Pulsed Localized Exhaust experiments, to study localized ion-beams produced in regions of large relative neutral-plasma convection. The experiments use space shuttle orbital maneuver subsystem engines to inject high-speed exhaust molecules into the ionosphere over ground radar sites, which provide measurements of the resulting ion velocity distributions and plasma turbulence. The simulations are used to reproduce and elucidate the observed ionospheric disturbances.

Methodology: Simulations are conducted using a multi-species, time-dependent, reactive-flow, direct simulation Monte Carlo (DSMC) method. DSMC is regarded as a numerical solution to the Boltzmann equations; it is a statistical method, in which individual molecules are tracked through physical space, and their interactions with other molecules and with surfaces are calculated. The basic algorithm includes the following steps: move molecules, sort/index molecules, allow collisions, and then sample molecules to calculate macroscopic properties. The method assumes that molecular motion is decoupled from molecular collision during each timestep, and that the collision process (where energy is redistributed among kinetic and internal modes) is probabalistic. The DSMC methodology is well-suited for parallelization via domain decomposition. Each processor conducts its own individual DSMC calculation, and communication between processors is only necessary when a molecule crosses processor boundaries. The 3-D code is parallelized, using MPI, and was developed under the HPCMO CHSSI program. It achieves close to ideal fixed-problem speed-up on 64 processors on the Altix.

Results: The shuttle exhaust is composed of water molecules at 120K, injected into the quiescent ionosphere (at 300 km altitude) at a rate of 50×10^{25} molecules/s. The ionosphere initially consists of O atoms at 1000K, where the background atmospheric density decreases with altitude. As observed experimentally by ground radar measurements, the simulations show that the injection of neutral, high-speed shuttle exhaust molecules into the background ionosphere results in large-scale ionospheric disturbances, and in the formation of an ion-ring velocity distribution and corresponding reduction in the density of ambient O atoms.

Significance: Ion-ring distributions are naturally-occurring phenomena in space. These calculations (and the experiments they support) focus on the artificial generation of ion-ring velocity distributions, and are intended to simulate the naturally-occurring phenomena. Insight into the mechanisms of their formation and destruction is important to better understand the physics of space plasmas.



Simulations were conducted in support of the Shuttle Ionospheric Modification with Pulsed Localized Exhaust (SIMPLEX) experiments. In these experiments, exhaust from the space shuttle Orbital Maneuvering Subsystem engines was injected into the ionosphere to produce ion-beams (mainly H_2O^+), and charge exchange with the ambient O^+ ions results in an unstable velocity distribution and plasma wave generation. These images, from a direct simulation Monte Carlo calculation, show the interaction between the neutral shuttle exhaust and background ionosphere, at 30 seconds after the release.

Title: Dynamics of Coronal Magnetic Fields
Author(s): C. R. DeVore[1], S. K. Antiochos[1], J. T. Karpen[1], J. A. Klimchuk[1], M. G. Linton[1], B. J. Lynch[2] and B. T. Welsch[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]University of California, Berkeley, CA
CTA: CFD

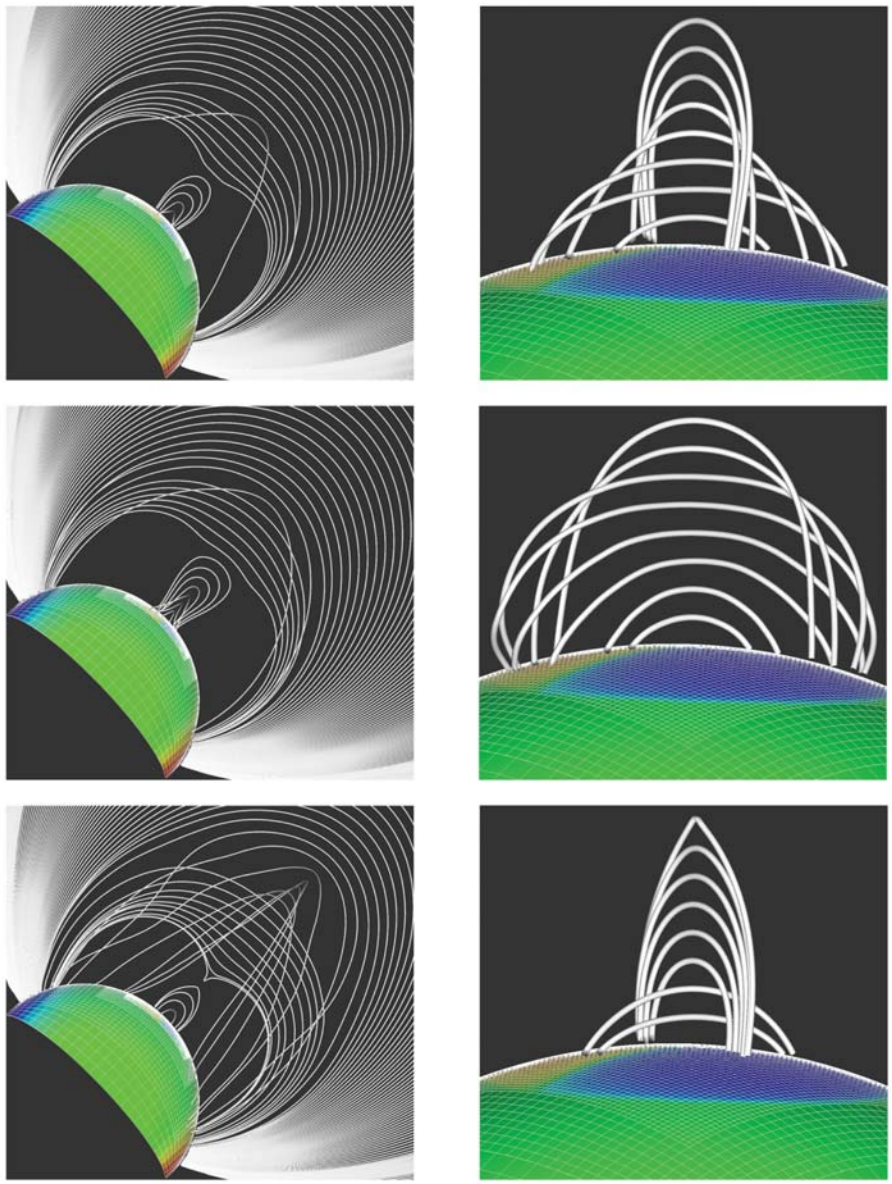
Computer Resources: SGI Origin [ASC, OH]; Cray XT3, SGI Origin [ERDC, MS]; Cray XD1 [NRL, DC]

Research Objectives: Magnetohydrodynamic simulations were conducted on multiprocessor computers of the evolution of magnetic configurations that serve as prototypes for solar activity. The objective is to improve our understanding of the dynamics of solar magnetic reconnection, coronal mass ejections, flares, and coronal heating. Resources also were used to enhance and test our state-of-the-art model for performing these complex simulations using adaptive meshing techniques.

Methodology: The numerical model, ARMS (Adaptively Refined Magnetohydrodynamics Solver), is a magnetohydrodynamics code that solves conservatively the evolution equations for mass, momentum, energy, and magnetic flux densities in three spatial dimensions and time. It uses a finite-volume formulation of the equations and flux-corrected transport (FCT) techniques to advance the variables. ARMS also employs techniques of adaptive mesh refinement, in which the grid adapts dynamically to the evolving solution for maximum efficiency and resolution. Our massively parallel implementation exploits distributed-memory systems via message-passing interface (MPI) communications.

Results: We attained several noteworthy computational milestones in our research program this year. The most dramatic success was the demonstration of simulated solar eruptions driven by very simple boundary motions within our nonlinear, time-dependent, three-dimensional ARMS model. An example is shown in the included figure, in which color shading shows the strength and sign of the Sun's radial magnetic field at the surface, white lines on the surface show the adapted numerical grid, and white cylinders reaching out into near-Sun space are magnetic field lines. The magnetic configuration consists of the Sun's background field, concentrated near the north and south poles, with an embedded pair of sunspots positioned at the equator. Clockwise rotational motions applied to both sunspots introduce the highly concentrated stretching of the field lines – 'magnetic shear' – evident in the top right panel. The excess magnetic pressure at low altitudes associated with this shear eventually overwhelms the magnetic tension in the overlying field lines at high altitudes. Eruption occurs when the sheared field lines suddenly rise rapidly into the high corona, as seen in the middle panels. Below the ejecta, the vertically very elongated field lines break and reconnect due to the resistivity of the coronal plasma. On the Sun, the resultant heating gives rise to flare hard radiation and particles. In our model, the reconnection also reforms the original magnetic structure, as seen in the bottom panels, which sets the stage for future such eruptions so long as the sunspot rotational motions continue. This demonstration is a true breakthrough for our science efforts and for the military and civilian space-weather communities, who seek to develop a fundamental understanding of violent solar events of this type that eventually will lead to improved forecasting and mitigation techniques.

Significance: Dynamical phenomena that affect the Earth and its near-space environment originate in the activity of magnetic fields in the Sun's corona. The Navy's interest in these matters stems principally from its reliance on space-based communications, navigation, and surveillance systems. Energetic particles and hard radiation also pose medical hazards to high-altitude pilots and astronauts in orbit.



A Simulated Solar Storm. Evolving magnetic field lines in a magnetohydrodynamic simulation of a solar eruption. Left: global view, right: close-up view of the source region. The time sequence is eruption onset (top); outward acceleration to high speed accompanied by rapid expansion of the inner structure (middle); and deceleration to rest with source reformation for subsequent eruptions (bottom). [C. R. DeVore *et al*., NRLDC]

Title: Large-scale Blast Simulations for DC-Analyst
Author(s): Douglas A. Schwer and K Kailasanath
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Cray XD1 [NRL, DC]; Linux Cluster [ARL, MD]

Research Objectives: The main research goal of the present HPC project is to study blast and fire suppression using water mist and other potential mitigants in large enclosures with obstructions, and to further the development of a tool that can be used in damage control scenarios. To that end, the fire and blast codes used in previous years are being combined into one tool that can be used for a wide variety of small and large-scale damage control scenarios.

Methodology: The FBM code (**F**ire and **B**last **M**itigation code) is constructed around the PARAMESH library that implements an adaptive mesh refinement procedure and parallelization using the MPI libraries and domain decomposition. Adaptive mesh refinement procedures are used so that fine detailed structure (such as shock waves or shock interactions) can be captured while including a large domain of interest. Built around this base are algorithms that have been used extensively in this lab for flames and blasts, including the Flux-Corrected-Transport (FCT) algorithm for convective transport, the CHEMEQ algorithm for fast chemical kinetics, diffusion, sooting, and radiation models. In addition, multi-phase flows are handled either through an Eulerian-Eulerian formulation known as the sectional approach, or through Lagrangian particle-tracking methods. For the recent research, the multi-phase flow has consisted primarily in the form of water mist for suppression of flames or blast mitigation. However, the models are more general and can be used with other mitigants or fuels. Complex geometric obstructions are handled through a VCE method.

Results: A direct comparison was done for the Eulerian sectional approach and Lagrangian particle-tracking approach for one-dimensional and multi-dimensional shock waves impinging on air seeded with glass particles or water droplets. Results showed that these two methods are nearly equivalent in terms of momentum and heat transfer, and vaporization, as long as enough sections are provided to represent the initial size distribution accurately. Larger differences between the two approaches were seen when droplet breakup was considered. In addition to the high-speed flow computations, low-speed fire simulations were also conducted with the FBM code. These simulations used the barely-implicit-correction-FCT (BIC-FCT) method for convection calculation and the Eulerian sectional approach for the dispersed-phase water droplets. The results from these computations looked at the effect of different mist injection locations on the effectiveness of water mist to suppress small-scale incipient fires.

Significance: These results are significant to the DoD/Navy because the Eulerian sectional approach is considerably more efficient than the particle-tracking approach for these types flooded environments, where water mist or some other multi-phase suppressant is dispersed over a wide area near the fire or blast location. By understanding the limitations of the sectional approach, it can be applied where appropriate to make many scenarios more tractable computationally, while avoiding application in scenarios where it is less appropriate. The fire simulations are significant because it increases understanding of how small fires are suppressed by water mist in realistic scenarios. The results also increase our understanding of how enclosed areas are flooded with water droplets injected using nozzles.

Title: Fine Scale Structure of the Air-Sea Interface
Author(s): Robert Handler and Geoffrey Smith
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: SGI Altix [NRL, DC]; SGI Origin [ERDC, MS]

Research Objectives: The research objectives of this multi-year effort are to understand the small-scale processes at the air-sea interface, to improve understanding of remote sensing signatures, and to improve flux modeling at the interface.

Methodology: The work presented here represents the numerical component of a balanced numerical-experimental research effort aimed at improved understanding of interfacial processes. The work is principally funded by the 6.1 project Non-equilibrium Processes at the Air-sea Interface. We use a pseudo-spectral code which solves the full 3D Navier-Stokes equations. The present version of the code includes buoyancy and surfactant effects.

Results: In FY07 we completed the following: (1) Preliminary development of an atmospheric LES model based on a spectral approach for the 6.1 project Small Scale Processes in the Lower Atmosphere Boundary Layer Using Millimeter-Wave Radar; (2) Performed preliminary LES runs on an idealized problem; (3) Completed the DNS of a sheared interface at three shear based Reynolds numbers (Re = 150,180,220) which represent a range of wind speeds from 2 to 3 m/sec; (4) Performed preliminary statistical analyses of these cases and generated 3D flow visualizations. The LES work is new for this year. In this effort, our ultimate objective is to have an advanced capability to accurately predict small scale turbulence in the atmospheric boundary layer which can then be compared with observations from LIDAR and millimeter wave radar. In our simulations of the air-water interface, the domain is approximately 1 meter long, 0.5 meters in width, and about 7 centimeters in depth. When we compare these results closely with those from an experiment that was performed at the University of Miami in their air-sea interaction laboratory, the agreement was quite good: (1) The cellular nature of the surface was similar in both cases; (2) The surface drift velocities were well predicted; (3) The streak spacing was well predicted. In addition, our DNS results revealed subsurface features such as the coherent vorticity field, which cannot easily be ascertained experimentally.

Significance: The primary Naval application of this work is associated with the development of inverse remote sensing algorithms and the prediction of air-sea interfacial heat, mass, and momentum fluxes. The models developed, along with the simulations, will be used to develop new techniques for interfacial flux measurements. One specific application would be to develop criteria than can be used to determine when and if subsurface wakes can be detected using thermal IR imagery.

Title: Direct Numerical Simulation of Fluid-Sediment Wave Bottom Boundary Layer
Author(s): Joseph Calantoni
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CFD

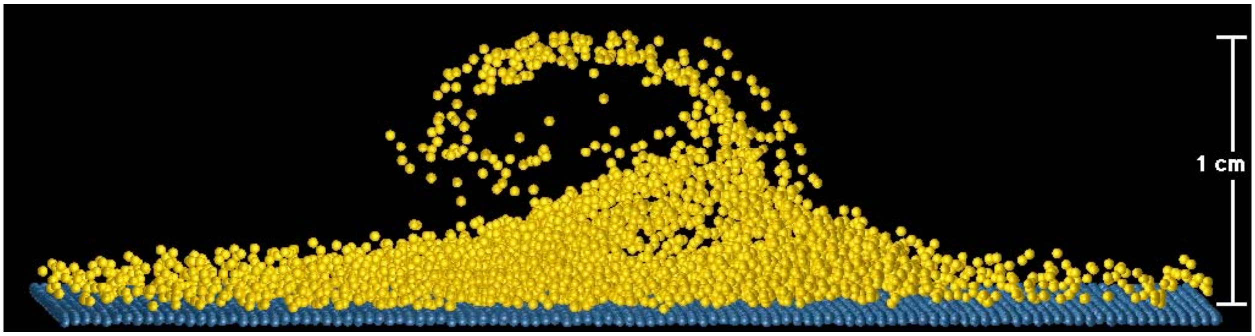
Computer Resources: Cray X1E [AHPCRC, MN]; Cray XT3 [ERDC, MS]

Research Objectives: The desire to develop predictive models for nearshore bathymetric evolution necessitates a better understanding of the physics of fluid-sediment interactions in the wave bottom boundary layer (WBBL). Our long-term objective is to develop robust formulae for predicting bulk sediment transport rates in the nearshore. Since such processes are difficult if not impossible to measure in-situ, we will perform numerical simulations of the two-phase (fluid and sediment) WBBL to improve existing parameterizations for bedload and suspended load transport rates in the nearshore. Fundamental concepts used in describing the phenomena of sediment transport such as the reference concentration, bed failure criterion, and a recently introduced concept of acceleration-induced transport can be addressed with our models. The models produce the high level of detail necessary to refine our present understanding of sediment transport processes and clarify new directions for measurement techniques needed to improve present predictive capabilities.

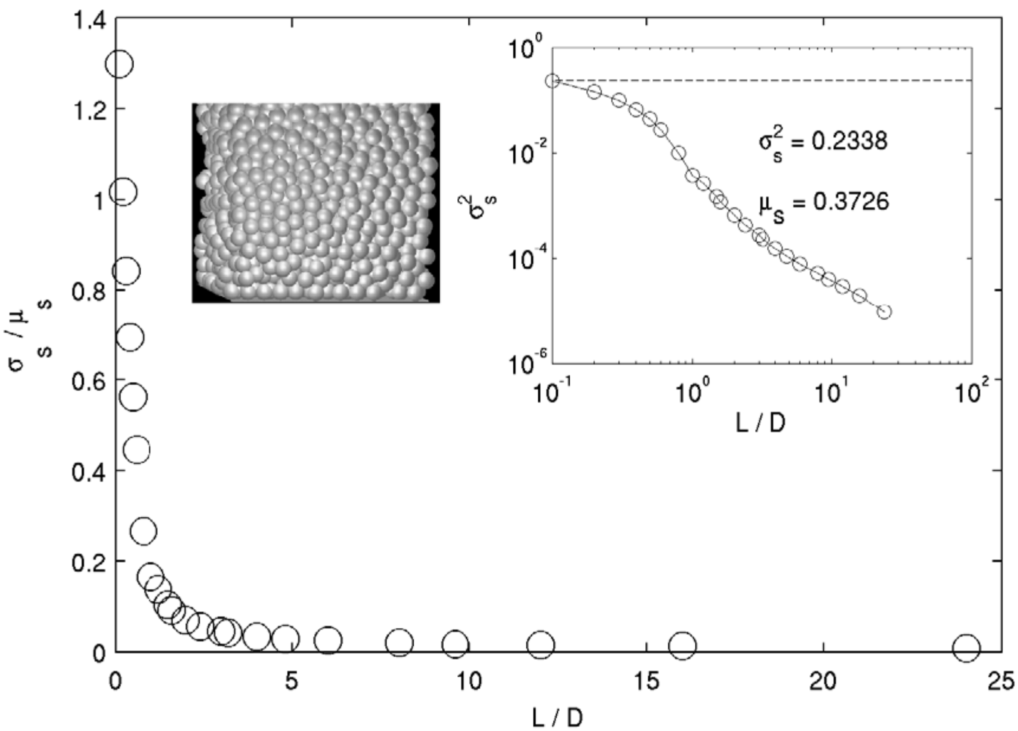
Methodology: Utilization and development of a suite of two-phase WBBL models for simulating sediment transport in the nearshore environment is ongoing with HPC resources. The three-dimensional sediment phase of the flow is simulated with a discrete element model (DEM) that allows individual grains to be uniquely specified (e.g., size, density, and shape). The fluid phase model varies in complexity from a simple one-dimensional eddy viscosity to a fully three-dimensional direct numerical simulation. Coupling between fluid and sediment phases varies from one-way coupling, where fluid flow drives particle motions without any feedback, to a system fully coupled at every fluid time step, where Newton's Third Law is strictly enforced.

Results: The majority of our CPU resources this year have been dedicated to development and testing of new codes. Model development continues along two lines. First, in collaboration with Dr. Donald N. Slinn at the Department of Civil and Coastal Engineering, University of Florida, we have recently implemented a three-dimensional turbulent fluid phase model, which has been successfully coupled to the sediment phase using one-way coupling, where fluid flow drives sediment motion without any feedback between fluid and sediment phases. Work is presently underway to fully couple the new turbulent fluid phase with the sediment phase. Second, the implementation of a parallel version of the DEM using the MPI standard has been successfully accomplished. DEM source code originally provided by colleagues at Sandia National Laboratories has been modified to implement boundary conditions relevant to sediment transport. We performed our largest simulation with over 8.5 million particles on 1440 cores of the Cray XT3 at the ERDC MSRC. Using the Cray Performance Analysis Tools (Cray PAT) we have identified areas of the code to target for optimization. Initial simulations with the parallel DEM have focused on bead packing geometries relevant to studies of acoustic wave propagation and attenuation in marine sediments. The results in the figure show statistics of porosity for random loose packs of spherical glass beads obtained from simulations.

Significance: Ultimately, all process-based models for nearshore bathymetric evolution are limited by shortcomings in fundamental knowledge of sediment transport. Model simulations provide an unprecedented level of detail for the study of sediment transport that is impossible to obtain with available measuring technologies in the field or laboratory. The computational resources consumed were in direct support of NRL base program "Coastal Dynamics of Heterogeneous Sedimentary Environments".



Shown above is a snapshot of particles from a simulation with the new turbulent fluid phase model. Here the particles are near neutrally buoyant (S = 1.03). The image is taken right after the fourth flow reversal of a sinusoidal wave and the formation of a turbulent eddy of about 1 cm in diameter is evident.



In the figure above, simulations were performed with the DEM using spherical particles with a diameter, D = 0.4 mm, having the material properties of glass beads in a vacuum. Particles were settled onto a square plane under the influence of gravity with periodic boundary conditions imposed in the horizontal directions. The particles were piled to form an approximate cube of particles. A series of simulations were performed for cubes of particles with side lengths of 6D, 12D, 24D, 48D, 96D, and 192D. Here we show statistics for the 48D cube simulation containing 132,711 particles with bulk porosity, $\mu_s = 0.3726$. Plotted is standard deviation divided by bulk porosity versus non-dimensional length. The standard deviation was computed over all the porosity values obtained by subdividing the 48D cube into smaller cubes of side length L / D. In the inset (right) porosity variance versus non-dimensional length is plotted with the dashed line indicating the theoretical value of porosity variance, $\sigma^2_s = 0.2338$. The inset (left) is a snapshot of the packed particle configuration for the 12D cube.

Title: Dynamic Phenomena in the Solar Atmosphere
Author(s): Spiro K. Antiochos, C. Richard DeVore and Mark G. Linton
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Cray XT3, Cray X1E [AHPCRC, MN]; SGI Altix, Cray XD1 [NRL, DC]; Cray XT3 [ERDC, MS]; SGI Altix, SGI Origin [ASC, OH]

Research Objectives: The goal of this HPC program is to understand and to model the solar drivers of the violent space weather that disrupts DoD and civilian communications, navigation and surveillance systems. The program is focused on understanding, and ultimately predicting, the physical mechanisms giving rise to the most important solar drivers: coronal mass ejections (CME) and X-class flares. The fundamental question that we are investigating with our numerical simulations is whether magnetic reconnection leads to the giant disruptions of the Sun's magnetic field that constitute a CME/eruptive solar flare event.

Methodology: During the past few years, we have developed a theoretical model for CME initiation: the "breakout" model. The model postulates that an eruption is due fundamentally to the catastrophic breakdown in a magnetic force balance in the solar atmosphere. The outstanding question, however, is the process that triggers the force balance breakdown. During this fiscal year we have made critical progress on several fronts. First we showed how our model operates in a fully 3D system with no symmetries. The eruption was driven by simply imposing a shear flow at the numerical boundary, which represents the solar photosphere. These are the first simulations to obtain a fast eruption in 3D with no questionable assumptions on the boundary conditions. They used ARMS, our state-of-art adaptive MHD code that was developed by the NASA and DoD HPC programs.

Results: With ARMS we simulated the evolution of a multipolar field consisting of a dipole at Sun center and an active region dipole near the surface. The field topology contained the usual fan separatrix with a magnetic null point in the corona. To energize this system, we applied a simple shear flow at the boundary that produced a magnetic structure similar to what is observed in the solar atmosphere, a low-lying filament channel with overlying quasi-potential field. As in our previous 2.5D results, we found that reconnection occurred at the coronal null which allowed the sheared field to "break out" in a fast eruption. The eruption produced a shock in front of the CME. The next step, therefore, is to include a solar wind in the ARMS code so that we can follow the eruption to the field of view of the LASCO and SECCHI coronagraphs, approximately tens of solar radii. Our results to date, however, already show a good qualitative agreement with the coronagraph observations.

In addition to the simulation of the eruption, we investigated the post-eruption magnetic reconnection that constitutes a flare. Observations of solar coronal flares occurring behind CME's have shown down-flowing voids in the corona, which are believed to be the signatures of descending magnetic flux tubes. We used 3D simulations with ARMS to study our hypothesis that these flux tubes have reconnected in the current sheet which forms behind the CME in the high corona. We performed three dimensional MHD simulations of a localized reconnection event in a Y-type post-CME current sheet. The reconnected field creates a downflow which rapidly decelerates as it hits the Y-line and the magnetic loops below it. We compared this deceleration with the observed deceleration of coronal voids when they hit coronal arcades. Our results provide strong support for NRL's EIS experiment on Hinode.

