# Space Propulsion and Power

Presented at the AFOSR Spring Review 2013, 4-8 March, Arlington, VA.
Space Propulsion and Power Portfolio
Research to Understand, Predict, and Control Complex interactions of the Matters in Space Propulsion Systems

Coupled Materials and Plasma Processes Far From Equilibrium

DUAL- MODE PROPULSION - micro chemical thruster

Electrosprays

Novel Energetic Materials

Reduced Basis and Stochastic Modeling of high pressure combustion dynamics

Distribution A: Approved for public release; distribution is unlimited
Coupled Materials and Plasma Processes Far From Equilibrium

Electrosprays

Novel Energetic Materials

Reduced Basis and Stochastic Modeling of high pressure combustion dynamics

Space Propulsion and Power Portfolio
Program Interactions and Trends

AFRL/RQ
NASA
Joint Workshop, Dec 2011

Sayir (RTD)
Luginsland (RTB)

AFRL/RQ
NASA

Berman (RTE)

Bedford/ONR
Joint Contractors Mtg, Aug 2012
Hawkins/AFRL/RQ
Petris/DTRA
Palaszewski / NASA
Pagoria/LLNL

Sayir (RTD)
Berman (RTE)
Anthenien/ AFOSR

AFRL/RQ
NASA

Fahroo (RTA)
Darema (RTC)
Li (RTE)

Distribution A: Approved for public release; distribution is unlimited
Sheath Potential Instabilities
~4 MHz

Wall Material (SEE emitter)

SEE beam

Plasma Sheath

Why do we care?

- Change the particle & energy fluxes!
- Change the stability and lifetime of device!
- Change the characteristics (SSA) of device!
Scanning Electron Microscope Images
“Black” regions – No SEE; “White” regions - SEE

Velvet fibers on the surface
strong SEE from fibers

Velvet fibers perpendicular to the surface– No SEE except from fiber tips

To avoid field emission leading to arcing $g, l_p < \lambda_D$

Plasma flow

![Diagram showing plasma flow and field emission](image)

**Hall thruster**

**Scanning Electron Microscope Images**

**High SEE boron nitride**

**Very low SEE velvet**

- Need to take into account spatial/temporal variations of plasma scale, $\lambda_D$ (Debye length), due to plasma design and instabilities

Kinetic simulations revealed a new regime of plasma-wall interaction with a very strong secondary electron emission. See yield $\gamma$ is the number of secondary electrons emitted per incident primary electron. Effective secondary electron emission $\gamma^*$ accounts for non-Maxwellian effects.

- Electrons acquire enough energy from the electric field parallel to the wall, causing $\gamma^* > 1$.
- Sheath collapse leads to extreme wall heating by plasma and plasma losses (bad).

Modeling of plasma-wall interaction (Kaganovich, Princeton) has been experimentally validated by N. Claire and F. Doveil, Aix-Marseille Université/CNRS.

M. D. Campanell, A. V. Khrabrov, I. D. Kaganovich, Physics of Plasmas 19, 123513 (2012)

Distribution A: Approved for public release; distribution is unlimited.
Small-Scale Turbulence and Inverse Cascade
Generating Large Scale Coherent Structures for Hall discharges (magnetron similar)

- Generated by nonlinear coupling between fast-growing unstable higher frequency modes and lower frequency modes
- These large-scale fluctuations correlate to measured transport properties

Fluctuation Dispersion – k(θ)

High turbulence + coherent structures (spoke?)

Just coherent structures (drift waves?)

Width of the power spectra in frequency space

Electron mobility

Anode-region

Plume region

Distribution A: Approved for public release; distribution is unlimited
Successfully synchronized continuous wave laser induced fluorescence to coherent structures in plasmas


- **Time-Synchronized continuous wave LIF Measurements of Velocity – First Results**

- Velocity fluctuations vastly different depending on probed location in magnetized plasma
- Physical probes can only measure the average velocity!
Self-consistent analytical theory used to optimize micro plasma source

- Critical research for in-space propulsion, plasma-enhanced combustion, plasma aerodynamics, small scale sensors, directed energy devices, plasma processing …

**Micro-scale plasma source**

- Goal: Develop efficient and stable cusp-confined micro discharge
  - New “stream function” magnetic field analysis developed to predict plasma behavior throughout discharge

**Optimization using analytical theory yields 2X increase in plasma production and stable plasma over baseline**

- Model trends experimentally validated


**Discharge Axis**

**Cathode**

**Anode**

**Exit Plane**

**Flux-aligned coordinate system**

**Optimized discharge**

**Baseline**

**Plasma density (normalized to bulk)**

Distribution A: Approved for public release; distribution is unlimited
Electrosprays, dual-mode propulsion (Lozano-MIT-YIP)

Molecular Dynamics Simulations reveal how to mitigate Fragmentation of Solvated Ions

When electric field (or electric pressure) \(>\) surface tension + internal liquid pressure

- **If fragmentation occurs, efficiency drops!**

Full-atom MD with \(E\) field

- **MD results suggest the use of complex ions, as there are more degrees of freedom to dissipate internal energy**

<table>
<thead>
<tr>
<th>Ionic Liquid</th>
<th>Taylor Cone</th>
<th>monomer</th>
</tr>
</thead>
<tbody>
<tr>
<td>dimer</td>
<td>neutral</td>
<td></td>
</tr>
</tbody>
</table>

- **EMI-BF\(_{4}\)**: Less complex dimer, 100% fragmentation
- **PMI-PF\(_{6}\)**: More complex dimer, 55% fragmentation

Can we obtain Taylor cone without a physical emitter or capillary?