Significance: The numerical results and comparison with observation provide strong support for our breakout model for the origin of coronal mass ejections. Furthermore, our simulations yield important new information on the amount and form of the energy that is released by these explosive events. These results have greatly advanced our understanding of the primary drivers of space disturbances.

Title: MHD Simulations of Flux Cancellation on the Sun
Author(s): Judith T. Karpen, Spiro K. Antiochos, C. Richard DeVore and Mark G. Linton
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Linux Cluster [MHPCC, HI]; Cray XD1 [NRL, DC]

Research Objectives: To identify the energetic, dynamic, and structural signatures of flux cancellation on the Sun.

Methodology: We performed 3D simulations of magnetic flux driven to reconnect near the photosphere. Our finite-difference code with adaptive mesh refinement, ARMS, solves the equations of ideal MHD (with numerical resistivity providing localized reconnection) in Cartesian geometry, via two fully multidimensional FCT modules. The code has been optimized for, and run on, several massively parallel MPI-based architectures. We began these studies by modeling the simplest possible system – a sheared flux tube embedded in a potential arcade in the lower solar atmosphere, driven to reconnect by subsurface flows converging on the polarity inversion line as observed on the Sun. To develop basic physical insight into the interaction between magnetic field and plasma under these conditions, we have begun by modeling cancellation of unsheared flux, by placing the outer radius of the sheared flux below the top of the circulation cells. In FY08 we will model cancellation of sheared flux using the same system but expanding the radius of the sheared flux beyond the top of the circulation pattern. A substantial part of our efforts and computer resources were spent in determining the optimal boundary conditions and system dimensions, and in developing a flow profile compatible with the wide range of subphotospheric properties as well as observed convective motions. We have made two production runs thus far, one strongly driven (but still subsonic) and the other driven at speeds comparable to observed values (horizontal vmax ~ 2 km/s). The following discussion concerns the more slowly driven simulation, as the case more directly applicable to the Sun.

Results: Although the data are still being analyzed, we have already learned much about the cancellation process. Our simulations demonstrate that convective-type subphotospheric flows can drive magnetic reconnection along the polarity inversion line of a finite arcade, resulting in increasingly complex 3D magnetic structure below and above the model photosphere. Plasmoids are generated above the photosphere by 2000 s, first appearing where the converging flows are strongest and later toward the far end of the arcade. Although the field and flow profile initially are highly symmetric, this symmetry clearly has been broken by ~3000 s into the calculation. A significant amount of fine structure develops in the axial direction, showing the importance of considering the full 3D system. In addition, by the end of the run (6000 s) much of the field has acquired substantial shear. We are still deciphering the origin of this shear; although the downflow through the center of the sheared fluxtube eventually transports sheared field to the base of the flow pattern and then upward, insufficient time has elapsed for this process alone to account for most of the observed shear.

Significance: Understanding 3D magnetic reconnection is a high priority for several research areas at NRL, including plasma, space, astro-, and solar physics, and is a Grand Challenge problem for the CFD section of the DoD HPC program. By increasing our understanding of the role played by flux cancellation in restructuring the coronal magnetic field, we enhance the Navy's ability to predict solar activity and longer-term variability with near-Earth and/or terrestrial impact.

CCM

Computational Chemistry and Materials Science

- Quantum chemistry and molecular dynamics methods are used to design new chemical systems for fuels, lubricants, explosives, rocket propellants, catalysts, and chemical defense agents.

- Solid state modeling techniques are employed in the development of high performance materials for electronics, optical computing, advanced sensors, aircraft engines and structures, semiconductor lasers, laser protection systems, advanced rocket engine components, and biomedical applications.

- These computational research tools are also used to predict basic properties of new chemical species and materials that may be difficult or impossible to obtain experimentally, such as molecular geometries and energies, spectroscopic constants, intermolecular forces, reaction potential energy surfaces, and mechanical properties.

Title: Gravitational Effects of Evaporation in Long Atomic Guides
Author(s): Spencer E. Olson and Fredrik K. Fatemi
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: Cray XD1 [NRL, DC]

Research Objectives: The goal of this work is to simulate evaporative cooling in exotic atom traps, including long, high-magnetic-field-gradient atom guides as well as blue-detuned all-optical traps. As an ensemble of atoms is cooled via evaporative cooling to temperatures far below the laser-cooling limit, it can undergo a phase transition into what is known as Bose-Einstein condensate (BEC). In this state, the quantum-mechanical properties of the ensemble become dominant and can be used to perform ultra-high precision sensing measurements. There are two directions that we are exploring with this computational work. First, we seek to find a best strategy to establish steady-state evaporative cooling in atomic guides for the purpose of continuous generation of BEC. Second, we explore evaporative cooling with atoms in all-optical traps formed by manipulating low-power lasers that are narrowly blue-detuned from atomic resonance. While spontaneous scattering in semi-near-resonant laser fields poses a particular problem, it should be mitigated by the fact that as atoms are cooled much less of the light is sampled by the ensemble.

Methodology: To simulate evaporative cooling of atoms in various trapping potentials, we employ a gridless implementation of direct simulation Monte Carlo (DSMC) developed by S. E. Olson. The gridless strategy abstracts the DSMC algorithm from the physical system and allows the code to be applied easily to arbitrary trapping potentials. Because of the computationally intensive nature of gas dynamics simulations, parallel computation has become standard. For the simulations of this work, HPC resources are used to obtain results within an acceptable length of time and statistical error rate. The abstraction of gridless DSMC enables an automatic and very scalable parallel algorithm to be wrapped around base code. The parallel wrapper, implemented with MPI, automatically adjusts the load balance of the groups of processes to minimize the total wall-clock time for a particular run. Because only nearest neighbors are allowed to talk, this parallel approach minimizes overhead and can attain a very high efficiency even with large numbers of processors as described by S. E. Olson.

Results: The results of these simulations have proven helpful in understanding evaporative cooling in both atom guides as well as semi-near-resonant blue-detuned traps. For atom guides, a set of five basic evaporation strategies, shown in Figure 1(a), were simulated to demonstrate, as shown in Figure 1(b), a promising evaporation strategy for creating steady-state BEC. For blue-detuned traps, simulations show that an ensemble, initially in the |F = 2i hyperfine state with T = 10 μK, can be efficiently cooled via evaporation (Figure 2). In addition, the forced evaporation tends to severely dampen the state changing photon scattering, as indicated by the stalled |F = 3i state growth in Figure 2. While the degeneracy in states tends to bring the |F = 3i fraction to 7/12, the evaporative cooling process stalls the state-changing events such that |F = 3i growth is held to ~ 10%. We have furthermore successfully compared simulations of state-changing off-resonant scatter in exotic blue-detuned traps to experimental results.

Significance: DOD/Navy interest in this work lies in the precision measurements that are made possible through the use of cold-atom systems. One of the best known applications of cold atomic physics is the precision measurement of time in atomic clocks. Although work on atomic clocks in the cold-atom physics community continues, a large effort, funded by DARPA and other DOD research entities as well as non-DOD entities, has shifted to focus on development of precision metrology of acceleration fields including magnetic, electric, and gravitational fields. Such measurements rely on the large coherence possible between quantum-mechanical states of cold atoms. This work seeks to contribute to the community effort by developing new and improved methods of obtaining ultracold atoms and BEC.

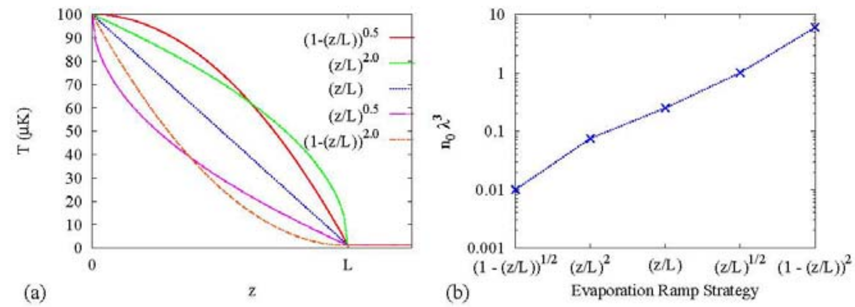


Figure 1: (a): Evaporation strategies. The curves here depict the approximate temperature that can be supported as a result of the variable evaporation threshold. By lowering the threshold in the forward direction, a forced evaporative cooling is imposed. (b): Final phase space density $n\lambda_{th}^3$ of the different evaporation strategies.

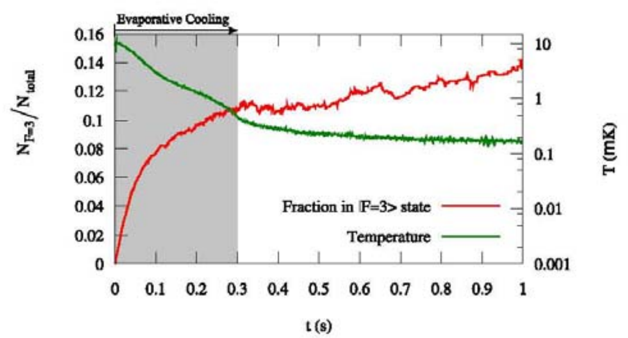


Figure 2: State population and temperature dependence of atoms trapped in a crossed, hollow-beam, blue-detuned trap during forced evaporative cooling. The evaporation threshold is lowered linearly in time for times $0 \leq t \leq 300$ ms.

Title: Molecular Dynamics Simulation Studies of Intra- and Intermolecular Forces in Biological Systems
Author(s): Jeffrey Deschamps[1] and Alexander D. MacKerell, Jr.[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC, [2]University of Maryland, School of Pharmacy, Baltimore, MD
CTA: CCM

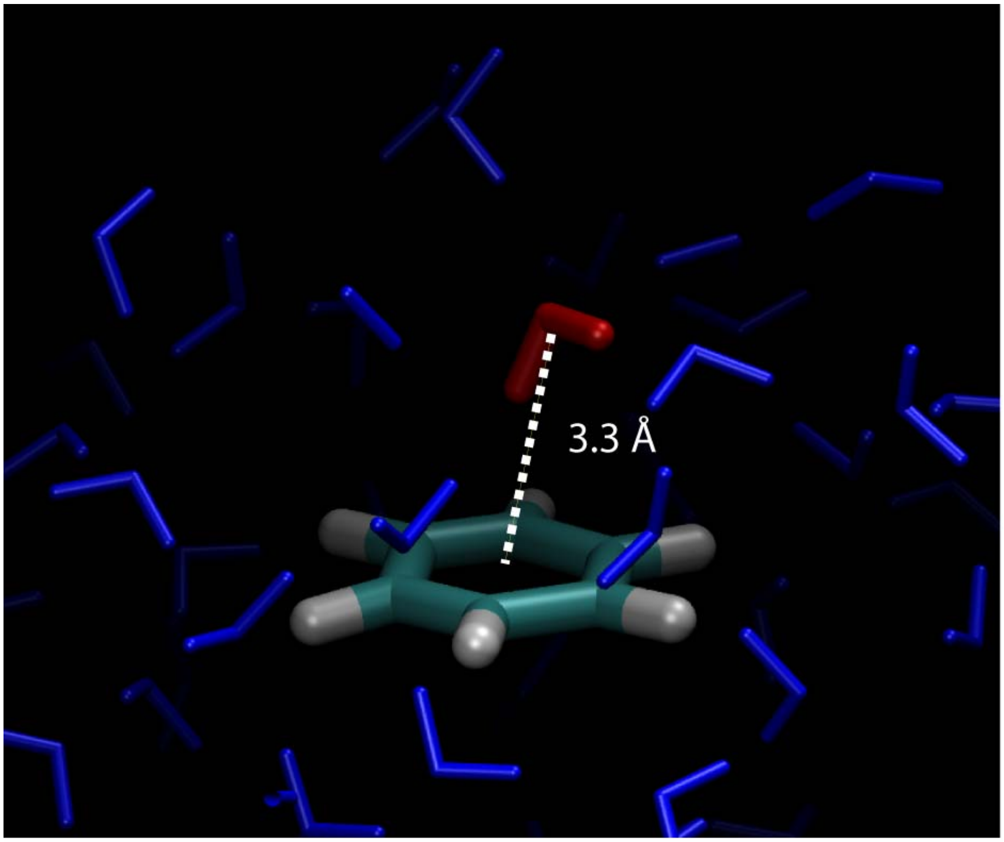
Computer Resources: SGI Origin, SGI Altix [ASC, OH]; Cray XD1 [NRL, DC]; Linux Cluster [MHPCC, HI]

Research Objectives: Molecular dynamics (MD) and quantum mechanical (QM) theoretical approaches were applied to obtain atomic details of the relationship of structural and dynamical properties to activity and reactivity of biological molecules, including opioids, proteins, DNA, RNA and lipids.

Methodology: QM and MD methodologies were used to study the chemical, structural and dynamical properties of selected molecules. QM studies were performed using the Gaussian suite of programs with optimizations performed to default tolerances. MD simulations were performed using the program CHARMM with empirical force fields developed as part of our ongoing research program. CHARMM runs in parallel on the SGI's, the Dell Cluster and the Cray XD1 architectures using MPI. Empirical force field development included a novel approach that treats explicit treatment of electronic polarization via a classical Drude oscillator. MD simulations were performed with both an explicit solvent representation, including counterions, in the presence of either periodic boundary or stochastic boundary conditions and using an implicit solvent model based on the Genearlized-Born Approximation.

Results: Significant advances have been made in empirical force field developments as well as in our studies of protein, DNA, RNA and opioid structure-function relationships. Developments in the additive force field involved progress on a comprehensive carbohydrate force field including QM calculations on tetrahydropyrans that will act as target data for the optimization. Optimization of the pyranose parameters is complete and the majority of QM calculations have been completed for the discaccharide portion of the force field. Significant progress was made in the context of the polarizable force field where parameters optimization has been completed for alcohols, ethers and aromatic compounds. This represents a significant step towards development of a comprehensive FF for biomolecules. With respect to the opioids, we completed development of a novel methodology to quantitatively predict efficacies and binding affinities of both traditional opioids and peptidic opioids. In addition, MD simulations were performed to understand the conformational properties of peptides designed to bind to quantum dots.

Significance: Computational studies of macromolecules via empirical force fields is a field what continues to rapidly grow. The empirical force fields being optimized as part of these ongoing studies will significantly impact this growing field allowing for more accurate calculations on a wider range of molecules. In particular, our development of a polarizable force field for macromolecules is yielding novel insights into microstructure details of the interactions of these molecules as well as setting the standard for the future development of polarizable force fields. The opioid studies represent an extension of our conformationally sampled pharmacophore (CSP) approach that will greatly increase its utility allowing for predictions of both binding affinities and efficacies. The CSP method has been used in a number of laboratories throughout the world and the development of the quantitative CSP should further increase the general utility of the method.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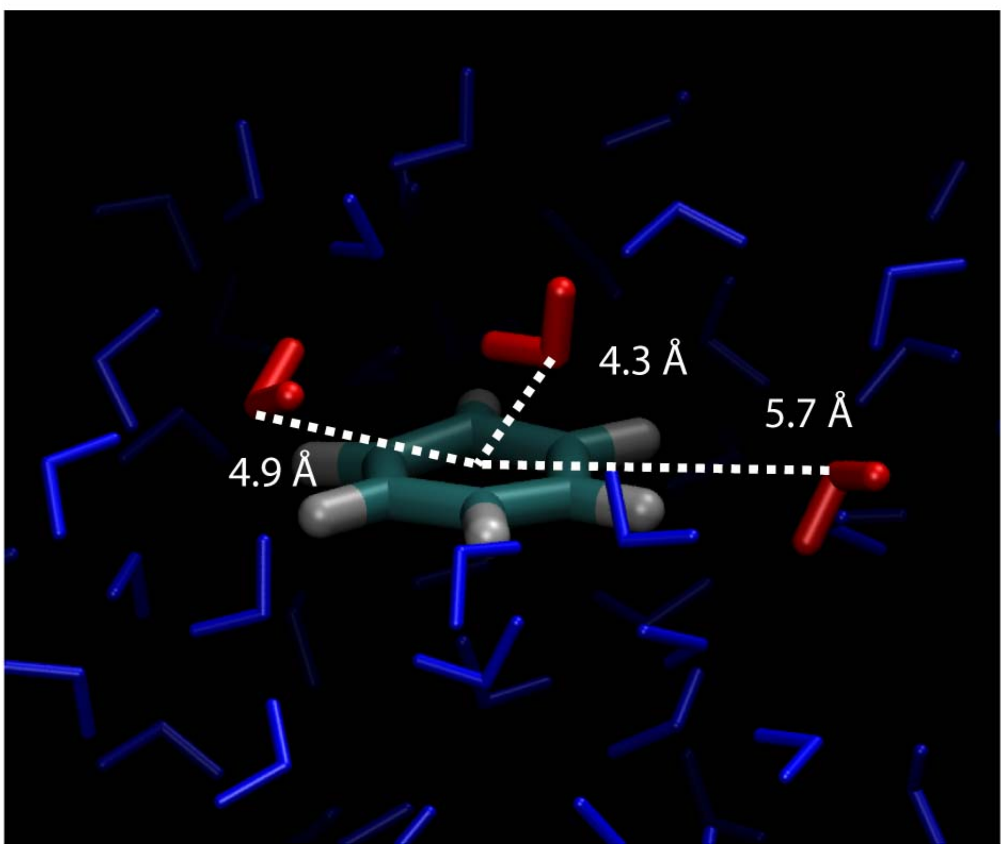
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Title: Structural Chemistry
Author(s): Jerome Karle and Lulu Huang
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI Origin [ASC, OH]

Research Objectives: Calculating Drug target interaction energies by the Kernel Energy Method

Methodology: *Ab initio* quantum mechanics is applied to obtain the interaction of drugs and their molecular targets, including peptides, proteins, DNA, and RNA, obtaining results of high accuracy. In this approach the computational difficulty of representing a molecule increases only modestly with the number of atoms. The calculations are simplified by adopting an acceptable approximation that allows a full biological molecule to be represented by smaller "kernels" of atoms. These results suggest that problems of medicinal chemistry, such as the rational design of drugs, may be illuminated by quantum mechanical analysis.

Results: The general case is illustrated by specific examples, namely, the HF/STO-3G calculations of three aminoglycoside drugs that attach to ribosomal A-site RNA nucleotide targets.

Significance: We have shown how to begin with a crystal structure and obtain there from quantum mechanical information not otherwise known, from the structure alone. Such information includes the energy of the structure, the interaction energy between a drug and its target, and the analysis of such interaction energy in terms of the contribution of each contributing kernel pair. The accomplishments of this work allow the relative importance of individual kernels to the drug interaction energy to be assessed. And, that is very useful for designing and developing new drugs.

Title: Water Mist Behavior in Fire Environments
Authors(s): James W. Fleming[1] and David Gilinson[2]
Affiliations(s): [1]Naval Research Laboratory, Washington, DC, [2]University of Maryland, College Park, MD
CTA: CCM

Computer Resources: SGI Origin, SGI Altix [ASC, OH]

Research Objectives: This project seeks to understand the suppression and flow behavior of water mist in flame environments as a function of water drop size and number density, drop size distribution, mist delivery configuration, environmental conditions including flow and temperature fields, and fire/thermal field interactions.

Methodology: The commercial CFD package FLUENT was used to design and model the flow field in a slot burner in order to optimize this burner geometry for optical diagnostics.

Results: We performed cold fuel/air/nitrogen flow computations on two grids: one grid simulating a conventional Wolfhard-Parker slot burner (burner with central fuel slot with parallel air slots on each side) and one grid simulating the same burner with additional purge flows at the ends of the fuel slot. At the fuel/air intersection at the ends of the fuel slot in a conventional Wolfhard-Parker slot burner, the existence of edge flames complicate the ability to carry out laser-based absorption experiments in this burner. These computations explored burner design conditions that could minimize the edge flame effects on the central main flame. We used the computational results to guide the design choice of purge slot width dimensions and nitrogen purge flow rate for optimal edge flame minimization with minimal impact on the primary slot burner flame. Future computations will complement experimental studies where water drops are added to the air flow in this burner to understand water drop flow behavior and flame suppression effectiveness.

Significance: The Department of the Navy is committed to water mist technology for all future ship classes and current ships where feasible. Ship yards need guidance for water mist fire protection system design. It is imperative for the Navy to optimize water mist systems so economy of ship design can be addressed for ships currently approved for construction and for future ship construction. Research is needed to optimize the design of these systems to maintain ship operability and crew safety. The project will bring an improved understanding of water mist fire suppression capabilities in order to expand this key technology to a greater number of DoD arenas requiring fire protection.

Title: Maintaining MBD-5 CHSSI codes for DFT Calculations Using Symmetry and Variational Fitting
Author(s): Brett I. Dunlap
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: Cray XD1, SGI Altix [NRL, DC]

Research Objectives: Develop fast and accurate density-functional calculations using variational fitting to reduce the formal rate at which the calculations scale to the cube of the number of occupied orbital's and to use completely analytic matrix elements to allow arbitrary accuracy.

Methodology: The codes solve the DFT equations using Gaussian basis sets to fit both the orbitals and the Kohn-Sham potential. The fits are robust, i.e., they do not change the energy to first order in the fitting error, and all linear-combination-of-atomic-coefficients are determined by variation. NRL's Solid-Harmonic-Gaussian DFT (SHGDFT) code [B. I. Dunlap J. Phys. Chem. A 107, 10082 (2003)] uses point-group symmetry most efficiently and computes forces efficiently using the solid-harmonic basis and generalized Gaunt coefficients. NRL's Helical Nanostructures (HENS) code [J. W. Mintmire, "Local-Density Functional Electronic Structure of Helical Chain Polymers," in Density Functional Theory Approaches to Chemistry, Eds., J. K. Labanowski and J. W. Andzelm, (Springer-Verlag, 1991), pp. 125-136] can efficiently compute the electronic structure of all carbon nanotubes by explicitly treating only the rotationally equivalent atoms of the first unit cell and the helical operation.

Results: Computed the sum-over-states polarizibility of fullerenes and fullerene onions up to C_{2160}.

Significance: Discovered that perturbation theory can be done in analytic density-functional theory at N^2- rather than the standard N^4-cost in methods that index arrays via particle-hole excitation.

Title: Simulation and Design of Molecular Scale Materials
Author(s): Mark R. Pederson[1], Tunna Baruah[2], Steven Richardson[3], Rajendre Zope[1] and Reeshemah Allen[1]
Affiliation(s): [1]Naval Research Laboratory, Washington DC, [2]Department of Physics, University of Texas El Paso, [3]Howard University, Washington DC
CTA: CCM

Computer Resources: Linux Cluster [ARL, MD]; SGI Altix [NRL, DC]

Research Objectives: Apply and further develop in-house density-functional-based (NRLMOL) molecular simulation package to problems of importance to the DoD mission.

Methodology: In-house density-functional-based molecular-simulation software (NRLMOL and MPNRLMOL) is used to analyze and predict the properties of molecular-assembled materials and nanoscale devices. For an arbitrary assembly of atoms, the optimal gaussian-type-orbital expansion of the Kohn-Sham orbitals is determined and the forces on each atom are calculated. The molecular geometry is then iteratively updated using either generalized conjugate-gradient methods or through the solution of Newton's equations. Details of the methodology include the analytical determination of the effective potential on a numerical integration mesh. Given the values of the potential and basic functions on this mesh, accurate numerical integration allows one to determine all matrix elements needed for construction of the secular equation. Standard matrix algebra methods are currently used to solve the secular equation. Once the wavefunctions for the electronic degrees of freedom are obtained, many properties are calculated using a variety of NRLMOL post-processing methods. These properties include interatomic forces, vibrational energies, electron-phonon interactions, magnetic anisotropies, exchange energies, radiative transition rates, approximate excited state energies, van der Waal's attractions and other polarizable phenomena.

Results: Work has continued toward more detailed understanding of the role of polarizabilities in nanoscale molecules. For example, we have carried out a detailed investigation of static dipole polarizability of lithium clusters containing up to 22 atoms. We have built a database of lithium clusters by optimizing several candidate structures for the ground state geometry for each size. The full polarizability tensor was determined for about 5-6 isomers of each cluster size using the finite-field method. In addition we have performed calculations on the polarizability of an organic photovoltaic molecule and shown that shown that the polarization effects on the charge transfer excitions are expected to be very large. Work on two new types of molecular magnets has been initiated. In one case the magnetic response of the materials suggests that there is a field-induced rearrangement of a Ni-Mo cage structure. For this study we have performed calculations on the vibrational spectra and calculated the exchange parameters as a function of distortion. In another case, we have studied a Mn-based molecular magnet to determine the lowest lying spin state of the molecule. Publications on these results are forthcoming. Work on the ultraviolet photoemission spectra of large organic donors is also in progress.

Significance: The properties of molecules and their interaction with the environment are of fundamental importance to many technologies being developed for future naval applications. These include possible nano- and molecular-scale devices for: (1) sensing, (2) energy conversion and storage, (3) information processing and archival and (4) medical applications. As methodologies for molecular-material prediction mature, the concept-to-delivery time lag will continue to decrease.

Title: Growth and Control of Metal Films on Semiconductor Substrates
Author(s): S.C. Erwin
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI Altix, HP XC Cluster [ASC, OH]

Research Objectives: To investigate the the fundamental physics of semiconductor surfaces.

Methodology: This computational research is based on the generalized-gradient approximation (GGA) to density-functional theory (DFT). Semiconductor surfaces exhibit strong distortions (.reconstructions.) from ideal structures. For this reason, the most appropriate approach for the problems studied here is the pseudopotential planewave method, as implemented in the VASP code.

Results: We used density-functional theory to study the structure of III-Sb (001) (III = Al or Ga) surfaces. Based on a variety of reconstruction models, we constructed surface stability diagrams for AlSb and GaSb under different growth conditions. For AlSb (001), the predictions are in excellent agreement with experimentally observed reconstructions. For GaSb (001), we showed that previously proposed model accounts for the experimentally observed reconstructions under Ga-rich growth conditions, but fails to explain the experimental observations under Sb-rich conditions. We proposed a new model that has a substantially lower surface energy than all ($n \times 5$)-like reconstructions proposed previously and that, in addition, leads to a simulated STM image in better agreement with experiment than existing models. However, this new model has higher surface energy than some of (4×3)-like reconstructions, models with periodicity that has not been observed. Hence we conclude that the experimentally observed (1×5) and (2×5) structures on GaSb (001) are kinetically limited rather than at the ground state.

Significance: The surfaces and interfaces of III-V semiconductors constitute some of the most important components of the semiconductor industry. For example, III-V heterostructure quantum wells are key components in a wide range of optical and high-frequency electronic devices, including field-effect transistors, resonant tunneling structures, infrared lasers, and infrared detectors. Many of these devices require extremely sharp and clean interfaces. For this reason, an understanding of the atomic-scale morphology of III-V semiconductor surfaces is critical to controlling the growth and formation of their interfaces.

Title: Structure, Formation, and Diffusion Mechanisms in Nanostructures and Thin Films
Author(s): Michelle Johannes
Affiliation(s): Naval Research Laboratory, Washington DC
CTA: CCM

Computer Resources: SGI Altix, HPC XC Cluster [ASC, OH]

Research Objectives: The main objective is to investigate the atomic structure, dynamics, and diffusion present in metal and semiconductor nanostructures, i.e., thin films, nanocrystals and nanowires. The nanostructure energetics, structure and diffusion will be analyzed, and the thermodynamics and diffusion mechanisms that account for these properties will be elucidated. From this information methods to produce nanostructures with desired features will be developed.

Methodology: The first-principles VASP code is used to calculate the structural energetics and simple diffusion processes in relatively small or symmetric systems. Moderate to large size simulations are approached through the tight-binding method. In these cases the NRL tight binding molecular dynamics (NRL-TBMD) code is utilized to simulate atomic motion or calculate structural energies.

Results: Density functional and tight binding simulations of fcc metallic structures were carried out with the VASP and NRL-TBMD codes to investigate how bond strengths depended on the position of the atoms with respect to surfaces or position inside a metallic cluster. These bond strengths are then used to determine the atomic concentration of different metallic species as a function of position inside bimetallic or trimetallic clusters such as CuRh alloy clusters. The VASP code was also used to calculate the energies of different structural phases of the shape-memory alloy NiTi to form a database for fitting a tight-binding parameterization for this system. This parameterization will be used for molecular dynamics simulations to investigate phase changes in shape-memory nanostructures.

Significance: The behavior of metallic nanoclusters is used for developing new materials with superior mechanical properties (hardness, etc.,) for the Navy. The mechanical properties of shape-memory alloys allows their use in switching, e.g., in actuators, used in electro-optical materials of interest to the Navy.

Title: Quantum Information Processing
Author(s): C. Stephen Hellberg and Kristopher E. Andersen
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

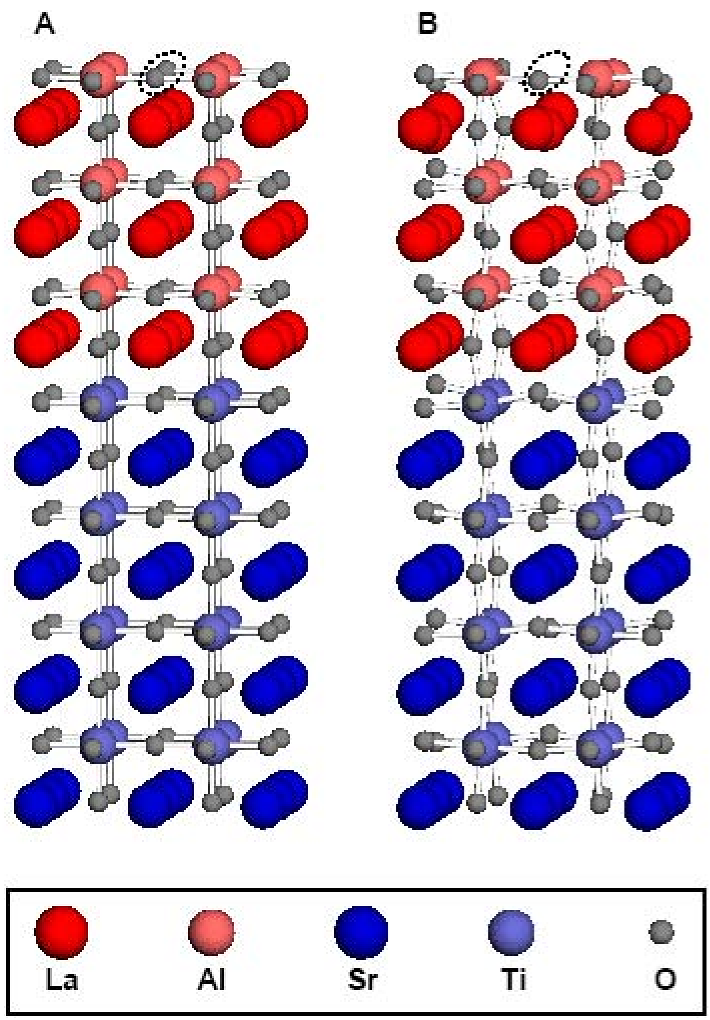
Computer Resources: SGI Altix, HP XC Cluster [ASC, OH]

Research Objectives: To improve nanostructions for quantum information processing and other applications. There has been great interest in growth of complex oxides for device applications. The success of semiconductions as technological materials is based on three important features: (1) their electrical conductivity can be tuned over a wide range; (2) insulating layers (i.e., SiO_2) can be formed readily; (3) devices can be scaled to nanoscale dimensions. Features (1) and (2) have long been present in oxides, but only recently have nanoscale devices been demonstrated in oxides. Our objectives are to understand and optimize nanoscale manipulation of oxides.

Methodology: We used first-principles density functional calculations to determine the ground state structure and electrical properties of $LaAlO_3$ grown on $SrTiO_3$. We used the VASP planewave code at the ASC HPC center. This code allows a system with many atoms (we used up to 423 atoms) to be simulated and, most importantly, relaxed accurately.

Results: We showed that $LaAlO_3$ thin films grown on $SrTiO_3$ have two stable structures: ideal films with no vacancies and films with a high density of oxygen vacancies on the surface. The ideal films have a large internal electric field due to the changed planes in $LaAlO_3$. In the films with vacancies, this field is relieved, resulting in an energy gain. However, there is an energy cost to forming vacancies. We showed that for $LaAlO_3$ films that are 3 monolayers thick (the same thickness used in the experiments) both structures are stable. The ideal films are insulating everywhere. However, the films with vacancies on the *surface* have metallic *interfaces*. This explains how an AFM can be used to write and erase metallic nanowires at the interface between $LaAlO_3$ and $SrTiO_3$.

Significance: The ability to pattern reversibly high-mobility electron gases at nanoscale dimensions provides new ground to develop devices for ultrahigh density information storage and processing. Integration with silicon-based devices is possible, as shown by reports of high-quality $SrTiO_3$/Si heterostructures produced by molecular-beam epitaxy.



Stable structures of a 3 monolayer $LaAlO_3$ film on $SrTiO_3$. (A) ideal film with no vacancies and (B) film with one surface oxygen vacancy per 2x2 unit cells. The oxygen vacancies cause a significant rotation of the oxygen octahedral which propagates deep into the STO. The ideal film is insulating everywhere, while the film with surface vacancies has a metallic *interface*, 3 layers below the surface.

Title: Multiscale Simulations of Material Properties
Author(s): N. Bernstein[1] and D. E. Farrell[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC, [2]Northwestern University, Evanston, IL
CTA: CCM

Computer Resources: SGI Altix, HP XC Cluster [ASC, OH]; Cray XT 3 [ERDC, MS]

Research Objectives: To understand and predict mechanical properties of materials using atomistic simulations.

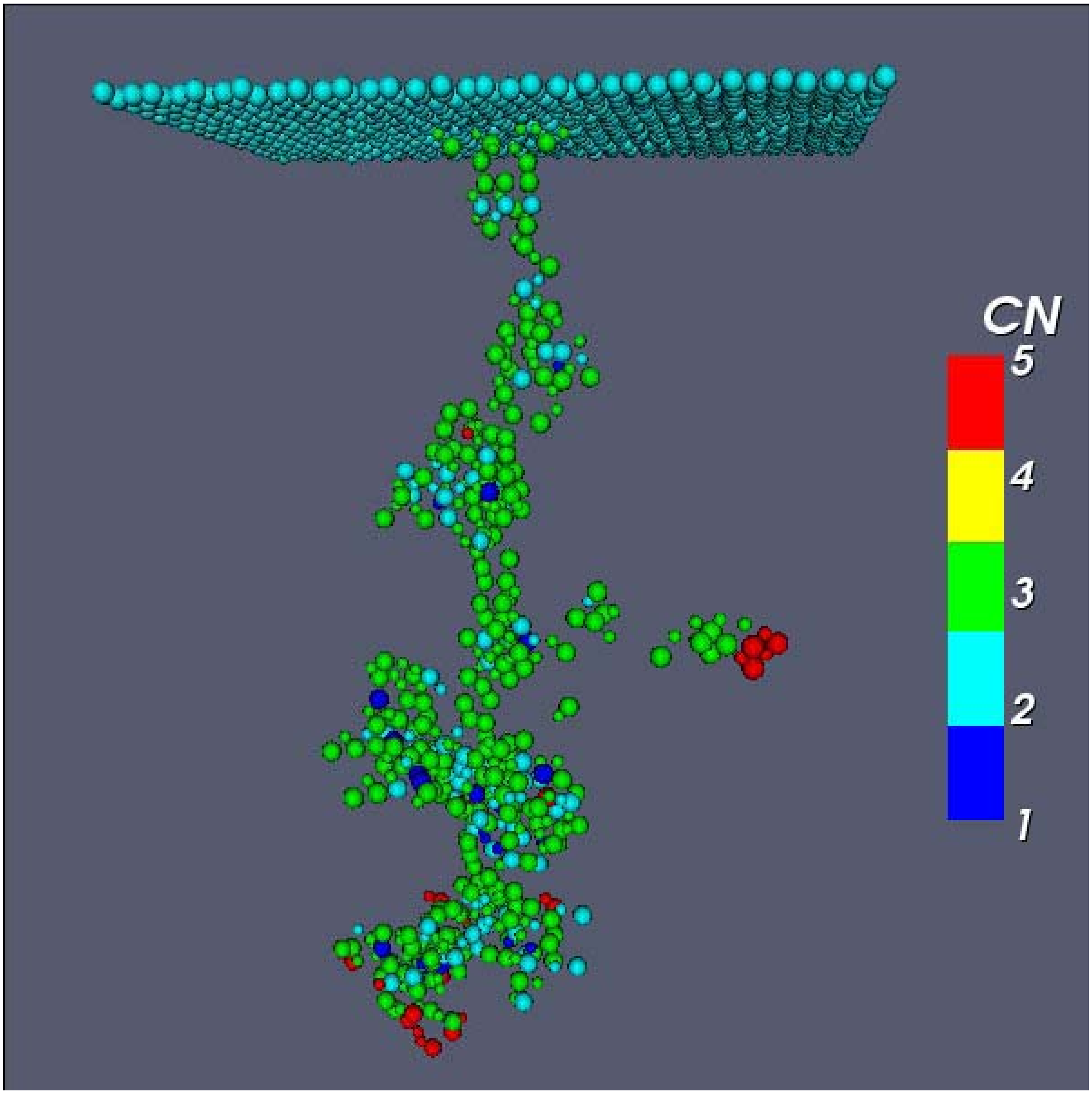
Methodology: Simulations used molecular dynamics (MD) and conjugate-gradient energy minimization with forces from combination of interatomic potentials, tight-binding, and first principles density functional theory. Some simulations were carried out using a single model. Others used coupling of length scales approaches, including LOTF and an energy-conserving local energy mixing method.

Results: Multiscale simulations of Si fracture along the cleavage plane showed an instability that occurs only at low speeds, in contrast to the more widely studied high-speed instabilities. The presence of this instability was confirmed experimentally, where it manifested itself as ridges that form when the crack is propagating sufficiently slowly. A mesoscopic model showed how the atomic scale rearrangement of bonds at the crack tip can lead to macroscopically observable ridges. The same methodology, using the learn-on-the-fly (LOTF) method coupling interatomic potentials with tight-binding and density functional theory forces near the crack tip, was used to simulate fracture in silicon carbide. Initial results show that chemical effects greatly modify the behavior of crack-tip bonds as compared with single component systems such as pure silicon studied before.

Silicon carbide has also been proposed for use as a structural material in neutron irradiated environments. Variable time-step MD was used to simulate the initial stages of material evolution after the impact of an impinging neutron. The system shows the formation of a damaged region (0.1~ps), and the subsequent relaxation and annealing of the point defects formed (10~ps).

Ductile materials such as metals usually depend on dislocation motion to enable plasticity and dissipate energy when the material is under mechanical load. The dislocations can become pinned by inclusions, but can get around them by climbing if point defects such as vacancies are present. The interaction energy of a vacancy in the presence of a dislocation in Al was computed using an embedded-atom type interatomic potential. To improve the accuracy of the calculation, a new method for coupling quantum-mechanical and interatomic potential descriptions of bonding, that enables for the first time accurate forces and conservation of energy in a solid-state system, was developed. Initial results show that the method should work well for the Al-vacancy-dislocation system.

Significance*:* Silicon is a well studied model system for brittle materials, such as the ceramics used in thermal-barrier coatings for engine turbines and as inserts for body armor. The previously unsuspected instabilities we observe in silicon show how atomistic details can affect macroscopic failure modes. Initial results for silicon carbide, and material used in technological applications, show that the complex atomic structure and chemistry will dramatically alter the fracture behavior. Silicon carbide has also been proposed as a first-layer material in fusion reactors, where it would have to maintain its mechanical properties in the presence of extreme heat and neutron irradiation. Metals, are ductile and can therefore be worked and fail gracefully, but some materials such as aluminum must be hardened, for example by the presence of inclusions, to be useful. Plasticity mediating dislocations respond to the inclusions by interacting with point defects such as vacancies. Computing these interaction energies requires an accurate multiscale method that gives well defined local energies, a combination that we have developed for the first time.



Visualization of a displacement cascade after the impact of a neutron into zinc-blende structure silicon carbide. Atoms are colored by coordination number.

Title: Calculation of Materials Properties via Density Functional Theory and its Extensions
Author(s): Michael J. Mehl
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

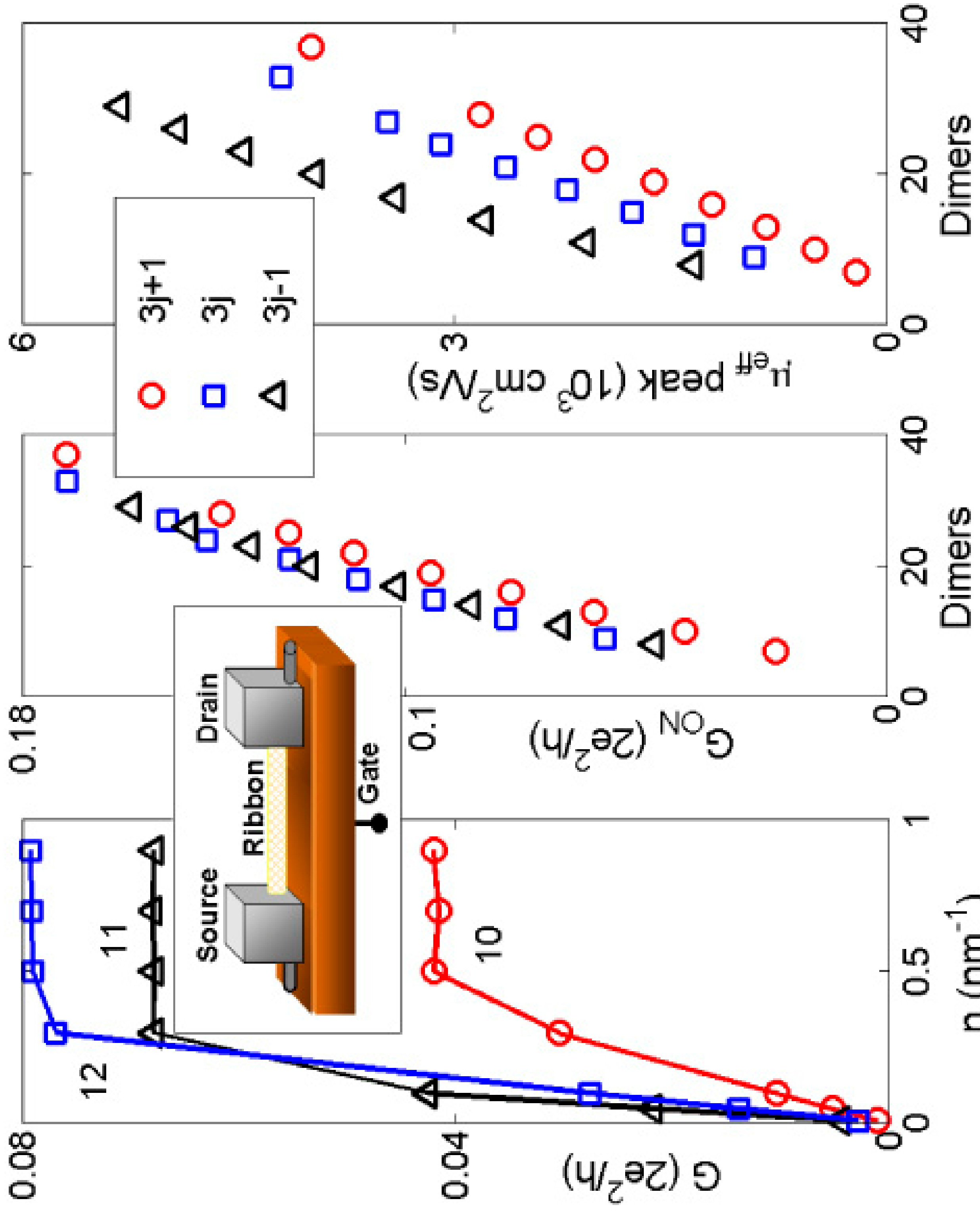
Computer Resources: SGI Altix, HP XC Cluster [ASC, OH]

Research Objectives: The determination of materials properties from accurate first-principles density functional theory (DFT) computations is limited by the small systems sizes, on the order of one hundred atoms, which can be fit onto modern computers. Even order of magnitude improvements in computational speed will only double the number of atoms in the system. Calculations of properties such as diffusion, the structure and motion of defects and dislocations, crack propagation and the electronic response of large-scale systems requires system sizes of up to one million atoms. The Center for Computational Materials Science has developed a variety of algorithms grounded in DFT and extended to handle all of these types of calculations. This project will use the techniques to study the properties mentioned above as well as other properties of materials of interest to the Navy.

Methodology: DFT computer codes will be used to expand our database of structural and electronic data high symmetry structures of systems under consideration, e.g., Fe/Cr/Ni/C for steels, or C/H for graphene nanoribbons. This database is used used to develop parameter sets for tight-binding and atomistic potentials using codes previously developed at NRL and to augment previously developed sets of parameters. The tight-binding method, which has accuracy comparable to DFT, will be used to study systems containing thousands of atoms where the quantum mechanical nature of bonding is important. Larger systems will be studied using atomistic potentials. Unexpected predictions of these models will be verified by DFT calculations if possible.

Results: We studied diverse systems such as iron and tin, and showed that the PAW-pseudopotential method used in VASP is in very good agreement with all-electron LAPW calculations. We are therefore confident that VASP can be used with high accuracy in the study of the effects of corrosion in steel, which will be represented by bcc iron. We also developed a tight-binding parameterization for carbon and hydrogen, using this to study the behavior of hydrogen-terminated graphene nanoribbons. We found that the electrical behavior of the ribbons depends crucially on the “family” of the ribbon, where the family number is 3N+j, the number of carbon dimers counted across the width of the ribbon. The electrical conductivity of the ribbons saturates for widths greater than about 0.5 nm, but each family retains its distinctive electronic behavior.

Significance: This research shows that the electronic response of graphene nanoribbons depends crucially on the size of the ribbon, with different response characteristics depending on the ribbon family. This means that electronic devices made from graphene ribbons can be tuned to give the desired response by carefully constructing the nanoribbon.



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Dimers
20
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μ_eff peak (10³ cm²/Vs)
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3j+1
3j
3j-1

Title: Liquid Microchannel Flows for Biofluidics Analysis
Author(s): Guan M. Wang and William C. Sandberg
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

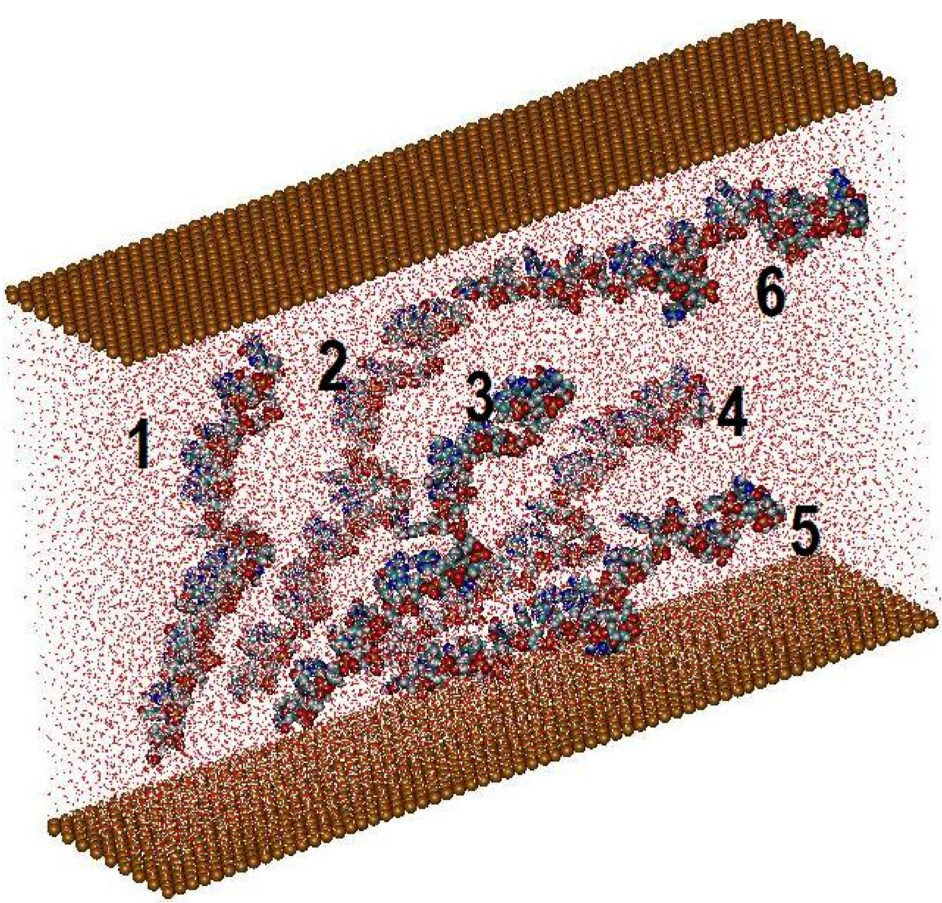
Computer Resources: SGI-Altix [NRL, DC]

Research Objectives: This computational research is aimed specifically at understanding and optimizing biomolecular transport, capture, and force discrimination in microfluidic/nanofluidic systems for biological warfare (BW) threat agent detection. The development of nanosensors requires understanding of the atomic interaction dynamics of the confining nanosensor geometry, the coupling of biomolecules to the device surfaces, the molecular dynamics of the carrier solvent, and the interaction of the sensor dynamics with the carrier solvent. As for simulations of biomolecules such as DNA, at the *atomic level*, the study of biomolecular properties has been confined to nearly equilibrium states only, i.e., no flow fields were applied to the solvents. There has not been a way, until now, of creating shear flows in nanochannels and there has also been no capability in existence, until now, for computing the nonequilibrium dynamics of either free or tethered biomolecules.

Methodology: We have developed a series of quantum and molecular methods to enable the equilibrium software CHARMM to handle non-equilibrium dynamics. These methods have been applied to cases of DNA molecules in shear flows in nanochannels.The typical complex system that we have studied consists of DNAs tethered to Au (111) surfaces through a linker molecule 6-mercapto-1-hexanol (MCH) and a water solvent with sodium and chloride ions. DNAs are single/double strands (ss/ds). For tethered dsDNAs only one strand is anchored onto surfaces. Free DNAs in shear flows are also explored for comparisons. The solvent contains mostly water molecules with added sodium and chloride ions to neutralize the system.

Results: We have carried out, for the first time, the all-atom computational investigation of multiple free DNA molecules in a nanochannel shear flow. The hydrodynamic forces on DNA molecules were directly calculated at the atomic level as were the backbone and side chain forces and torques along the length of the DNA molecules. Spontaneous coiling and uncoiling transitions were observed for one of the molecules, while others exhibited a range of extension, compression, and rotational motions.

Significance: The computations of the dynamics of single and multiple free ssDNA molecules in a shear flow, including the extensional and relaxational time-history, provides the first atomic-level information available to assist in understanding the behavior of long-chain polymer molecules in a shear flow and may lead to insights into the dynamical behavior of biomolecules in biomolecular ionic liquids, such as occur in actual arterial flows.



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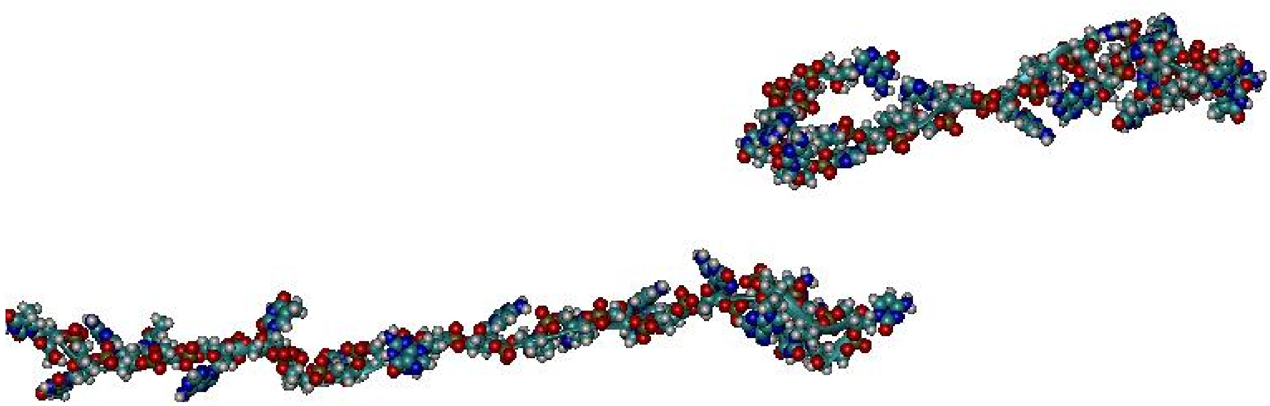


b.

Figure 1: a) Six free DNA molecules in a nanochannel shear flow of water molecules and a distribution of sodium and chloride ions. b.) selected instantaneous conformations exhibited by DNA molecule 6 as it flows along near one of the channel walls.

Title: Quantum-Chemical Simulation of Surface-Science Experiments
Author(s): Victor M. Bermudez
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: Cray XD1 [NRL, DC]; SGI Origin, SGI Altix [ASC, OH]; Linux Cluster [ARL, MD]

Research Objectives: The objective of this program is to perform quantum-chemical calculations as an aid in interpreting surface-science experiments. One example is the analysis of ultraviolet photoemission spectroscopy (UPS) data resulting from chemisorption of organic molecules on semiconductor surfaces. Extracting structural information from such data requires molecular-orbital calculations for different models and comparison with experiment. Another example is the assignment of the vibrational modes of chemisorbed species, as observed in infrared spectroscopy. This requires that one compute the energy-minimized structure and obtain the normal-mode energies for comparison with experiment.

Methodology: The CRYSTAL98 and CRYSTAL03 software packages have been used extensively. These are designed for both Hartree-Fock (HF) and Density Functional Theory (DFT) calculations on periodic structures in one, two or three dimensions. The GAUSSIAN03 software package is used for similar calculations on isolated molecules and clusters.

Results: A large amount of effort has been devoted to a DTRA-funded program on the quantum-chemical modeling of the adsorption of chemical warfare agents (CWA's) and simulants on surfaces. Real CWA's are far too dangerous for routine experimental study. *Ab initio* quantum-chemical theory can relieve much of the burden of working with real CWA's through the use of modeling. *Ab initio* calculations, using DFT with the B3LYP functional, have been applied to the adsorption of the CWA simulant dimethyl methylphosphonate (DMMP) and the corresponding real agent Sarin on γ-Al_2O_3. The goals are to determine the accuracy with which the adsorbed molecules can be modeled and to conduct a "side-by-side" comparison of the bonding of these species to γ-Al_2O_3. Free-standing Al_8O_{12} and $Al_{20}O_{30}$ clusters give reasonable descriptions of the adsorbate structure and properties, and the results are not strongly dependent on cluster size or basis set quality. For either molecule, the energetically favorable mode of adsorption is Al-O=P dative-bonding, in agreement with experiment. The adsorption energy of DMMP on the Al20O30 cluster (-57.5 kcal/mol at the 6-311G(df) level) is greater than that of Sarin (-49.2 kcal/mol). The infrared-active normal-mode frequencies for free DMMP and Sarin have been used to verify the reported mode assignments for these species. For the adsorbed molecules, the ν(P=O) stretch shows a red-shift (relative to the gas phase) of ~60 cm^{-1} (observed) vs. about 84 cm^{-1} (calculated). The calculated shifts for other modes are much smaller and generally agree with experiment. Similar calculations have been performed to study the adsorption of trichlorophosphate, DMMP and Sarin via hydrogen bonding to Si-OH groups on the amorphous SiO_2 (a-SiO_2) surface. Two SiO_2 models are used: a small $Si_5O_7H_8$ "cagelike" cluster and a larger $Si_{21}O_{56}H_{28}$ structure designed to approximate the local environment in a-SiO2. Adsorption energies, bonding geometries, and adsorbate vibrational modes are obtained, and anharmonicity is explicitly included in the treatment of the SiO-H stretching mode. The computed results for the adsorption-induced shift in frequency of the SiO-H stretch and of the molecular P=O stretch are compared with the available experimental data. For all three species, the most stable adsorption geometry involves hydrogen bonding between two Si-OH groups and the O atom of the P=O group. As an example, the figure shows the lowest-energy configuration of Sarin adsorbed on *a*-SiO_2.

Significance: These are the first studies (either computational or experimental) to report a "side-by-side" comparison of the adsorption behavior of a simulant and the corresponding real CWA.

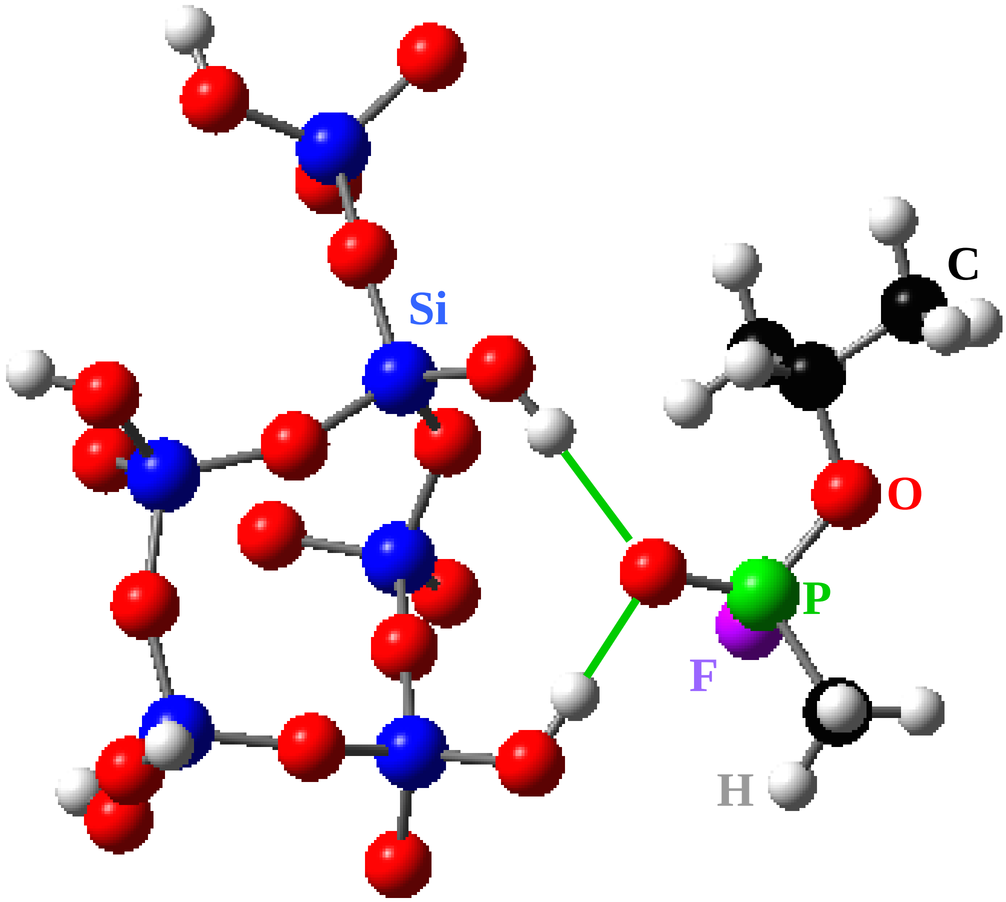


Figure 1. Results of the *ab initio* quantum-chemical modeling of the adsorption of Sarin on *a*-SiO_2. The different elements are labeled and color-coded. Only a small section of the *a*-SiO_2 model is shown. The actual model used was much larger ($Si_{24}O_{48}$). The heavy green lines show the hydrogen-bonding interaction between the O atom of the phosphonyl (P=O) group and *two* SI-OH groups. The structure shown is the lowest in energy. Other structures involving H-bonding to the F atom or the O atom in the C-O-P bond are less stable.

Title: Computer Simulation Modeling of Fluid Flow through Porous Media
Author(s): J.F. Gettrust[1] and R.B. Pandey[1,2]
Affiliation(s): [1]Naval Research Laboratory, Stennis Space Center, MS, [2]Department of Physics and Astronomy, University of Southern Mississippi, Hattiesburg, MS
CTA: CCM

Computer Resources: IBM P4 [NAVO, MS]

Research Objectives: Our objectives are to understand the self-organizing morphology/structures of constituents as they continue to flow (dynamics) in a complex system. In such a non-conservative, non-equilibrium steady-state driven system, the parameters affecting the flow, phase changes, and structures are: composition and distribution of the sediments, characteristics of fluid constituents, i.e., interactions and miscibility, concentration, temperature, pressure gradients, etc. Major questions we address (as part of our continued efforts) are: How do density profiles evolve? How do flow rates of constituents depend on these parameters? Where does the linear response of flux rate, i.e., Darcy's law, apply and where does it fail? How do different phases (solid, liquid, and gas) emerge and how do they depend on these parameters?

Methodology: We use Monte Carlo and lattice gas methods. For most of our studies, the porous medium is modeled by direct simulation methods to incorporate assumed structural morphology and appropriate porosity. We have started using realistic porous matrices, generated directly from reconstituted laboratory samples as resolved by X-ray computed tomography. Many independent samples are often required to evaluate the average quantities for such stochastic systems. Message passing interface (MPI) seems an ideal tool to parallelize our programs.

Results: As before, density and velocity profiles, correlations, and flow of fluid through open media are studied in a three-dimensional lattice. We have examined the self-organizing structures in multi component immiscible systems with different molecular weights. Interaction among constituents (driven by concentration and pressure gradients) leads to a multi-phase self-organized system in a steady-state where a dissociating solid phase from the source is separated from a migrating gas phase toward the top by an interface of mixed (bi-continuous) phase. Onset of phase separation and layering is pronounced at low bias range. The flux density of these constituents responds linearly in the low bias regime, but becomes non-linear and eruptive at high pressure. The response depends on the molecular weight of the fluid constituents. The flow of a simple (one component, hard-core) fluid through the reconstituted laboratory sample is also examined by computer simulation. The response of the flux density to the pressure bias appears qualitatively similar to that of the laboratory measurements.

Significance: The problems of flow in heterogeneous systems are complex and lack appropriate analytic predictive tools. Our computer experiments make specific predictions for density profile and flow rate of gas (applicable to the dissociation of methane hydrate). Measuring the dissociation of methane hydrate within sediments and understanding its distribution and flow are difficult issues but very important to some of the Navy projects that are being carried out here. In the absence of systematic field observation, our computer simulation studies provide an understanding of how methane gas flows and is distributed in porous media in appropriate physical (parametric) conditions. These studies also help advancing the frontier of knowledge in issues crucial to NRL as well as to the understanding of (generalized) fluid flow within complex media.

Title: Materials for Energy Storage
Author(s): Michelle Johannes
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI Altix [ASC, OH]

Research Objectives: The objectives of this program are to use density functional theory (DFT) to understand the properties and performance of energy storage and generation materials. We concentrate specifically on a computational search for better Li ion and fuel cell electodes, Since electrochemical properties such as intercalation potential, capacity and conductivity can be calculated prior to synthesis, this project is intended to save time, effort and money in the laboratory by predicting well-optimized cathode compounds.

Methodology: First principles pseudopotential methods are employed to calculation the quantities of interest. The majority of the work will be done using the Vienna Ab-Initio Software Program (VASP). Post-processing is done using personal codes.

Results: This project has had several notable successes in battery research in the past year. The first is the completion of a DARPA funded seedling program aimed at increasing the capacity of cathode materials relative to the industry standard, $LiCoO_2$. In this program, I used DFT to investigate the intercalation potential and capacity of 16 different potential cathode compounds. Based on the computational results, I predicted a three-fold increase in capacity for a Ni/Cu based compound. My colleagues in chemistry synthesized the material and, at low discharge rate, the capacity indeed proved superior to $LiCoO_2$, by even more than the predicted factor of three (3.8 to be exact). The HPC resources were also used in a recent comparison of the voltage profiles of Li_2RuO_3 and RuO_2. The two compounds contain identical elements and local structures but show both qualitatively and quantitatively different discharge curves. DFT studies of the two structures revealed the underlying chemical and physical factors that determine the sharp differences. These factors can be generalized and used as guidelines in the search for materials with good discharge profiles.

Good results were also obtained from work on fuel cell catalysts. It is well known that a small amount of sulfur can "poison" a catalyst surface. However, the extent of the poisoning was recently shown to be strongly dependent on the surface type. Time on this project was used for several very large calculations of different fuel cell catalysts surfaces with a sub-monolayer coverage of sulfur. The adsorption energies of the reactive components of catalysis were calculated and compared to those on a clean surface. The relevant property of a good, sulfur tolerant surface was found to relate to the geometry of the surface in the immediate environment of the sulfur poison and not to the electronic properties of the clean surface, as was previously though.

Significance: The discovery of a new battery cathode material with nearly four times the capacity of $LiCoO_2$ could have extremely widespread significance, not only for the military but for commercial applications such as cell phones, laptops and music players, all which use these batteries. Further computational and experimental work is needed to stabilize the battery for high rate use, but the promise revealed by our preliminary results is strongly encouraging.

Developing sulfur tolerant fuel cells is becoming increasingly important as fuel cell technology moves out of the laboratory, where conditions can be made pristine, and into the real world, where impurities and poisons are common. Understanding the factors that contribute to cathode poisoning will be very significant to the development of usable catalysts.

CEA

Computational Electromagnetics and Acoustics

- High-resolution, multidimensional solutions of Maxwell's equations to define the electromagnetic fields about antenna arrays; electromagnetic signatures of tactical ground, air, sea, and space vehicles; electromagnetic performance and design factors for EM gun technology; electromagnetic signature buried munitions; high-power microwave performance; and interdisciplinary applications in magnetohydrodynamics and laser systems.

- High-resolution, multidimensional solutions of the acoustic wave equations in solids, fluids, and gasses to model the acoustic fields for surveillance and communication, seismic fields for mine detection, and the acoustic shock waves of explosions for antipersonnel weapons.

Title: Large-Scale Computational Electromagnetics
Author(s): Richard S. Schechter, Sung-Taek Chun, Mark Kragalott and Michael S. Kluskens
Affiliation(s): Naval Research Laboratory, Washington DC
CTA: CEA

Computer Resources: SGI Altix [ASC, OH]; Linux Cluster [ARL, MD]

Research Objectives: The objective is to use large-scale simulations of electromagnetic wave propagation to model such problems as the performance of complex antenna arrays and their radiated fields. Other problems include modeling wave propagation in new types of materials such as electromagnetic bandgap (EBG) and left-handed materials (LHMs). Another objective is to improve the accuracy and fidelity of these simulations by devising algorithms that are more accurate and testing them against benchmark or known solutions.

Methodology: The finite-difference time domain (FDTD) technique is a widely used method in computational electromagnetics. The method is well suited for modeling wave propagation in heterogeneous media, antenna modeling, and scattering problems.

Results: The FDTD method was successfully employed in modeling LHM metamaterial lenses, composed of split-ring resonators (SRRs) and wires on circuit boards. This represents the first time that large-scale 3D simulations of laboratory-size metamaterial lenses, with all the details of the wires and SRRs, has been performed. The results demonstrate the focusing effect of these new materials and the sensitivity of the focusing to frequency and thickness of the lens.

A large Vivaldi 11 by 11 array element antenna was modeled in 3D using an MPI code, Conformal Finite-Difference Time Domain (CFDTD). Additional structures were added to make the simulations closer to NRL experiments. These large models contain up to 1.8 billion cells. The computations were utilized in a high-priority project to measure and predict wideband RF mutual coupling. These antennas are ultra-wideband (UWB).

Significance: In LHMs, electromagnetic waves have negative phase velocity and a negative refractive index. These properties can be used for a variety of microwave and optical applications such as beam steerers, modulators, band-pass filters, microwave couplers, and antenna radomes. Large phased array UWB antennas are important to the Navy.

Title: High-Accuracy Finite-Difference-Time-Domain Calculation of Electromagnetic Fields
Author(s): Michael I. Haftel
Affiliation(s): Naval Research Laboratory, Washington DC
CTA: CEA

Computer Resources: SGI Origin [ERDC, MS]; SGI Origin [ASC, OH]

Research Objectives: To develop the High Accuracy Scattering and Propagation (HASP) code for the 3D Maxwell's equations and to calculate the fields in and scattered from objects of naval or technological interest, including RF cavities and advanced materials.

Methodology: A highly accurate FDTD algorithm for solving Maxwell's equations (up to 10000 times more accurate than the Yee algorithm) is written into the HASP code. The algorithm has been implemented to take maximal advantage of parallel processing using Fortran 90. This code has been applied to calculating electromagnetic fields around and in complex 2D and 3D objects, including complex cavities and advanced materials such as photonic crystals and plasmonic materials.

Results: We used the HASP code to simulate the optical fields and optical transmission through nanoarrays of coaxial rings embedded in thin metallic films. A number of different ring geometries (inner and outer radii, film thickness, and periodicity) were simulated. The simulations were coordinated with experimental measurements for nanoarrays in silver films to verify that the enhanced transmission at wavelengths much larger than the aperture diameters are due to closely coupled cylindrical surface plasmons (CSP's) propagating on the inner and outer surfaces of the rings, and this coupling is more efficient as the inner and outer ring radii approach each other. A number of simulations were also carried out for metamaterials in the RF and microwave regime that demonstrated that the CSP enhanced-transmission effect, normally associated with the optical and IR regimes, can be reproduced at low frequency by coaxial apertures in films consisting of periodic high-dielectric structures embedded in a (nearly) perfect conductor.

Significance: This work indicates how nanostructured arrays can enhance the optical properties of materials well beyond the diffraction limit. This will impact the design and performance of optical materials and devices used by the Navy for sensing and transmission. Also, these studies impact the design of metamaterials in the IR, microwave, and RF regimes for similar applications.

Title: Electron Beam Source and Transport Simulations
Author(s): Jesse Neri and Steve Swanekamp
Affiliation(s): Naval Research Laboratory, DC
CTA: CEA

Computer Resources: Linux Cluster [ARL, MD]

During FY07 we used HPC computer time to run parallel electromagnetic particle-in-cell calculations for to study the coupling of radiographic electron beam loads to inductive adder accelerators. These simulations show the detrimental effects of the vacuum electron flow on the quality of the x-ray source. Furthermore, these simulations aid in the design of hardware to minimize the flow current in the diode and hence improve the overall quality of the radiation sources. The high-quality radiographic sources are a critical component in the NNSA Stockpile Stewardship Program.

Research Objective: The goal of the current program is to identify the issues and mechanisms of coupling high-quality radiographic electron beam loads to magnetically insulate vacuum transmission lines, which have their own inherent vacuum electron flow. The issues at hand include the impedance matching between the load and accelerator and effects of vacuum electron flow on the radiographic performance of the loads.

Methodology: The MPI parallel LSP particle-in-cell code is used to model the accelerator output feed and radiographic load section of the NRL Mercury and Sandia RITS-6 devices. The problem requires modeling of substantial portions of the accelerator to establish a characteristic vacuum electron flow, and capture the physics of the load impedance behavior on the vacuum electron flow. High spatial resolution is required in the simulations to obtain the effects of the flow electrons on the loads, which forces small time steps for the simulation. The simulations are driven with the measured voltage waveforms of the accelerators, and the simulation results are compared with the measured currents and x-ray pulses from the experiments.

Results: The simulations reproduce the basic results of the experiments and clearly identify vacuum flow electron as the culprits in degrading the impedance and radiographic qualities of the loads. The RITS-6 simulations show that the late-time oscillations in the machine current and x-ray output are from the vacuum electron flow entering the load, lowering the load impedance, which then limits the flow of vacuum electrons to the load, and the impedance recovers, then the process repeats.

Significance: The simulations help to interpret the experimental results, where direct measurements of electron flows are difficult. The simulations then help to design the hardware in the load region that is used to minimize the coupling of power flow electrons in to the loads, leading to improved radiographic performance. The predictive capabilities of the simulation save time and money in the design and construction of the experiments, and lead to obtaining radiographic systems that meet program requirements.

Title: Acoustic Propagation in Littoral Sub-Mesoscale Model Environments

Author(s): Roger M. Oba[1], Colin Shen[1], Patrick Gallacher[2] and Alex Warn Varnas[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC, [2]Naval Research Laboratory, Stennis Space Center, MS

CTA: CEA

Computer Resources: SGI Altix [NRL, DC]

Research Objectives: This supports the acoustical component of computational work for the 6.2 Project entitled "Integrated Sub-Mesoscale / Acoustic Modeling Predictive Capability for Littoral Regions" which has an objective of integrating a full 3D acoustic propagation modeling with physical oceanographic modeling of a 4-demonstrating numerical 4D (space and time) predictability of acoustic properties using a physics based, 4D, synthetic littoral environment. The resulting computations are being used in model/data comparison and predictive capability validation.

Methodology: The physical oceanographic realization of a 4D littoral environment are being calculated by one of the 4D non-hydrostatic oceanographic computational codes being used by C. Shen and T. Evans (NMCO), P. Gallacher (NRL-MIT), and A. Warn Varnas (EULAG). The 6.2 project links the ocean dynamics to the acoustics by mapping temperature and salinity distributions to the sound speed field through an equation of state for each temporal update of the environment. The resultant sound speed fields are input to FOR3D, a continuous wave, parabolic, spatially 3D acoustic code. The temporal/spatial sampling of oceanographic and acoustic models have significantly different scales, and mediating this gap has been successfully accomplished. Preliminary determination of what time sampling is required for the combined model in order to faithfully produce acoustic features of interest has been done. Comparison of the package predictions to coupled ocean/acoustic field data set of AsiaEx provides benchmarking in data-model is ongoing. The experimental data show certain oceanographic / acoustic relations and these will be used provide model package validation using appropriate acoustic measures. Some model evaluation can then be made according to predictive ability using skill scores.

Results: In FY07, the oceanographic models are using ASIAEx site parameters and environment, and the resulting acoustic results have been used in metrics for comparison to data. Acoustic modeling of the first successful hydrodynamic runs revealed estimates of array performance that were consistent with experimental data in terms of array signal gain, signal gain fading and beamwander during oceanographic events. Substantial contributions toward proof of concept.

Significance: The Navy has considerable interest in acoustic system performance in littoral regions where oceanographic variability often appears as non-stationary, horizontally anisotropic contributions to the ambient sound speed distribution. In this proposal, we consider a viable solution to the problems of developing physically accurate synthetic environments and combining them with acoustic computational models. The success of the New Start would provide the Navy with a better awareness of littoral acoustic performance and measures of the expected performance in a quantitative form. This is the first step to developing a true predictive capability in shallow water.

Title: Modeling 3-D Range-Dependent Acoustic and Electromagnetic Propagation with the Parabolic Equation Method
Author(s): Joseph F. Lingevitch
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: Linux Cluster [ARL, MD]

Research Objectives: The objective of this research is to develop efficient parabolic equation based models for computing reference solutions to reverberation problems of interest to the Navy. The reference solutions are used to develop improvements to standard Navy reverberation modeling.

Methodology: Recently, we have developed a 2-D parabolic equation method for computing acoustic reverberation (backscatter) from range-dependent features such as a rough sediment interface in a waveguide. This numerical technique is orders of magnitude faster than solving the full wave equation and is of great value for solving acoustic propagation problems in the ocean.

Results: The geometry of a 2-D reverberation problem of interest is shown in Figure 1. This problem involves a pressure release flat ocean surface and a constant velocity water layer over a sand sediment layer. The water and sediment are modeled as fluid media with material properties as shown in Figure 1. The interface between the water and the sand is given by $H(x) = 50 + \gamma(x)$ meters where $\gamma(x)$ is a zero-mean Gaussian distributed random variable, with variance h^2, and correlation length scale l. The two cases of interface roughness that we consider for this problem are: 1a.) h = 0.32 m, l = 400 m and 1b.) h = 0.14 m, l = 10 m. A point source is located at depth z = 15 m, with source function given by

$$S(t) = e^{-\frac{(\Delta\omega t)^2}{2}} \cos(\omega_0 t) \;\; \mu\,\text{Pa} \;@\; 1\text{m},$$

where $\omega_0 = 2\pi f_0$ is the circular frequency of the source with bandwidth $\Delta\omega = 2\pi f_0 / 20$.The quantity of interest is the expected value of the reverberation intensity at x = 0 m and depths z = 5, 25 and 45 m for $f_0 = 250$ Hz . The solution to this problem is computed by averaging the reverberation for 100 realizations of the ocean bottom. The PE algorithm described above used to compute frequency domain solutions over the bandwidth of the source and to a maximum range of 10 km. The time-domain backscattered pressure is computed by Fourier synthesis. For this problem we solve for 1500 frequencies between 220 Hz and 280 Hz with a frequency spacing of 1/30 Hz (1500 frequencies). Since the maximum range in the PE calculation is 10km, we compute the first ~ 13 s of reverberation. In Figure 2, the reverberation intensity time series averaged over 100 realizations of the bottom roughness are shown for Problems 1a, 1b at three receiver depths (5, 25, 45 m).

Significance: In standard Navy reverberation models, approximations are introduced to efficiently compute the expected value of the reverberation intensity. These models utilize scattering and boundary loss kernels which approximate the scattering and loss from rough surfaces. In order to validate these models benchmark quality solutions of the full scattering problem are required. The parabolic equation reverberation algorithm discussed above is one method for generating these benchmark solutions. This method is about 2 orders of magnitude more efficient than finite element solutions of the same problems. The two calculations shown in Figure 2 each required about 10,000 hours of time on the JVN cluster. We estimate that a finite element solution for the same problem would require 1,000,000 hours for each calculation.

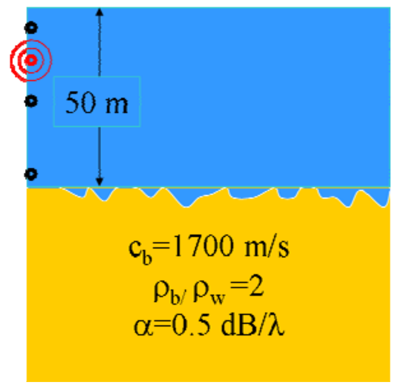


Figure 1. Geometry for a 2-D reverberation problem with a point source located at depth z = 15 m. The receivers are located at x = 0 and z = 5, 25, 45 m. The surface of the water is flat with a pressure release boundary condition. Two cases of roughness parameters are considered for the interface between the water and sand sediment layer: 1a.) h = 0.32 m, l = 400 m and 1b.) h = 0.14 m, l = 10 m.

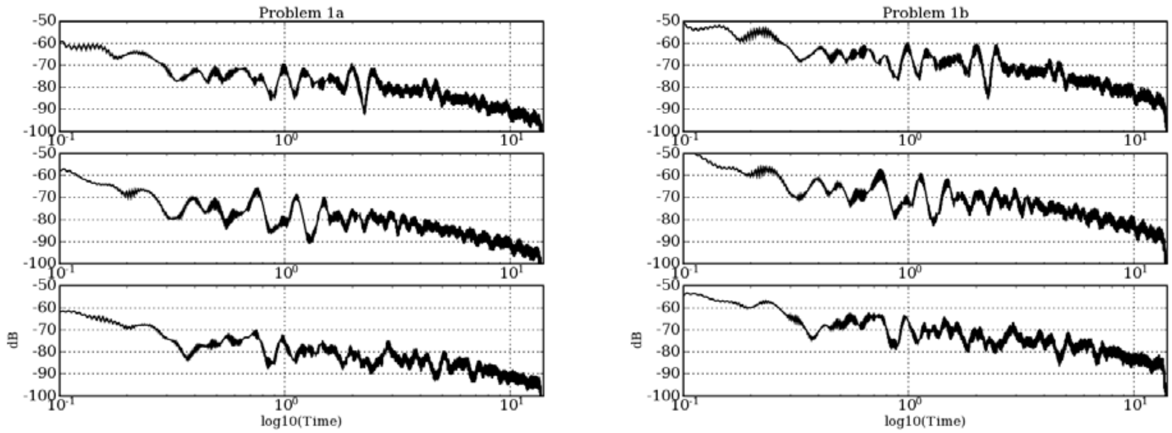


Figure 2. Expected reverberation intensity time series averaged at depths z = 5, 25, 45 m computed by parabolic equation reverberation algorithm for a) Problem 1a and b) Problem 1b. Each curve is an average over 100 realizations of the bottom roughness.

Title: Three-Dimensional Elasto-Acoustic Modeling
Author(s): Saikat Dey[1] and Luise S. Couchman[2]
Affiliation(s): [1]SFA Inc., Crofton, MD and [2]Naval Research Laboratory, Washington DC
CTA: CEA

Computer Resources: Cray XD1, SGI Altix [NRL, DC]; Linux Cluster [ARL, MD]

Research Objectives: Numerical modeling of large-scale structural-acoustics problems using STARS3D. Applications include radiation and scattering from complex elastic (rigid) structures; seismic-acoustic propagation modeling, and Páde-approximation-based rapid frequency-response computation.

Methodology: STARS3D utilizes hp-finite element approximations providing high accuracy solutions for mid-to-high frequency domains. Homogeneous infinite exterior medium is handled using infinite elements while inhomogeneous infinite exterior is modeled using perfectly matched layer (PML) technique. Rapid wideband frequency-sweeps are realized using a reconstruction method based on Páde-approximations.

Results: Figure 1 depicts two results. The first one (left) is a broadband target-strength computation for a rocket-like shell considered to be rigid. The second one (right) involves seismic propagation and shows accurate Páde-approximation-based reconstruction of wideband, large-range surface frequency-response due to a buried point-force.

Significance: 1) Target-strength computations presented in Figure 1 are used in the SERDP program aimed at detecting unexploded ordinances (UXO). 2) The ability to rapidly and accurately simulate seismic-acoustic propagation is enabling better design and optimization of Unattended Ground Sensor (UGS) systems.

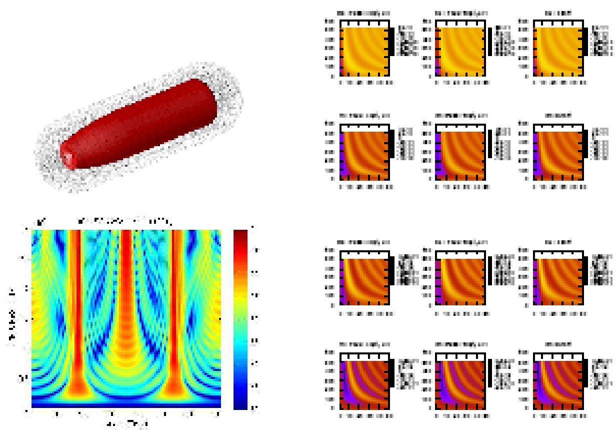


Figure 1: Wet-surface and surrounding mesh for 5-inch rocket (top left); STARS3D target-strength computation (bottom left) assuming sound-hard rigid scattering. Pade-based reconstruction of wideband seismic frequency-response z-displacement (top right) and x-displacement (bottom right).

Title: Acoustic Error Modeling
Author(s): Josette P. Fabre
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CEA

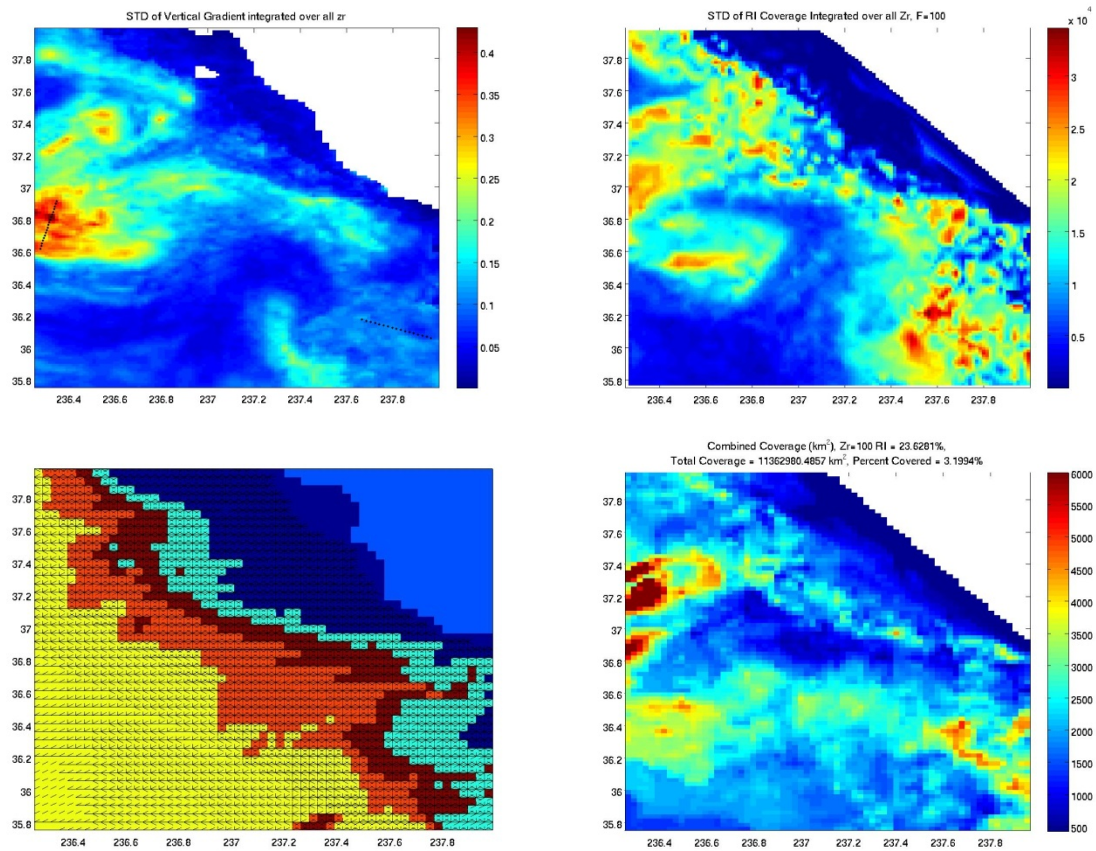
Computer Resources: IBM P4 [NAVO, MS]

Research Objectives: To quantify errors in acoustic fields based on errors in the input environmental fields, for example, sound speed, bathymetry, surface and sediment structure as well as derived parameters such as sonic layer depth, below layer gradient and depth excess. This information will provide a valuable asset to both the operational and research communities providing uncertainty estimates of predicted acoustic fields. These uncertainty estimates will provide guidance on sampling (take measurements in areas of greatest error/uncertainty) as well as provide confidence in performance predictions. The current effort estimates error due to variations in the sound velocity and fields derived from sound velocity only. Ensembles of acoustic fields are computed based on oceanographic ensembles to describe acoustic error. This project includes visualization of the acoustic field as well as research into reduction in computation time based on the acoustic field properties. Now that the initial work has been proven successful, the project can be expanded to include error due to bottom and surface description(s). Additionally, these efforts will be expanded to support optimal search track planning and Tactical Decision Aid analysis.

Methodology: Several steps are taken to develop the capability described above. First, ensembles of oceanographic fields are computed, this is done under a separate sub-project (NRLSS018). These fields are combined with bathymetry, sediment description and wind information to develop input files for the acoustic models. The development described here requires use of several acoustic propagation models: including but not limited to the Navy Standard Parabolic Equation (NSPE) model and the Kraken Normal Mode model. All of these programs predict transmission loss (TL). These programs are written in Fortran and are not parallelized. However, for this project, each model must be run for each geographic position, bearing, frequency and source depth. This results in hundreds of thousands of runs. In order to maximize the computers capabilities the routine that creates the input files also creates a batch file for submission to the LSF and shell scripts for assigning each serial job to a processor on the designated nodes. The LSF script then submits each shell script to the Parallel Operating Environment (POE) and multiple serial runs are submitted in parallel. Additional research is being conducted in taking advantage of isotropy in the environment to reduce the number of runs. Normal mode properties are computed and clustered using standard techniques and the number of runs is reduced by determining how range dependent an area is and running range independent runs (which are faster than range dependent runs) where the environment is weakly range dependent. Some of these results are also provided below as well as in the referenced papers.

Results: Several methods of estimating uncertainty due to the acoustic propagation have been developed. These methods have been tested in several areas and are currently being applied during a Navy Fleet Exercise being conducted in the Western Pacific. Maps of acoustic uncertainty due to sound speed uncertainty are being used with Kalman Filter techniques to prepare glider measurement guidance. Examples from an exercise in Monterey Bay are given in the figure below. This capability is being expanded and transitioned to the Naval Oceanographic Office in FY08.

Significance: In 2000, ONR initiated a program in this important area of research, uncertainty. Until recently, scarce measurements were input to models and the output was used for predicting the performance of a system. The prediction was not always accurate and the source of the error was unclear. The capability here directly addresses this problem by providing guidance for sampling strategies as well as providing variability (due to variability in sound speed only) of acoustic predictions.



Examples of acoustic variance for a Navy exercise area in the Western Pacific. Top left shows the variability (standard deviation) of vertical sound speed gradient (color) versus longitude and latitude integrated over 10 receiver depths, top right shows the variability (standard deviation) of range independent coverage (units of m2) (color) versus longitude and latitude integrated over 10 receiver depths for 100Hz. The lower left shows clustered regions determined using modal properties of the acoustic propagation and bottom right shows coverage computed to take advantage of the isotropy in the sound speed environment as determined by the clusters.

Title: Low Grazing Angle Radar Backscatter
Author(s): J. V. Toporkov and M. A. Sletten
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: SGI Altix [NRL, DC]; SGI Origin [ERDC, MS]; SGI Origin [SMDC, AL]

Research Objectives: The project seeks to gain and improve understanding of the ocean radar backscatter at low grazing angles (LGA) through direct numerical simulations of surface scattering processes. Sea echoes can be a hindrance in ship-borne or coastal radars as they mask target responses. Yet, ocean backscatter is the main source of information in many remote sensing applications. Detailed knowledge of the properties and behavior of sea backscatter is essential for successful performance of all such systems, many operating in the LGA regime. Analysis of clutter realizations simulated under well-defined and well-controlled conditions provides comprehensive descriptions of statistical and temporal properties of the backscatter and illuminates the trends with variations in system or environmental parameters. Numerical results serve as excellent benchmark cases when assessing applicability and accuracy of approximate scattering models. Flexibility of the numerical technique allows simulating radar backscatter at various wave lengths across the electromagnetic spectrum.

Methodology: The technique combines an ocean surface model that includes non-linear hydrodynamics with computationally efficient, exact calculation of the electromagnetic backscatter. In this work, the wind-driven surface is represented by realizations of a Gaussian random process described by a certain model wave spectrum, e.g., Pierson-Moskowitz. The small-scale roughness (important at centimeter electromagnetic waves such as X band) is shaped by wave-wave interactions modeled by the non-linear Creamer transformation applied to a Gaussian realization. The electromagnetic field scattered by a given surface profile at a particular frequency is found by iterating the second-kind integral equation for the induced surface current. This technique is formulated from first principles and, as such, automatically accounts for many phenomena (multiple scattering, shadowing) known to be problematic for analytical treatment. The numerical method shows robust convergence even as incident field direction approaches grazing. To simulate pulse scattering, surface response is calculated at a number of frequencies, and Fourier synthesis is used. Temporal evolution of a surface realization is represented by a sequence of profiles, with scattering calculations repeated for each profile. Simulations are limited to a two-dimensional situation but have direct relevance to commonly occurring three-dimensional geometries.

Results: Scattering of a wide-band HF signal by a time-varying ocean surface was the focus of the simulation efforts. The problem setup imitated a dipole transmitting antenna being placed on a tower or a ship, cf. Figure 1. Coherent radar returns were calculated over a 200-second span, allowing time-dependent analysis of the signal magnitude and evaluation of the Doppler spectra, cf. Figure 2. One interesting feature of the simulated backscatter is the “fading effect”, i.e., occasional drop in the received signal magnitude for all ranges (Figure 2a). This phenomenon is consistent with some field observations and may be caused by large wave crests occurring in the vicinity of the antenna. Availability of detailed surface profiles (an advantage of a numerical experiment) makes further detailed investigation possible. Other efforts included analysis of previously generated Monte Carlo sets of X-band and L-band backscatter to evaluate clutter statistics and their behavior. HPC resources were also used to process collected InSAR data.

Significance: Detailed knowledge of the LGA sea clutter and understanding of its behavior are essential for predicting and improving the performance of ship-borne radar systems and are vital for enhancing the quality of ocean-related remote sensing products. Direct numerical simulations replicate the input data as seen by such a sensor, establish correlations of these data with the wave fields being probed, and guide development of advanced clutter models and data retrieval techniques.

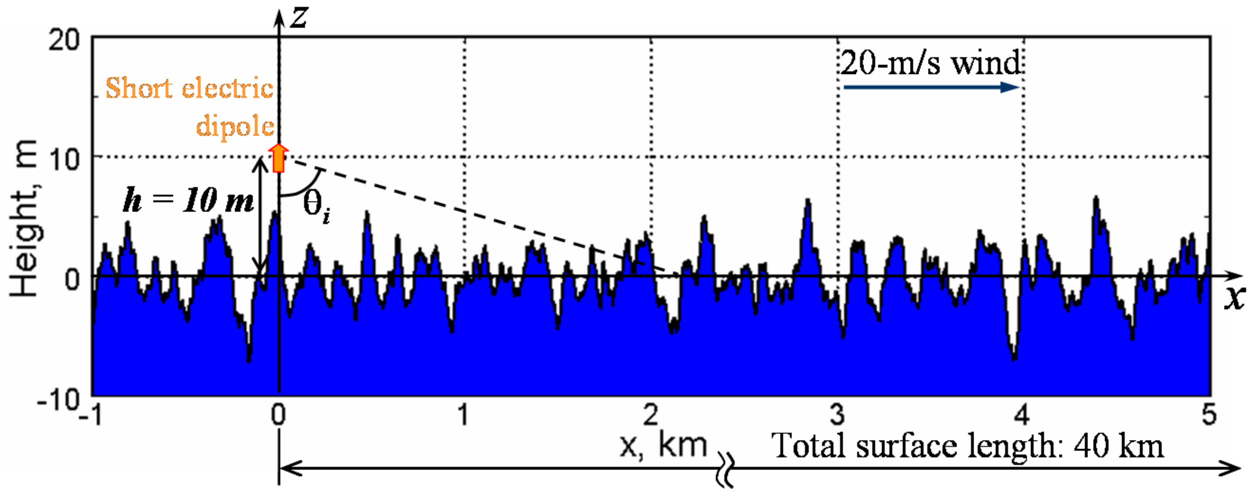


Figure 1. Problem set-up

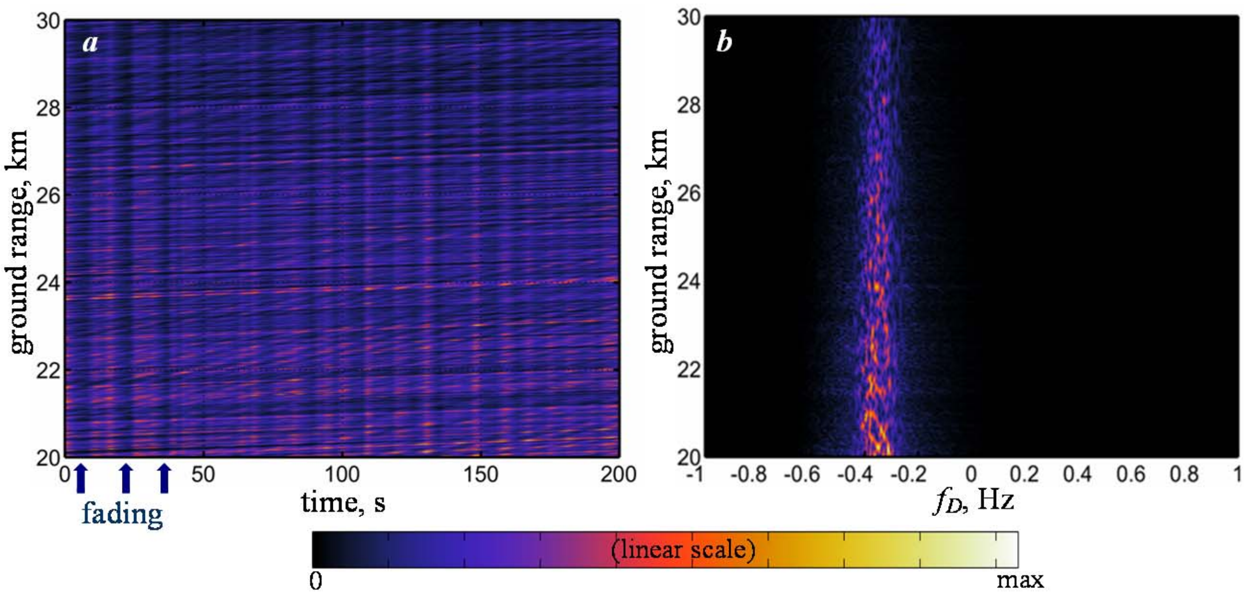


Figure 2. a) Magnitude of range-resolved backscatter vs. time; b) Doppler spectrum of the coherent return. Range resolution is 15 m.

Title: Intense Laser Physics and Advanced Radiation Sources
Author(s): Daniel F. Gordon
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

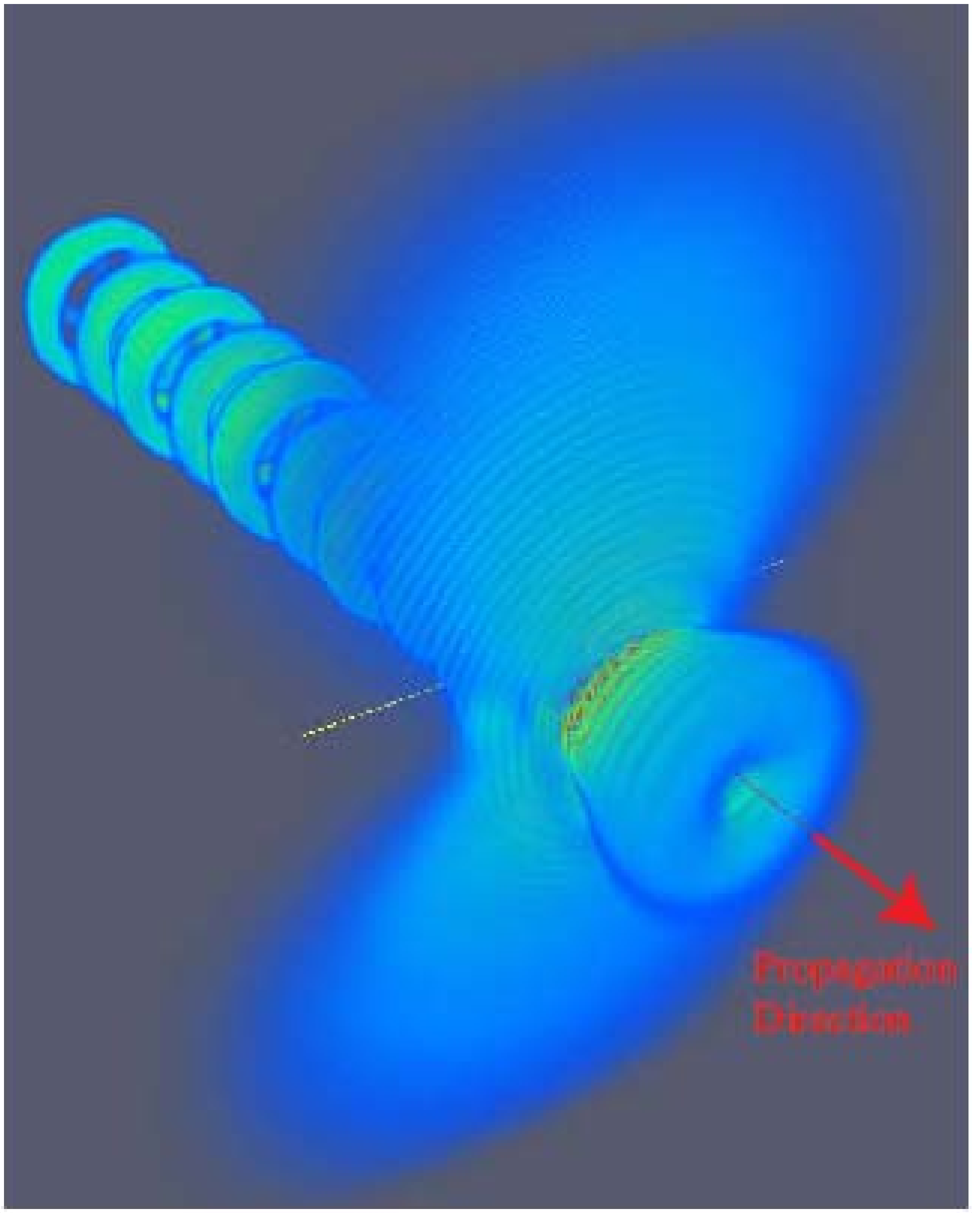
Computer Resources: IBM P4 [NAVO, MS]; Cray XT3 [ERDC, MS]; Linux Cluster [MHPCC, HI]

Research Objectives: The primary objectives of this program are to model the propagation of intense, short-pulse lasers in plasmas and other nonlinear media, and to provide computational support for experiments on the NRL Table-Top-Terawatt (T3) laser and Terawatt-Femtosecond-Laser (TFL). Current areas of research include plasma based accelerators, terahertz radiation generation, and laser guided discharge modeling.

Methodology: HPC resources are utilized using an object oriented parallel framework called turboWAVE which contains modules designed to solve a variety of problems. Both fully explicit and ponder motive guiding center particle-in-cell modules are used to model relativistically intense laser pulses propagating in plasmas. Fluid modules are used to model atmospheric discharge physics. The framework supports non-uniform grids and sliding re-zones for problems with extreme space-scale separations.

Results: HPC resources in 2007 have been used primarily for laser wakefield accelerator modeling. Several 3D PIC simulations were carried out in an effort to explain new and interesting results from recent NRL experiments. In these experiments, a 2.5 TW laser pulse was focused into a gas jet and 1.5 MeV electrons were observed in a well defined jet oriented at about a 40 degree angle with respect to the laser axis. These electron characteristics are interesting because they could conform to the requirements for injection into a standard laser wakefield accelerator. The simulations reproduced the experimental results, except that the simulated electrons were emitted into a cone rather than a jet. We have hypothesized that the disparity may be due to ionization physics which was not included in the simulations. We are carrying out additional runs to test this hypothesis. The simulations also revealed an interesting effect that was not considered by the experimental diagnostics. Namely, a well defined cone of second harmonic radiation was observed originating from an electron cavitation region ("plasma bubble"). This second harmonic radiation might make a useful experimental diagnostic if its characteristics can be related to the characteristics of the cavitation region. Work on laser guided discharges was also continued into 2007. The characteristics of streamer propagation as computed by the SPARC code were compared with a new NRL transmission line model and satisfactory results were obtained.

Significance: Laser-driven accelerators and radiation sources have potential applications for ultrafast (femtosecond) imaging of chemical and biological systems. High energy electron beams might be useful as a gamma ray source for detection of special nuclear materials. Laser guided electrical discharges could have applications for non-lethal weapons or for mitigation of natural lightning.



Volumetric rendering of the electric fields produced by an intense laser pulse focused into a gas jet. The ring-like structures near the axis are due to the plasma wake-fields. The wing-like structures represent conical emission at the second harmonic of the laser. This second harmonic emission is interesting because it is emitted in regions of strong electron cavitation. Such cavitation regions ("plasma bubbles") can be used as ultra-high gradient accelerating structures.

Title: Infrasound Signal Propagation Modeling
Author(s): Douglas P. Drob, Joseph Lingevitch and Geoffrey Edelman
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: Linux Cluster [ARL, MD]; SGI Altix [NRL, DC]

Research Objectives: Advance the state-of-the-art in infrasound propagation modeling techniques in order to improve capabilities to detect, locate, and characterize infrasonic sources.

Methodology: Develop parabolic equation and acoustic ray tracing propagation codes to investigate observed infrasonic signals produced by natural and man-made infrasound sources, with particular emphasis on explaining the observed seasonal and local-time variations. Continuing efforts are required to update and archive global environmental specifications to support the development of the infrasound propagation codes. This includes mesoscale weather modeling capabilities to increase the resolution of atmospheric specifications, thus improving the accuracy of the resulting propagation calculations. Comprehensive numerical simulations over a variety of geophysical parameter spaces (e.g., frequency, season, local-time) are required to understand the observed variations of infrasound propagation characteristics that result naturally from atmospheric variability.

Results: Significant progress was made on the production of multiday mesoscale specification for the analysis of ground-truth infrasound events. Specifications of arbitrary regional domains of interest can be generated with the Weather Research and Forecasting (WRF) model using observational inputs from global scale weather models. Figure 1 shows an example of the static sound speed at an altitude 10 meters above the land/sea surface with a corresponding east-west cross-section of the meridional (north-south) wind component. A new infrasound propagation code based on the Tau-P method was written and tested. Capable of both interactive and batch calculation, the code employs root finding and Romberg integration techniques to handle the inverse square root singularities. Using 4x daily atmospheric specifications from September 13, 2002 to April 31, 2007; calculations of the celerity, azimuth deviation, and turning height for all detection azimuths up to 35° elevation were performed for representative international monitoring network stations. These calculations are performed in the reference frame of the receivers via a transformation of the underlying equations. Figure 2 shows a comparison of the calculated wave ducting heights for an Antarctic station using the NRLMSISE/HWM-93 climatology and near-real-time G2S environmental specifications. The G2S environmental specifications paint a very different picture from those of the climatology.

Significance: The results indicate that the performance of automated infrasound event association and source location algorithms can and should be improved by the ability to continual update station travel time curves to properly account for the hourly, daily, and seasonal changes of the atmospheric state.

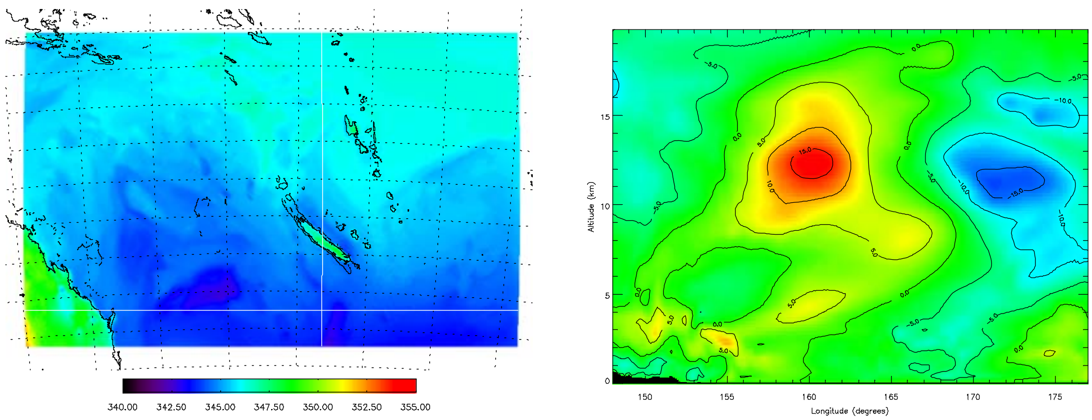


Figure 1. An example of the static sound speed at an altitude 10 meters above the land/sea surface, and a corresponding east-west cross-section of the meridional (north-south) wind component.

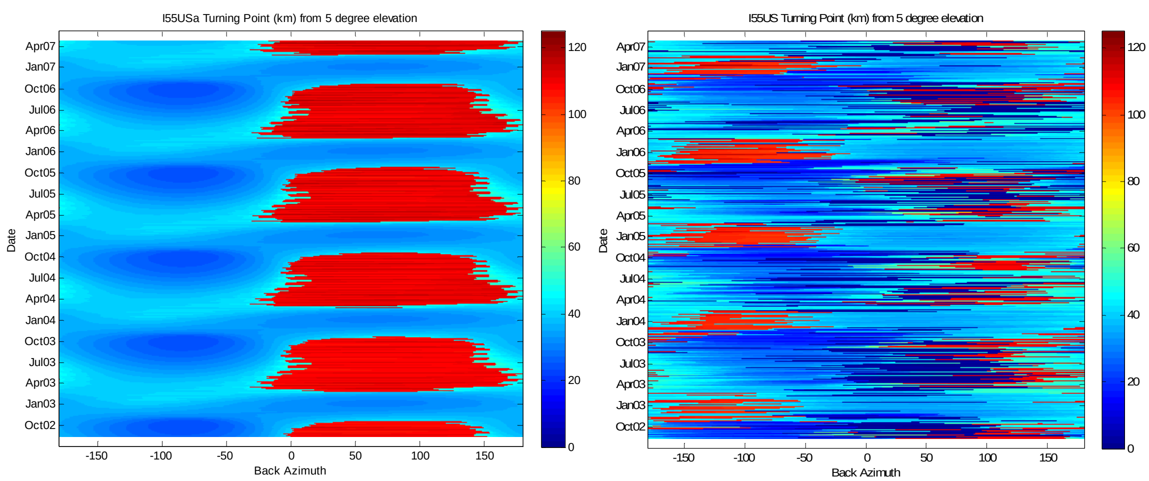


Figure 2. A comparison of the infrasound signal turning point (altitude in kilometers) for a station located in Antarctica using the NRLMSISE/HWM-93 climatological models and the near-real-time G2S environmental specifications.

Title: Validation of Tactical Decision Aids
Author(s): Josette P. Fabre
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CEA

Computer Resources: IBM P4 [NAVO, MS]

Research Objectives: Develop a physics-based environmental acoustic metric to evaluate TDAs which support planning and operations of acoustic autonomous and distributed systems in a time evolving scenario.

Performance of acoustic systems is governed by the environment. Accurate characterization of the environment and modeling of the acoustic propagation provides guidance for system deployment as well as operational and measurement tactics. There are many TDAs in existence and under development to support the Fleets' operational and near-operational systems. There is not, however, any accurate metric for evaluation of such TDAs.

In particular, autonomous underwater vehicles (AUVs) (ONR Undersea Persistence Program) are becoming available for Navy operations. Deployment of these AUVs will require knowledge of the environment in addition to providing information about the environment and the acoustics. As operations begin, data will be assimilated and decisions will be made based on this improved knowledge of the environment. The metric developed under this effort will provide validation for the data assimilation process.

Methodology: The primary thrust of this effort will be to develop a metric for evaluation of the environmental acoustics. There are several ways to accomplish this task. Very early in the project, the best ways will be explored and identified. The initial part of the project is being spent developing an algorithm that will operate on the environmental volume (sound speed, sediment and bathymetry) and providing comparison parameters for sensor placement analysis. As a simple example, we consider the signal excess (SE = SL – TL – AN + AG - RD) in a volume. Because we know the governing equations for TL and the other parameters can be considered constant, this expression can be taken and encompassed in a mathematical form and from that, parameters can be derived that are unique to the volume. These parameters can then be computed for other realizations (sensor placements) and compared. The optimal placement will be derived based on known environments and significant analysis will be conducted to ensure that these parameters (metrics) are well understood. A secondary thrust of this project will be to develop a data set for which all quantities are known and can be used for testing of acoustic TDAs. The primary development of this data set will involve oceanographic modeling, data assimilation and acoustic modeling.

Results: A metric to evaluate the accuracy of TDAs is being finalized and tested. Additionally methods of estimating uncertainty due to the acoustic propagation have been developed. Brute force methods are also being computed to compare against the new metrics. This work will be further tested on Fleet data in the coming months.

Significance: "In Joint Vision 2020, the Department of Defense's strategic plan to ensure battlespace dominance in the 21st century, a key element is information superiority enabled by emerging technologies...." "An important aspect of information superiority is situational awareness. This implies knowing where you are, where allied and coalition forces are and where enemy forces are. It means understanding the environment, from the sea floor to the top of the atmosphere." [Heart of ForceNet: Sensor Grid, Advanced Command and Control By RADM STEVEN J. TOMASZESKI]. Additionally, TDAs help us to understand the environment, and a way to evaluate the TDAs performance is needed.

CWO

Climate
Weather
Ocean Modeling

- Modeling of the Earth's climate and weather to improve scientific understanding of the oceanic and atmospheric dynamics and developing an oceanic and atmospheric prediction capability for both military operations (safety of flight, mission planning, optimal aircraft, ship routing, weapon system design) and civilian applications (fisheries forecasts, pollutant tracking, global change studies, and weather forecasts).

- Modeling of various properties of the ocean (temperature, salinity, currents) to improve the processing gain for acoustic antisubmarine warfare (ASW).

Title: Coastal Ocean Physics
Author(s): Colin Shen, Richard Mied, and Thomas Evans
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CWO

Computer Resources: IBM P4 [NAVO, MS]; SGI Altix [NRL, DC]

Research Objective: To understand submeso- to shelf-scale coastal ocean processes responsible for the flow patterns seen in optical and radar images of the sea surface and to simulate these processes with numerical models.

Methodology: The Fourier/Chebyshev transform method is used to solve the governing equations for submesoscale processes. The process model simulates three-dimensional, nonhydrostatic, rotating stratified flow. A semi-Lagrangian, higher order finite-difference method is used for the nonhydrostatic coastal waves/current simulation. This nonhydrostatic model for coastal oceans known as NMCO has both a free surface and a variable bottom topography and is capable simulating motions at all scales in a coastal ocean. This model developed at NRL-DC is fully parallelized. It has previously been validated and published in the literature (Shen and Evans, J. Comp. Phys., 2004).

Results: (1) The coastal ocean model, NMCO, is presently being used to model coastal ocean's sound speed environments affected by internal solitons. The specific focus of this year's study has been the simulation of soliton propagation in the area of Asian Seas International Acoustics Experiment (ASIAEX) in the South China Sea, in support the acoustic project, "Integrated submesoscale/acoustic modeling predictive capability for littoral regions." Observations show that internal solitons affect the acoustic array signal gain in this area. To simulate their effects on acoustics, an internal soliton similar to that observed is prescribed and integrated forward in time. The result shows that the soliton loses speed and amplitude as it propagates into increasingly shallower water, and at the same time, becomes dispersive giving rise to secondary waves. The soliton also develops curvature, being refracted by the bathymetry. These changes in soliton are consistent with observations and are shown to have effects on the acoustic array signal gain similar to those measured during the ASIAEX experiment. (2) The 'Velocity Projection' method (VP) developed at NRL-DC has been broadened to use sea surface tracer data, such sea surface temperature and colors, as input for determination of three-dimensional coastal currents. The method was previously limited to the sea surface velocity data measured by shore-based HF radars. With the tracer images available from satellite remote sensing, it is now possible to apply the VP method to wide areas of coastal oceans. Because the VP method accounts for the dynamics of the currents and use multiple-image sequence, it is shown capable of producing more accurate estimate of surface velocity vectors as opposed the conventional approaches which consider only kinematics. A demonstration of the applicability of the method to the actual tracer images is made with a sequence of satellite images of the sea surface temperature field on the continental shelf off the New Jersey coast. The computed surface current velocity vectors are compared to the vectors measured directly by the shore-based HF radars. Both speed and angle of the vectors obtained from VP are significantly closer to the measured than those given by the conventional methods, in particular the averaged angular error can be as low as only a few degrees whereas the error with the conventional methods is well over ten degrees. The results has been submitted to the Continental Shelf Research for publication

Title: Model Hindcasting in Smart Climatology

Author(s): James Dykes[1], Lucy Fitzgerald Smedstad[1] and Germana Peggion[2]
Affiliation(s): [1]Naval Research Laboratory, Stennis Space Center, MS and [2]University of New Orleans, LA

CTA: CWO

Computer Resources(s): IBM P4, IBM P5 [NAVO, MS]

Research Objectives: This project aims to develop concepts and techniques that clearly define smart climatology for strategic planning for ASW, SPECOPS and MIW, enabling superior analysis of environmental variability to support tactical decision planning. Ultimately, smart climatology is to take into account the effects on strategic planning of tactical extremes in ocean and atmospheric conditions caused by the large-scale climatic variations. A demonstration of this project is planned to provide the guidance for future potential transition of an end-to-end capability to the war fighter. The portion of this project requiring HPC resources involves running (MetOc) models for long historical periods with the goal of providing quick-turn-around results on demand.

Methodology: MSRC resources were utilized in generating the data and information based on running atmospheric and oceanographic models over a long period of time in the past, also known as hindcasts. A high resolution tactical scale climatology dataset required for knowledge extraction was generated by an air/ocean/wave coupled system, which has been constrained by relevant large-scale climatic variations. The system components include COAMPS®, WAVEWATCH III, NCOM, and SWAN for creating strategic and tactical climatologies in data-sparse and data-void areas, creating a three-dimensional depiction of the atmosphere and the ocean over a three-year period (1997 through 1999). This period is limited in time to cover the anomalous events of an extreme El Niño and La Niña for demonstration, and is expected to expand in later work. Certain parameters are extracted depending on the mission scenario. Ultimately, all the models will be closely coupled under ESMF, but for now they were run separately. The ocean models used forcing provided by either NCEP/NCAR Reanalysis or COAMPS® run at NRL Monterey. Global NCOM output provided the boundary conditions for the regional NCOM.

Results: WAVEWATCH III was run for the period 1993 through 2002 to provide spectral boundary conditions for a series of three SWAN nests for an area centered near the Taiwan Straits. Each WAVEWATCH III run took ~16 hours of wall clock time using eight processors on the IBM P4+ (kraken) per model year. Previously created restart files allowed for multiple year runs at once. NCOM nests using Global NCOM for boundary conditions were run from midway in 1997 through 1999. Each NCOM run took 60 hours of wall clock time using four processors on kraken per model year. Although COAMPS was run on a Linux cluster in Monterey, preliminary results of COAMPS on the IBM P5+ (babbage) show typical run times for a 48-hour period were about 50 minutes on 16 processors. All the resulting model output files including the complete atmospheric model outputs were stored on the Sun-Fire-15000 (vincent) server occupying about 15 terabytes total. This server provided a convenient means for data sharing amongst team members. The processed output is passed on to NRL 7440 personnel who are designing and building software to aid in analysis of the data.

Significance: The model output will be used in pattern analysis procedures resulting in information that will allow us to examine and validate the types of data and statistics that may impact strategic planning.

Title: East Asian Seas NCOM Transition Project
Author(s): Shelley Riedlinger and Richard Allard
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM P4 [NAVO, MS]

Research Objectives: To understand the processes which affect coastal and semi-enclosed seas through a combined use of ocean models, field observations and satellite data. The goal of this project is to use this understanding to develop and improve state-of-the-art nowcast/forecast systems for Navy relevant coastal regions. In this effort we also seek to further validate the East Asian Seas (EAS) Navy Coastal Ocean Model (NCOM) model and to identify improvements to the model. The EAS is also used as part of the relocatable multi-nest modeling system and other high resolution models.

Methodology: The EAS ocean model has a horizontal resolution of 1/16°, and includes tides, monthly river discharge and receives initial and boundary forcing from the Global NCOM. EAS is forced with atmospheric forcing from the Navy Operational Global Atmospheric Prediction System. In these studies, the EAS model is run with changes to input fields and model parameters. Comparisons of model results to data are used to determine the significances of the changes. In addition, work continues with universities and field campaigns to obtain additional data and better understanding of the important physical processes in the EAS region.

Results: Sensitivity studies of changes to input fields and model parameters have shown slight improvement in temperature profiles. Collaboration with universities has increased the availability of data for further validation. The PhilEx Cruise and drifter studies suggest that the EAS model produces reasonable general circulation, but better agreement is desired. It has been shown that EAS16 can be used as part of a nested model setup to provide higher resolution results in straits, bays etc.

Significance: The EAS NCOM has shown remarkable skill as a Navy Search & Rescue tool as evidenced in the Indonesian jet airliner crash in January 2007. EAS model currents were ingested by a NAVOCEANO surface drift model to estimate the aircraft's black box based on trajectories of wreckage.

EAS-NCOM DRIFTERS FOR 01 JAN 2007 – 10 JAN

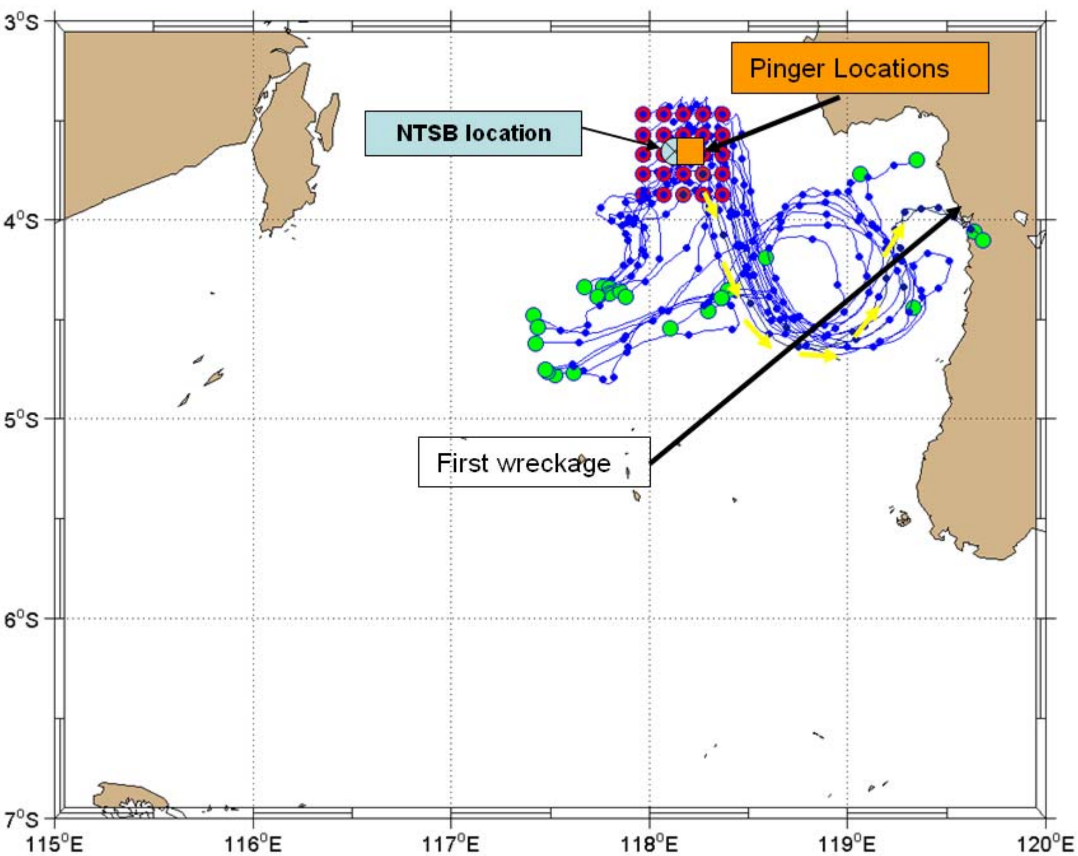


Figure 1. A forecast plot of the possible drift tracks for objects on the surface based on the EAS NCOM. Movement is based strictly on ocean model surface currents (no windage). The 24-hour surface current forecasts are concatenated to create a 10-day forecast. The field is "seeded" with a series of locations at 0700Z 01JAN07 (RED dots) and run forward in time to 10JAN07 (GREEN dots). Each BLUE dot represents 24 hours. Note that in this scenario, two objects slightly southeast of the NTSB location would drift toward the beach where the FIRST WRECKAGE piece was discovered. There is a counterclockwise eddy in the area that appears to capture a number of objects. Figure courtesy of the Naval Oceanographic Office.

Title: Eddy-resolving Global and Basin-scale Ocean Modeling
Author(s): Alan J. Wallcraft, Harley E. Hurlburt, Jay F. Shriver and Lucy F. Smedstad
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

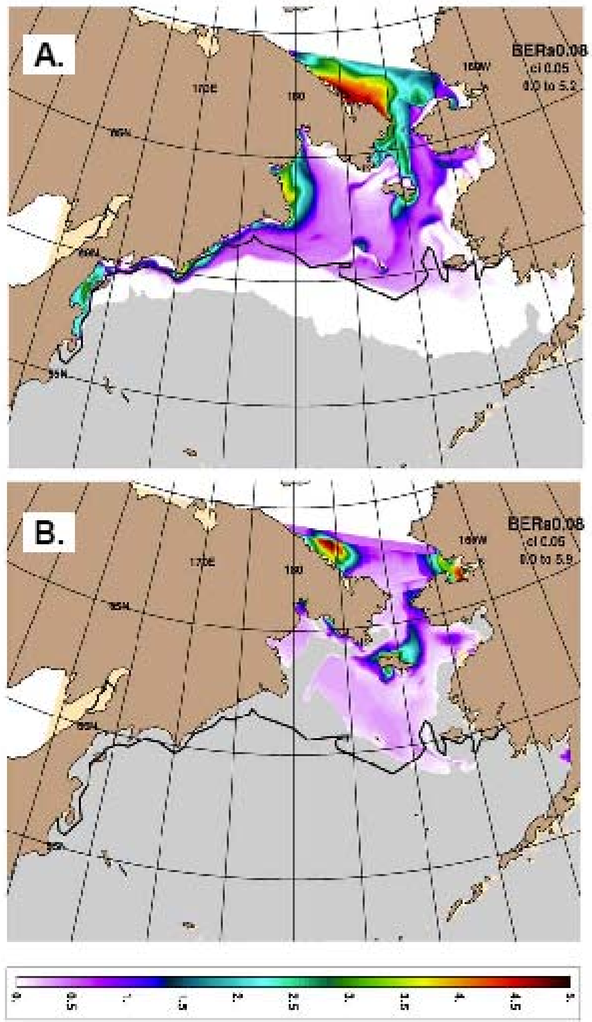
Computer Resources: IBM P4, IBM P5 [NAVO, MS]; Cray XT3 [ERDC, MS]; IBM P4 [ARSC, AK]

Research Objectives: Modeling component of a coordinated 6.1-6.4 effort on the "Grand Challenge" problem of eddy-resolving global and basin-scale ocean modeling and prediction. This includes increased understanding of ocean dynamics, model development, model validation, naval applications, oceanic data assimilation, ocean predictability studies, observing system simulation studies, and nested models.

Methodology: The appropriate choice of vertical coordinate is a key factor in OGCM design. Historically, we have used the NRL Layered Ocean Model (NLOM) because of its efficiency in computer time per model year. Layers are optimal for deep water but not for coastal domains, so as more computer power becomes available we are transitioning to models with hybrid vertical coordinates. The NRL Coastal Ocean Model (NCOM) allows both terrain-following and Z-levels in the vertical, and HYCOM has a completely general vertical coordinate (isopycnal, terrain-following, and Z-level) via the layered continuity equation.

Results: 32 publications (submitted to in print) excluding abstracts, 28 refereed. Global modeling: The 1/32° near-global upgrade to the original NLOM 1/16° system has been running in near real-time since Nov 2003, and was made operational at NAVO on 6 Mar 2006. Real-time and archived results are at: **http://www.ocean.nrlssc.navy.mil/global_nlom**. The fully global NCOM system with 1/8° mid-latitude resolution has been run daily by NRL in near real-time since November 2001, and was made operational at NAVO on 19 Feb 2006. It assimilates 3-D T\&S fields derived via MODAS synthetics from NLOM SSH and MODAS2D 1/8° SST. See: http://www.ocean.nrlssc.navy.mil/global_ncom. Experiments were performed to determine the impact of modifications to assimilation in this system. Specifically, we used mixed-layer depth (MLD) forecasts to modify the synthetic profiles assimilated by Global NCOM. Significant improvements were found in MLD, sonic-layer depth and below-layer gradient, key indicators of operational product performance. Additionally NCODA was used to assimilate in-situ observations. Based on the evaluations, these capabilities are completing FY07 transition to operations in preparation for OPTEST. Development of 1/12° global HYCOM began in 2005 and continues this year under DoD Challenge. Since December 2006 we have run a global HYCOM nowcast every day, and since February 2007 we have performed a nowcast and a 3-day forecast every day in real time. See: http://www7320.nrlssc.navy.mil/GLBhycom1-12/skill.html. Outside DoD Challenge, we continued to run at 0.72° globally to test through flow at straits, different mixed layer models, layer structure, and corrections to the atmospheric forcing. We also used 0.72° and 1/12° Arctic-only and 1/12°Bering Sea regions to test sea-ice issues. This includes the CICE sea-ice model 2-way coupled to HYCOM. Data Assimilation: We continue to use the Gulf of Mexico as our primary testbed for NCODA data assimilation, with sea-ice assimilation testing in the Bering Sea. The fully global 1/12° NCODA/HYCOM system is running under DoD Challenge. CONESTS and SEED: Using a 1/25° Gulf of Mexico HYCOM domain with and without NCODA data assimilation covering hurricane Ivan in 2005, we demonstrated the effectiveness of using data assimilation on the upper-ocean response to hurricane forcing and performed validation of model simulations with and without data assimilation against ADCP SEED observations.

Significance: Data Assimilative eddy resolving models are important components of global ocean monitoring and prediction systems. Military and civilian applications include ship routing, search and rescue, antisubmarine warfare, coastal and mine warfare, fisheries forecasts, pollutant spill risks, El Nino forecasting, ocean observing system simulation, and global change studies.



Ice thickness in meters on April 16, 2004 from 1/12° HYCOM Bering Sea: a) 2-way coupled to LANL's CIC, b) using HYCOM's internal thermodynamic ice model. Grey indicates no ice, and the thick line is the National Ice Center's ice edge analysis. There is no assimilation of ice or ocean data into the models, which re nested in 1/12° Global HCOM and forced by NOGAPS atmospheric fields.

Title: Progress of Global Ice Modeling
Author(s): Pam Posey and Lucy Smedstad
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM P4 [NAVO, MS]; SGI Origin [ERDC, MS]

Research Objectives: (1) to contribute to the development of the next generation Navy coupled ice-ocean model, (2) to test the new Navy Polar Ice Prediction System 3.0 (PIPS 3.0) model on computers compatible with the types of machines that will be available at the Navy operational centers, and (3) to gain an understanding of seasonal and inter-annual variations of coupled ice-ocean systems in the Arctic and its marginal seas.

Methodology: The overall approach is to take advantage of recent model improvements to eddy-resolving, hybrid-coordinate global ocean models (such as NCOM) and to ice models (the viscous-plastic Hibler and elastic-viscous-plastic LANL model). These improvements embraced numerical schemes, model physics, small-scale parameterization, ridging scheme and adaptation to massively-parallel machines. A major effort during this year was coupling CICE (PIPS 3.0) to global NCOM. Model physics verification will include testing the effect of particular choice of ice rheology and thermodynamics, and the nature of atmospheric forcing (wind stress over ice, prescribed vs. bulk heat flux formulas, feedback effects, etc.) Simulations and process studies include runs on both seasonal and inter-annual time scales. The effect of atmospheric forcing on the ice-ocean model codes is examined by running multi-year simulations (2-5 years) to evaluate the development of ice thickness and ice concentration. The main verification data sets for ice come from SSMI microwave data on ice concentration, Arctic buoy data on ice motion, and submarine sonar data on ice-thickness.

Results: The LANL CICE model was chosen for the new PIPS 3.0 based on its advanced ice thickness structure (multi-level), EVP ice rheology, ice ridging and its improved thermodynamics. The purpose of the new PIPS 3.0 is to forecast a better representation of the ice edge, ice drift and to provide guidance for determining areas of lead formation. A high resolution (9 km) and multi-level ice thickness formulation should provide the means to predict areas of possible lead opening and closing and improved ice edge growth/decay. During this year, the LANL CICE model was tested on an Arctic grid, similar to that used in the PIPS 2.0 model but at higher resolution (9 km vs. 25 km), that was coupled to a climatic ocean. During FY07, a file-transfer coupling system was developed between PIPS3.0 and NCOM. NCOM ocean fields (salinity, temperature and ocean currents) were passed and used by PIPS and then ice fields (ice thickness, ice concentration, ice/ocean stresses and heat fluxes) were in turn passed and used by the next forecasted run of NCOM. This file-transfer system was run from March 1, 2006 through present. Results from both the ice and ocean model were compared to real-time data. Figure 1 presents the ice concentration (%) for March 31, 2006 for the operational PIPS2.0, and the NCOM/PIPS3.0 system compared to an ice analysis map from the National Ice Center of the Eastern Siberia for the same time period.

Significance: This project is applied to the testing and validation of existing sea ice forecast systems and the development of new systems. In addition, this project provides insight into the ice and ocean circulation of the Arctic both regionally and in the global sense.

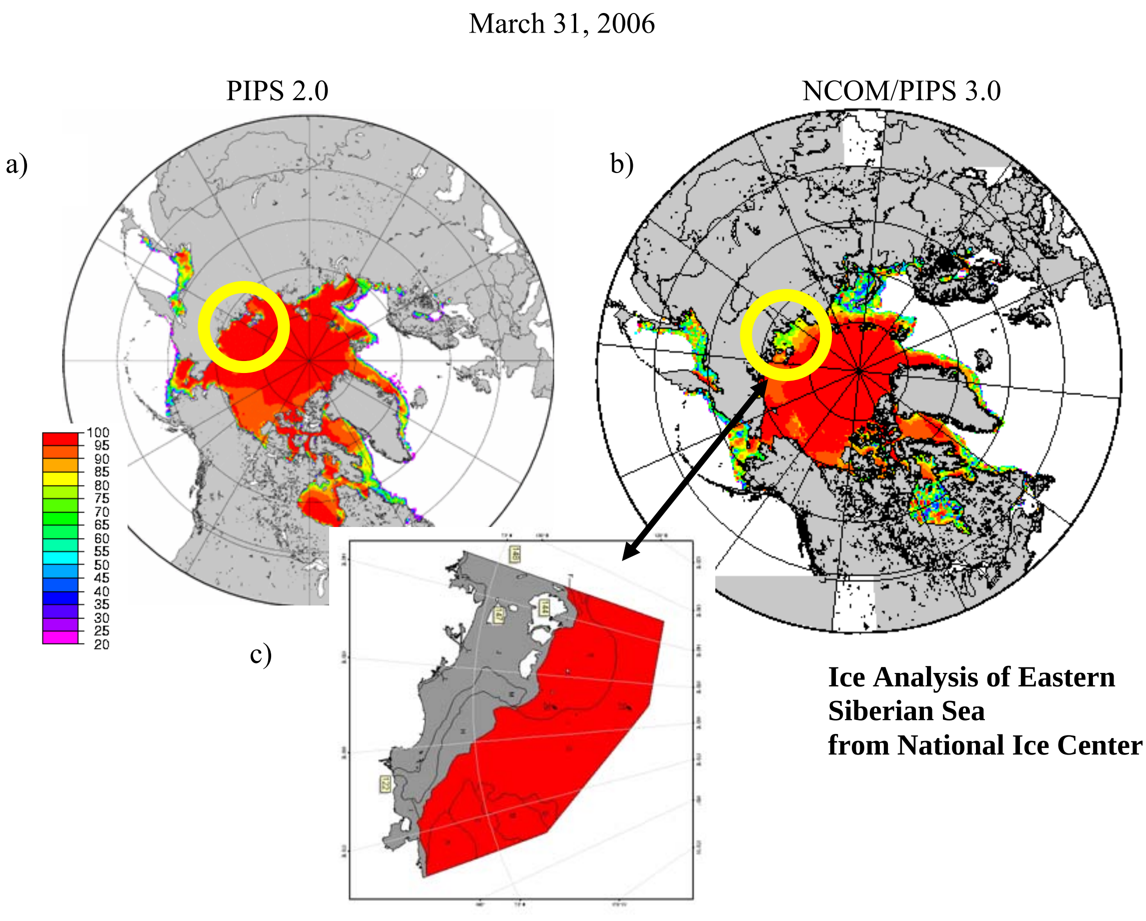


Figure 1. March 31, 2006 ice concentration (%) for a) the operational PIPS 2.0 system, b) the NCOM/PIPS 3.0 system and c) an ice analysis of the eastern Siberian Sea from the National Ice Center. The coupled NCOM/CICE (b) shows a more realistic ice concentration as compared to the ice edge analysis (c).

Title: Finite Element Coastal Modeling
Author(s): Cheryl Ann Blain[1], T. Christopher Massey[1] and Robert Linzell[2]
Affiliation(s): [1]Naval Research Laboratory, Stennis Space Center, MS, [2]Planning Systems Inc., Slidell, LA
CTA: CWO

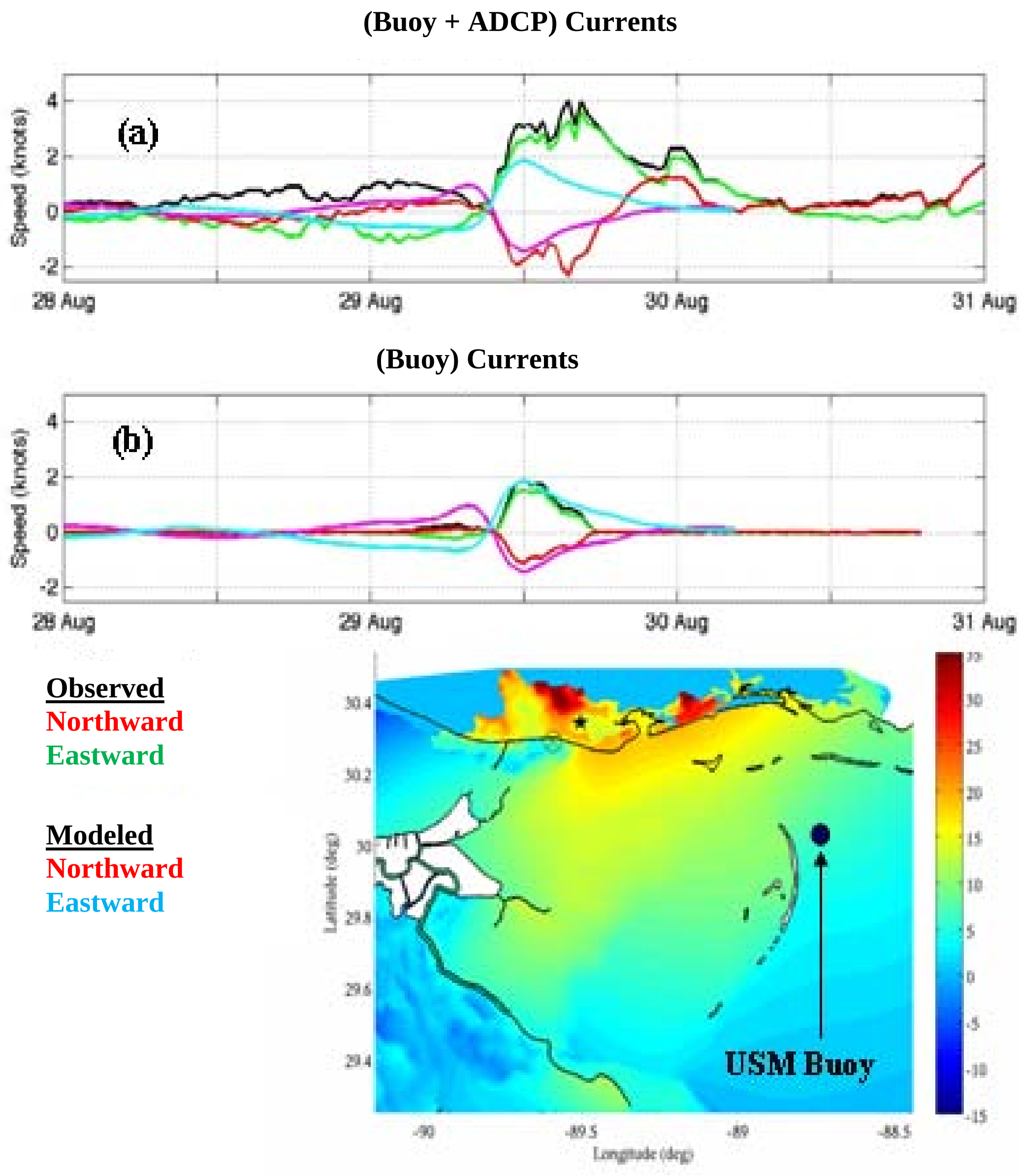
Computer Resources: Cray XD1 [NRL, DC]; IBM P4, IBM P5 [NAVO, MS]; Linux Cluster [MHPCC, HI]

Research Objectives: The objectives are to more fully understand and predict the complex dynamical processes occurring in coastal waters through the development and application of advanced, finite element-based numerical coastal ocean models. The bulk of the high performance computing work undertaken this FY has focused on benchmarking the two- and three-dimensional, depth-averaged shallow water equation model, ADCIRC, for transition to the Naval Oceanographic Office.

Methodology: The finite element coastal circulation model, ADCIRC, has a successful history of accurately modeling both tidally-induced currents and water levels [Mukai *et al*., 2002; Blain *et al*., 2004] as well as the development and propagation of storm surge and inland inundation generated by hurricane force winds [e.g., Blain *et al*., 1994; 1998; Westerink *et al*., 2005]. A set of three benchmark problems that spans the range of barotropic dynamics is selected to validate water level and current computations by the ADCIRC model. Current observations from Univ. Southern Mississippi, USGS high water mark data and several NOAA water level gages render hurricane Katrina (August, 2005) a particularly rich benchmark for validating the prediction of storm surge and inundation. A NOAA benchmark for Delaware Bay [Zhang *et al*., 2006, NOAA Tech Rep. NOS CS 24] is adopted for validation of two-dimensional tidal currents and water elevations in a shallow embayment subject to river discharge; historical data is available at 16 water level stations and 44 current meter locations. The final benchmark, Rattray Island, Great Barrier Reef, AU [White and Deleersnijder, 2007] is an Unstructured Grid Model Community Benchmark focused on three-dimensional tidal currents and vertical mixing using field data recorded by 26 current meters over a two-week period. Standard quantitative error measures based on model-data comparisons are the basis for ADCIRC model validation.

Results: The computed ADCIRC model currents represent well the intensifying northwest current during the approach of hurricane Katrina and the subsequent sharp directional change to the southeast once storm winds reversed direction (right (a)). The ADCIRC predicted currents also matched movement of the buoy itself (right (b)), lifted off the sea floor and carried by the current and waves, primarily after the storm tracked inland and inundated waters rushed off the land back into the sea. Time series comparisons for water levels and currents at each station in Delaware Bay reveal excellent skill scores (near 1, the best possible). Interestingly, once comparisons over the estuary as a whole (considering all stations) are conducted for individual constituents, model skill is notably degraded for non-dominant tidal constituents. This result reflects the inhomogeneous, non-linear response of the tidal constituents to friction within the estuary. Modification to the benchmark will have to account for spatially variable frictional characteristics within the estuary which should improve the tidal solution by constituent.

Significance: Coastal ocean models, such as ADCIRC, once transitioned to NAVOCEANO, the primary operational center for Navy oceanographic prediction systems, are applied at spatial resolutions ranging from hundreds of meters to tens of meters. The results are detailed maps of currents and water levels in shallow waters and inundated areas that aid in mission planning and execution for Special Warfare, Mine Warfare and amphibious operations. Non-naval interest in riverine and coastal environments relates to sediment transport, search and rescue operations, pollutant dispersal, and coastal restoration.



ADCIRC modeled currents (magenta-northward, cyan-eastward) compared to measured currents (red-northward, green-eastward) during passage of hurricane Katrina at a location seaward of the Mississippi coast barrier island (map). Landfall of hurricane Katrina occurred on the MS-LA border at 10 am 29 august 2005 (CDT). Time units are local, CDT, and currents are given in knots. Note: Buoy data courtesy of Dr. S. Howden, USM.

Title: Coupled Ocean-Acoustic Dynamics
Author(s): A. Warn-Varnas, S. Piacsek and J. Cazes
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM P4, IBM P5 [NAVO, MS]

Research Objectives: The principal goals of this project are to acquire an in-depth understanding of how changes in ocean parameters couple into changes in acoustic propagation, and to exploit this understanding to develop much more efficient 4-D ocean acoustic predictions. Specific goals include (a) the understanding of the generation and propagation of solitons in the Yellow Sea, and the Straits of Messina and Luzon; (b) an understanding of how changes in ocean parameters couple into changes in acoustic parameters; (c) the exploitation of this understanding for generating more efficient 4-D ocean acoustic predictions, and (d) to search with coupled ocean-acoustic models for losses and enhancements of acoustical energy and to explain the loss and enhancement mechanisms.

Methodology: Perform joint ocean-acoustic modeling with very high resolution soliton models, with grid spacings of a few meters in the vertical and tens of meters in the horizontal. Among the models employed will be the 2.5 D nonhydrostatic sigma coordinate model of Lamb (1994) and the 3D nonhydrostatic sigma-coordinate model of Smolarkiewicz (2001). These models predict the soliton signal in terms of temperature, salinity, and current. The local soliton models will be nested in temperature and salinity fields derived from data or the MODAS-NCOM data-assimilative model results. Tidal forcing will initially be provided by analytic functions, and later by barotropic tidal models or tidal data bases. The calculated sound speeds from oceanographic predictions will be used in acoustical field calculations for various environmental situations.

Results: In Strait of Messina simulation studies with a horizontal resolution of 50 m and .8m to 4m in the vertical were undertaken. These resolutions are an improvement over the previous 100 m resolution in the horizontal. This enables an improved representation of solitary wave evolution and propagation. In Strait of Messina studies an increase in thermocline and halocline depth yielded a higher phase speed for solitary waves on the right side and a modified evolution dynamics on the left side with a lower phase speed. Previous acoustical calculations with coarser horizontal resolution exhibited different ray patterns in cross range vertical planes. In an analogous study acoustical intensity dependence on frequency is pursued with a two-layer model. In the study a feedback method is developed that can indicate whether solitons are likely to adversely affect acoustic propagation. In Luzon Strait and South China Sea region horizontal resolution studies were conducted. It was found that mesh size is an important factor both in the principal propagation direction (E-W,x) or perpendicular to it (N-S,y): A $dx < 500$m is necessary to produce and maintain solitons, and a $dy < 5$ km is necessary to represent sill widths and achieve good curvature effects of wave fronts. At 500 m depth in Luzon Strait the predicted temperatures, salinities, and vertical velocities, using dx=167m and dy=2km, exhibit structures and curvatures similar to satellite observations.

Significance: MCM, Special Warfare, UAV's and shallow water acoustics are affected by interaction with solitary wave trains.

Title: Dynamics of Coupled Models
Author(s): John C. Kindle
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM P4, IBM P5 [NAVO, MS]

Research Objective: Investigate the coupling of dynamical ocean and atmospheric models. Provide a foundation for the development of scientifically valid, dynamically coupled atmosphere-ocean models.

Methodology: Emphasis in this project will be on evaluating the quality of surface momentum and heat fluxes from the atmosphere model component of the Coupled Ocean-Atmosphere Mesoscale Prediction System (COAMPS) model, and studying the response of the Navy Coastal Ocean Model (NCOM) to such surface forcing. Much of the project focus will be on the Pacific West Coast (PWC) region, and on the Arabian Sea-Indian Ocean in support of a multi-institutional NASA funded project of which NRL is a primary participant.

Results: We participated in design; planning and execution of the ONR sponsored MB2006 experiment in the Monterey Bay area. Real-time predictions of oceanic conditions in the Monterey Bay area were conducted in support of the experiment. A hierarchy of different resolution nested NCOM-based oceanic models in the Pacific Ocean was used for predictions, and observations from gliders, AUVs, aircraft surveys and ship cruises were assimilated by using the Navy Coupled Ocean Data Assimilation System (NCODA).

In collaboration with the 6.1 Core "Coupled Bio-Optical and Physical Processes" project, we conducted the analysis of the MB2006 experiment observations and model results, and compared them with post-experiment analysis of other two experiments AOSN II (2003) and AOSN I (2000). The following issues were investigated: COAMPS predictions of momentum, short and long wave radiation fluxes and their comparisons with the available mooring observations; estimation of the heat budget of the three dimensional upwelling center and evaluation of relative contribution of different terms to the heat budget, impact of data assimilation on surface and subsurface properties of the NCOM based model.

Additionally, a high resolution (~ 4 km) implementation of the regional NCOM-CCS model was accomplished in collaboration with the Dynamics of Coupled Models project. This implementation extends the domain to 52N and uses the DBDB2 2 minute bathymetry. In collaboration with the 6.2 NRL core project "CONESTS", a comparable HYCOM model was implemented using the same domain, bathymetry and horizontal resolution.

A regional NCOM model for the Indian Ocean at 12km resolution was implemented in order to examine the coupled air-ocean and biological responses to climate related changes in the strength of the Arabian Sea Southwest Monsoon to recent changes in the Eurasian snow cover. The Regional Indian ocean model, which receives boundary conditions from global NCOM, uses MODAS data assimilation also includes a 9-component biological model. In FY08, high resolution sub-nests for the northern Arabian Sea will also be developed. The work is in support of a mutli-institional NASA funded project, to which the significant HPC resources are an important contribution.

Significance: Understanding and predicting the dynamics of the air-sea surface boundary layer is important for short and long-term weather forecasting. This is critical for operations and weapon deployment, especially in the coastal and littoral zones. Improved large to mesoscale forecast skill is critical to both military and civilian use of the oceans, particularly on the continental margins.

Title: COBALT
Author(s): John C. Kindle
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM P4, IBM P5 [NAVO, MS]

Research Objective: The primary objective of proposed research is to understand the physical dynamical influences on the biodynamical processes and optical properties of the North Pacific eastern boundary current regime.

Methodology: This project will apply nested, coupled physical-bio-optical models of the coastal region together with in-situ and remotely sensed observations and data assimilation techniques for both physical and bio-optical fields to examine the research issues described above.

Results: In collaboration with scientists from various institutions (Princeton, NPS, Woods Hole, Scripps, Harvard, MBARI), we participated in design; planning and execution of the ONR sponsored MB2006 experiment in the Monterey Bay area. Real-time predictions of oceanic conditions in the Monterey Bay area were conducted in support of the experiment. The NCOM model outputs were used by the Princeton group to predict behavior of the coordinated glider fleet, and results were displayed on the Princeton Glider Prediction page. This represents the first case where model predictions were utilized for coordinated dynamical control of gliders in an automated manner. In collaboration with the 6.1 Core Air-sea coupling in the Coastal Zone project, we conducted the analysis of the MB2006 experiment observations and model results, and compared them with post-experiment analysis of other two experiments AOSN II and AOSN I.

The nested high resolution model for the Monterey Bay (NCOM-ICON) has been tested and evaluated during upwelling and relaxation events observed in the Monterey Bay area. In collaboration with the 6.1 Core Air-sea coupling in the Coastal Zone project, issues investigated during the past year include: coupling to the Navy atmospheric model COAMPS, NCOM-based model simulations on a curvilinear-orthogonal grid, use of sigma versus hybrid (sigma-z) vertical grids, coupling with a larger-scale model on the open boundaries, and bio-physical coupling in the NCOM-based ecosystem model.

A coupled ecological-physical numerical model with improved simulation of PAR (photosynthetically active radiation) propagation through the water column is able to successfully reproduce surface chlorophyll patterns observed via satellite as well as simulate the well-know phenomenon of a subsurface maximum chlorophyll concentration. Additionally, a high resolution (~ 4 km) implementation of the regional NCOM-CCS model was accomplished in collaboration with the Dynamics of Coupled Models project.

The nonhydrostatic NRL-MIT modeling system was embedded within multiply nested NCOM domains in the northern South China Sea (SCS) and in the Mid Atlantic Bight (MAB). The SCS hindcasts showed the growth and transformation of transbasin Nonlinear Internal Waves (NLIWs) generated in the Luzon Straits and the local generation of NLIWs near DongSha Is.

Significance: This effort will provide new capability for underwater ASW target vulnerability and detection and the effective use of E-O sensors. Additionally, this effort will support effective use of Navy laser system performance for underwater imaging for MCM operations and hydrographic laser bathymetry systems.

Title: Data Assimilation Studies
Author(s): William F. Campbell
Affiliation(s): Naval Research Laboratory, Monterey, CA
CTA: CWO

Computer Resources: IBM P4 [NAVO, MS]

Research Objectives: Our objective is to investigate methods to improve the use of remotely sensed data for global and mesoscale numerical weather prediction, including the addition of new data types, aid the development and testing of the NRL four-dimensional variational (4DVar) data assimilation system and to develop improved ensemble based forecast error covariance models. This system can also be used for basic and applied research leading to an improvement in our understanding of processes. Our goal is to assimilate traditional data and data from new sources efficiently and effectively, to provide the best atmospheric analysis, and ultimately improve numerical weather forecast performance.

Methodology: The NAVDAS-AR (NRL Advanced Data Assimilation System – Accelerated Representer) is our new 4DVar assimilation system, which is being developed and tested with our global model NOGAPS (Navy Operational Global Atmospheric Prediction System) for simulations and prediction of the atmosphere on a global scale. NAVDAS-AR is also used as a testbed for new mesoscale ensemble forecasting techniques. In addition, new types of data (such as ozone and GPS radio occultation) from advanced satellite instruments are being assimilated, and NOGAPS is being extended through the mesosphere to accommodate this data. Both NOGAPS and NAVDAS-AR incorporate MPI (Message Passing Interface) and are efficient and scalable to hundreds of processors.

Results: In FY07, both NAVDAS and NAVDAS-AR were successfully compiled on the IBM P4+ (Kraken) at NAVO. In addition, cycling data assimilation experiments using NAVDAS and NOGAPS-ALPHA (Advanced Level Physics and High Altitude) have been run successfully on Kraken. NAVDAS was modified to allow for flexible specification of vertical resolution and pressure levels up to 93 km. Microwave limb sounder (MLS) ozone and temperature, along with solar backscatter ultraviolet (SBUV) ozone, have been assimilated, and compare favorably with results from GMAO (NASA Global Modeling and Assimilation Office) and the Met Office.

Significance: HPC computing allows for the rapid development and testing of NRL’s core systems: NOGAPS, NAVDAS, NAVDAS-AR, and COAMPS. The extension of NOGAPS and NAVDAS/NAVDAS-AR through the mesosphere impacts missile re-entry, unmanned high-altitude reconnaissance, and the high altitude transport and dispersion of debris from explosions and natural phenomena such as volcanic eruptions. Data assimilation extensions and improvements will result in more accurate forecasts, which are of vital importance to the DoD.

Title: Coastal Mesoscale Modeling
Author(s): James D. Doyle
Affiliation(s): Naval Research Laboratory, Monterey, CA
CTA: CWO

Computer Resources: SGI Origin, SGI Altix [ASC, OH]; IBM P4, IBM P5 [NAVO, MS]; Linux Cluster [MHPCC, HI]; SGI Origin [ERDC, MS]

Research Objectives: Our objective is to develop and validate a coastal/littoral data assimilation and prediction system that can be used to provide high-resolution (<5 km) analysis/nowcast/short-term (0-48 h) forecast guidance for tactical sized areas of the world. This system can also be used for basic and applied research leading to an improvement in our understanding of atmospheric and oceanic processes. Further improvements to the mesoscale prediction system will result from the basic and applied research.

Methodology: The Coupled Ocean/Atmosphere Mesoscale Prediction System (COAMPS®[1]is being developed further for independent and coupled simulations of the atmosphere and ocean for the mesoscale. The atmospheric component of COAMPS is made up of a data assimilation system composed of the following elements: data quality control, multivariate optimum interpolation and three-dimensional variational analysis options, initialization, and a multi-nested, nonhydrostatic model. This model includes parameterizations for moist processes, surface and boundary-layer effects, and radiation processes. The NRL Coastal Ocean Model (NCOM) is currently being used for the simulation of the mesoscale ocean circulation response to the COAMPS forcing in one-way and two-way interactive modes. Ocean coupling is being developed using the Earth System Modeling Framework (ESMF). The COAMPS code maximizes efficiency through use of Message Passing Interface (MPI) technology.

Results: In FY07, COAMPS was demonstrated to be an accurate data assimilation and forecast system capable of predictions and simulations on a variety of scale from 0.3-9 km for land-sea effects, topographically driven flows, and tropical cyclones. High-resolution simulations of flow over terrain and mountains were conducted in conjunction with the Sierra Rotors Project (SRP) and the Terrain-Induced Rotors Experiment (T-REX), both of which were focused on the dynamics of sub-rotor and rotor circulations. The measurement program for SRP took place in 2004 and for T-REX in 2006. During T-REX, COAMPS was run in real time at high resolution (2 km grid increment) and the forecasts were used to select observing periods and for mission planning for three research aircraft taking measurements above the Sierra Nevada Range. Analysis of these real time forecasts is in progress. The dynamics of mountain-wave induced rotors were simulated over the Sierra range with a grid increment of 60 m. These simulations reveal the presence of small-scale sub-rotor vortices that are suspected to be aviation hazards, which were very similar in structure to observations from T-REX ground based instrumentation (Figure 1). In other studies, air-sea interaction in the Adriatic Seas was explored using the COAMPS/NCOM one-way and two-way coupled system. The coupled simulations demonstrate that the atmospheric winds and temperature were more accurately forecasted in a two-way coupled mode than with one-way coupling. High-resolution forecasts using COAMPS were used as part of the ONR Coupled Boundary Layers/Air-Sea Transfer (CBLAST) field experiment that led to improvements in the performance of near-surface temperature and winds forecasts.

Significance: COAMPS will play a significant role in providing atmospheric forecasts in support of Navy missions involving the deployment of weapons systems, strike warfare, radar propagation, and search and rescue. Research and development performed at HPC sites have led to measurable improvements in the predictive skill of COAMPS that will benefit its operational performance.

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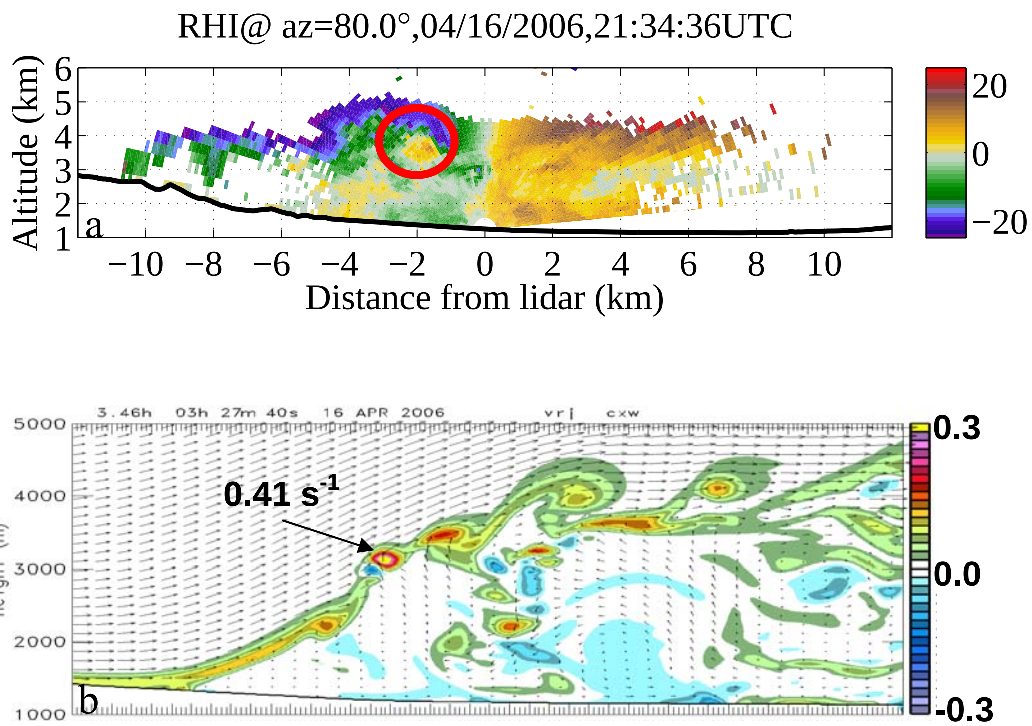


Figure 1. Doppler lidar radial velocity (m s^{-1}) from the DLR lidar (courtesy of A. Doernbrack and M. Weissmann) (top panel). Blue and green colors (negative velocities) correspond to flow towards the lidar and yellow and red colors (positive) away from the lidar). Vertical cross section of wind vectors and y-component of the horizontal vorticity (s^{-1}) (color scale shown at right) for a three-dimensional COAMPS simulation after 3 h 28 min. of integration (bottom panel). The horizontal grid increment is 60 m. Both cross sections are oriented approximately west-east with the west direction (mountain slopes) along the left portion of the plot.

Title: Development of a Middle Atmosphere in the Navy Operational Global Atmospheric Prediction System (NOGAPS)

Author(s): Lawrence Coy[1], Stephen Eckermann[1], John McCormack[1], David Siskind[1], Douglas Allen[2], Gerald Nedoluha[1], Karl Hoppel[1], Andrew Kochenash[1], Jun Ma[1] and John Lindeman[1]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC, [2]Dordt College, IA
CTA: CWO

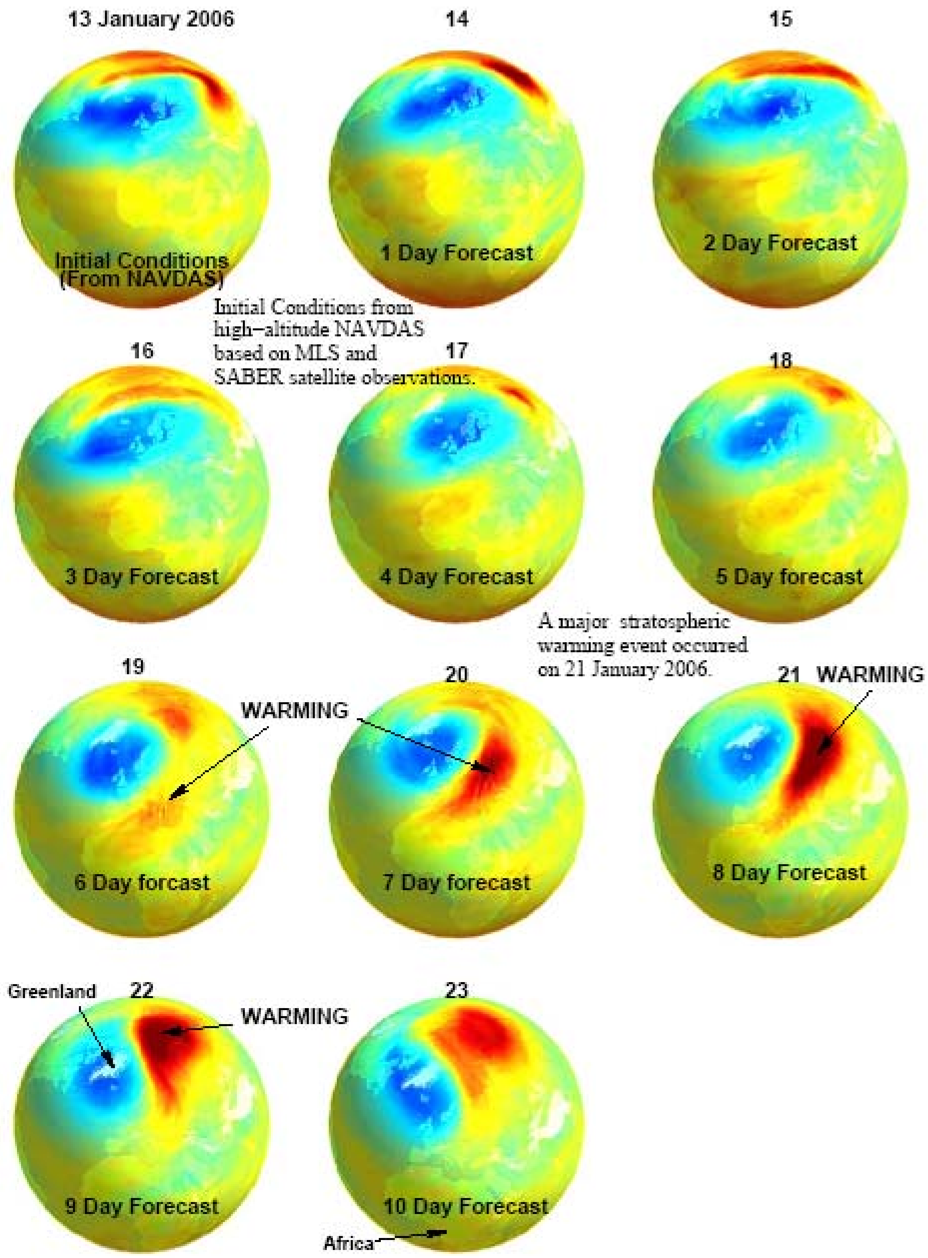
Computer Resources: SGI Altix [ASC, OH], [NRL, DC]; SGI Origin [ERDC, MS], [SMDC, AL]; Cray XD1 [NRL, DC]; IMP P4 [NAVO, MS]

Research Objectives: For FY07, the aim of the project was to test and develop an extended altitude version of the Navy's operational weather forecast model, NOGAPS-ALPHA (Navy Operational Global Atmospheric Prediction System- Advanced Level Physics High Altitude) in support of 6.1 and 6.2 research sponsored by ONR and other agencies. The inclusion of altitudes up to 120 km requires new physics for radiative heating, tracer transport (including ozone and water vapor), and sub-model resolution parameterizations which must be tested with model runs. Global, high-resolution, ground-to-space, winds and temperatures provided by these new NOGAPS-ALPHA capabilities facilitate research on the fundamental physics and "weather" of the upper atmosphere, and provide developmental forecast-assimilation capability for the near-space environment.

Methodology: The NOGAPS-ALPHA global atmospheric circulation model solves for the future state of atmosphere through time integration of the hydrostatic meteorological primitive equations on a sphere. The Fortran 90 NOGAPS code makes heavy use of MPI for parallel processing. Typically 20-80 processors are used for development runs: however, the code scales well and over 200 processors are used when the model is run operationally. Model time steps are in the range of 1 to 5 minutes. The atmospheric state at a given time requires on the order of 1-10 million numbers for its specification. We also interface NOGAPS-ALPHA to the NASA Global Modeling and Assimilation Office's ozone data assimilation system (DAS) code and the NAVDAS (NRL Atmospheric Variational Data Assimilation System) to perform full forecast-assimilation experiments to high altitude and with prognostic stratospheric chemical capabilities.

Results: In FY07, we have developed, tested, and compared ozone and water vapor photochemistry parameterizations, including those we created based on NRL's two-dimensional chemistry-radiation-dynamics model. We have added and tested high altitude radiative cooling code to NOGAPS-ALPHA. We have also developed the ability to assimilate high-altitude ozone, water vapor, and temperature observations from satellite platforms using NAVDAS. Ozone data assimilation research using the new GOATS (Global Ozone Assimilation Testing System) has been published. Other research published in peer-reviewed journals include NOGAPS-ALPHA hindcasts of resolved gravity waves and disturbed polar mesosphere meteorology have been compared to corresponding satellite observations, and NOGAPS-ALPHA forecasts have been used to study the response of the global atmosphere to a total solar eclipse.

Significance: This research directly supports on NRL's 6.1 ARI atmospheric coupling program by extending NOGAPS through the middle atmosphere (altitudes~15-100 km), and NRL's 6.2 data assimilation new start by using NOGAPS-ALPHA with NAVDAS and GOATS to assimilate higher altitude ozone and temperature data. Changes resulting from this research will be progressively transitioned into the operational NOGAPS to address the Navy's need for improved weather forecasts at all altitudes and real-time specification of the atmosphere from ground to space. For example, CHEM2D-OPP, the ozone photochemistry parameterization scheme developed at NRL-DC as part of this HPC project has been incorporated into NOAA's operational forecast system, the main weather forecast system for the US and has been transitioned to FNMOC's NOGAPS-based operational forecast system.



Temperature in the middle stratosphere forecasted by NOGAPS-ALPHA. Warmest temperatures are dark red. The warmest observed temperatures at the North Pole were observed on 12 January 2006, in good agreement with the NOGAPS-ALPHA forecasted warming. Warm air is being drawn out of the tropics and further heated by compression as it moves poleward. Note that this “forecast” was really a “hindcast” as it was run as an experiment after the warming occurred.

Title: Atmospheric Process Studies
Author(s): Young-Joon Kim, Justin McLay, Carolyn Reynolds and James Ridout
Affiliation(s): Naval Research Laboratory, Monterey CA
CTA: CWO

Computer Resources: SGI Origin [ASC, OH]; Cray X1E [ARSC, AK]; IBM P4, IBM P5 [NAVO, MS]

Research Objectives: The research objective of this project is to develop and test a state of the art global data assimilation and prediction system that can be used to improve our understanding of the fundamental dynamical and physical processes that operate in the atmosphere. Specific tasks include extending the data assimilation and prediction system up to an altitude of 100km and improving probabilistic prediction.

Methodology: The Navy Operational Global Atmospheric Prediction System (NOGAPS) was developed for basic and applied atmospheric research and for operational numerical weather prediction. NOGAPS, which serves as the primary modeling system in this project, is continuously being upgraded through improving both the physical parameterizations and dynamical core and also by extending its vertical dimension. As part of this project, a new horizontal discretization method, the spectral element method, is being investigated as a replacement to the spectral transform method currently used in NOGAPS. The new method is being tested through experimentation with the NRL Spectral Element Atmospheric Model (NSEAM). Cloud-resolving and mesoscale simulations of convection are being run using the high-resolution Coupled Ocean/Atmosphere Mesoscale Prediction System (COAMPS®[1]) to aid in physical parameterization development and the study of equatorial atmospheric waves. New methods for ensemble design are being tested in order to provide improved probabilistic forecast.

Results: Significant accomplishments were made in a number of areas. First, NSEAM has been coupled to the NOGAPS physics. A series of aqua-planet experiments have been performed. These experiments indicate significant eastward and westward-propagating equatorial waves and compare well to aqua-planet experiments with other models. Second, the new method for creating ensemble perturbations to the initial state, the Ensemble Transform (ET), is demonstrably superior to the operational method in terms of ensemble mean error, spread-skill relationships, and other metrics, and should be transitioned to operations in FY07. The use of stochastic perturbations in the parameterization of deep convection results in a significant improvement to ensemble performance in the tropics under a variety of metrics, and will be considered for transition to operations in FY08. Third, NOGAPS and COAMPS have been used to better understand equatorial Kelvin waves, and to document their forecast sensitivity to model resolution and the parameterization of deep convection. This work included some convective parameterization development, which should lead to improved simulations of these waves. Fourth, NOGAPS's model top lid has been raised to include the middle atmosphere and its drag mechanisms have been calibrated to improve the momentum budget.

Significance: The continued development of the global model will have a significant impact on weather forecasting and will also aid in the advancement in understanding the physical processes in the atmospheric system. Improvements to the computational efficiency on distributed memory machines will greatly facilitate future computationally intensive forecast capabilities, such as ensemble forecasting. We expect that the extension of NOGAPS to 100 km will improve tropospheric prediction, as well as provide improved forecast guidance in the middle atmosphere. Improvements to the Navy ensemble forecasting system will significantly increase the utility of weather forecasts for the many users who need information on forecast reliability and uncertainty.

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Electronics Networking and Systems/C4I

- Provide comprehensive outreach to existing HPCMP users in the DoD.
- Pursue aggressive outreach to existing HPCMP users in the DoD to expand the ENS user-base in size and technical scope.
- Expand ENS technical focus to include device-level simulation, nanoelectronics, and nanophotonics.
- Provide core support to existing CEA/ENS activities involving global modeling of device/EM environment.

Title: Numerical Studies of Semiconductor Nanostructures
Author(s): T. L. Reinecke, S. Badescu, E. Alldredge, L. M. Woods and R. Rendell
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: ENS

Computer Resources: SGI Altix, HPC-XC Cluster, SGI Origin [ASC, OH]; Cray XD1 [NRL, DC]; Linux Cluster [ARL, MD]

Research Objectives: To calculate the geometrical structures and the electronic and spectroscopic properties of adsorbates on nanostructures produced at NRL for applications as chemical sensors. To understand the electronic and optical properties of realistic semiconductor nanostructures for use in quantum information technology.

Methodology: *ab initio* electronic calculations are used for the electronic and structural properties of adsorbates on carbon nanotubes and on metal clusters. Numerical calculations for single particle properties, and many-body techniques for the effects of interactions between excitations are used for semiconductor nanostructures in quantum information technology.

Results: Highlights of this year's work include:
1. *Ab initio* calculations using density functional theory have been used to study adsorbate atoms on carbon nanotubes. Calculations have been done for the adsorption of acetone and alcohols on carboxyl functionalized nanotubes created by nanotube purification. New density functionals that accurately represent weak binding have also been used to study adsorption on pristine nanotubes. Alcohol adsorption at pristine sites shows a dependence on size of the adsorbate molecule that is consistent with recent NRL experimental data. This result is currently being written up jointly with experiment.

2. *Ab initio* calculations are being done to understand the effects of molecular interactions with metals on their Surface Enhanced Raman scattering. Equilibrium structures of simple benzene derivatives and their Raman scattering have been calculated and compared with experiments at NRL. We find that the Raman enhancement is due to a combination of electromagnetic and charge transfer (chemical) effects, which often cannot be separated. These results help to explain key NRL experiments and are being written up jointly with them.

3. A theory of the optical properties of coupled quantum dots has been developed and detailed numerical calculations have been made for comparison with NRL experiment. Optically controlled spins in coupled quantum dots are of importance for two qubit gates in quantum information. Coupled spin properties, non-linear optical properties and electric field dependences of the spin splitting have been calculated. They explain key NRL experiments and were published jointly with experiment in a number of papers this year.

4. Detailed numerical calculations of the photon modes were made for disordered arrays of micron-sized semiconductor microcavities for comparison with experiment. The disorder consisted of systematic variations in the sizes of the microcavities. The calculations provided a new picture of the localization of photon modes based on a series of impurity photon bands for the different cavity sizes. These results have been published with the corresponding experiment.

Significance: Improved understanding of the interactions between adsorbates and nanostructures has provided the basis for new classes of chemical sensors. Controlled coherent coupling between spins in quantum dots will form the basis for the two qu-bit gates from quantum dots needed for quantum computing.

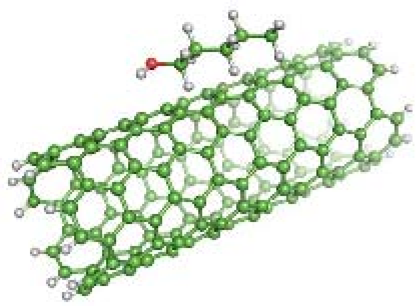

Figure 1. Structure of a 1-pentanol molecule adsorbing to the surface of a pristine (5,5), nanotube.

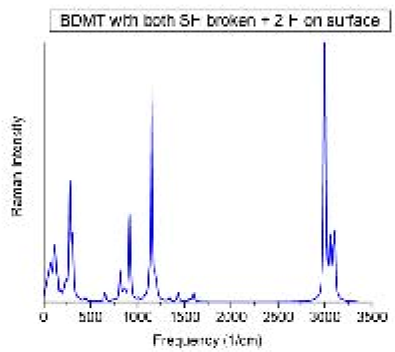

Figure 2. Surface Raman Spectrum of 1,4-BDMT (1,4 benzene-dimethyl toluene) adsorbed on a AG_{20} cluster.

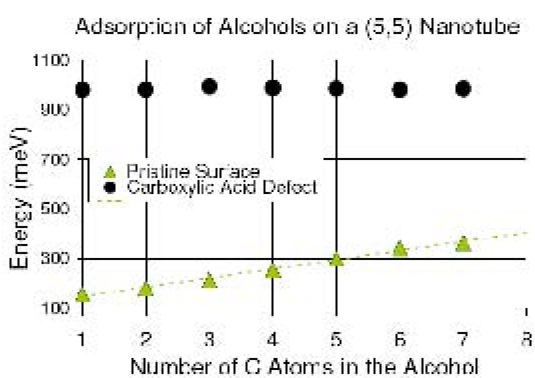

Figure 3. Comparison of the adsorption energy of 1-alcohols (methanol through 1-heptanol) binding at a carboxyclic acid defect and at a pristine surface of a (5,5) nanotube.

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Marine Geosciences Division (Code 7400)

Marine Meteorology Division (Code 7500)

Space Science Division (Code 7600)

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Major Shared Resource Centers (MSRC)

Distributed Centers (DC)

REPORT DOCUMENTATION PAGE

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14. ABSTRACT

These reports summarize the accomplishments of the NRL Principal Investigators who received computer allocations on the DoD High Performance Computing Modernization Program Shared Resource Center in FY07.

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