- Ionic liquid becomes superparamagnetic with an addition of ferromagnetic Fe2O3 nanoparticles!
Center of Excellence (Univ. of Michigan) – King (Michigan Tech)
First stable ionic-liquid ferrofluid synthesized by Hawkette, et al 2010 (Australia)

- Ethylmethylimidazolium acetate (EMIM-Ac) with bare (uncoated) Fe$_2$O$_3$ nanoparticles (Michigan Tech)

"Normal field instability" peaks (no electric field) can be rounded or they can be very sharp (shown in inset).

When an electric field is applied these peaks will get even sharper.

- Weak magnetic field with high-surface-tension ionic liquid ferrofluid shown. Normal-field instability peaks (left) are rounded in this case.
- Application of moderate electric field sharpens peaks due to electrostatic force (right)

B = 400 Gauss
E = 0 V/mm

B = 400 Gauss
E = 600 V/mm
Q1: Emitter tip density (tips per mm\(^2\)) is a function of surface tension, nanoparticle magnetization, and magnetic field. Can we synthesize an “ideal” ILFF for space propulsion that has high thrust density (milli-Newton per mm\(^2\))? 

Q2: An ILFF is a complex ferromagnetic, electrically conductive, and non-homogeneous colloidal fluid. What are the velocities of the molecular and macro species emitted when the fluid is electrosprayed and what is the beam divergence?
A Brief History of Nanoenergetic Materials

Examples from AFOSR program:

- **1st Generation**
  - Nanometer-sized Al powder/conventional propellants
  - Some performance gain, variable results

- **2nd Generation - Top down approach**
  - Quasi-ordered nanometer-sized inclusions in energetic matrix
  - Coated nanometer-sized metal powders
  - Controlled oxidation, improved storage lifetime

- **3rd Generation - bottom-up approach**
  - Organized multiscale processing to enable the insertion of nanoenergetic materials into larger units
  - 3-dimensional nanoenergetics for reaction control
  - Controlled reactivity, Improved manufacturability/processing

Distribution A: Approved for public release; distribution is unlimited
2nd Generation: Aluminum with nanoscale inclusions of fluoropolymers improves propellant performance (Son/Purdue)

- Experiments validate the hypothesis that aluminum with nanoscale fluorocarbon inclusions in a solid propellant yield reduced ignition temperature, increased burning rates, and smaller agglomerate size.

- Other nano-inclusion materials will be explored, including piezoelectric polymers to achieve smart/functional control of rate or sensitivity.

3rd Generation:
FY 2012 MURI: Smart, Functional Nanoenergetics Design from the atomistic / molecular scale through the mesoscale

biological example of multiscale effects

Multiscale Energetic Composites Fabricated on Porous Silicone Substrates (Yetter/ Penn State)

Gecko

- Rows of setae from a toe (micron)
- Spatulae (nm)

pillars were ~ 35 µm tall and have 8 µm square bases separated by ~8 µm.

Pore Diameters ~ 20nm and filled with oxidizer Mg(ClO$_4$)$_2$


Distribution A: Approved for public release; distribution is unlimited
Third Generation: Organized Multiscale Energetic Al Composites for Combustion Control

Step 1: Generation of passivated Al clusters
- Al-77 Cluster

Nanoscale passivated Al Cluster using ligands
- Pyrophoric and extremely fast reactivity
- Energetic gas generators with large ΔH of combustion
- Bond energy at ligand head controls IGNITION TEMPERATURE of cluster
- Passivating ligand provides additional energy during combustion

Aerosol of Al cluster and gas generator molecules

Step 2: Generation of mesoscale energetic composites

Mesoscale composite of Al cluster and gas generator for incorporation in solid and liquid propellants
- Energetic gas generators with large ΔH of combustion
- Gasification and decomposition temperatures of gas generator molecules control energy and temperature of mesoparticle disruption

Aerosol based self-assembly – a bulk manufacturing process

Distribution A: Approved for public release; distribution is unlimited
Copied Materials and Plasma Processes Far From Equilibrium

Novel Energetic Materials

Electrosprays

Control of Coherent Structures:
- Stable Plasma Propulsion with extended lifetime
- Plasma Photonic Crystals

- Non-Equilibrium Plasmas in Liquid Propellants
- Miscible liquid boranes in propellants
- Transformable Energetic Materials via co-crystallization or molecular blending

Reduced Basis and Stochastic Modeling of high pressure combustion dynamics

- Quantum Lattice Modeling for Multiphase reacting flows

Space Propulsion and Power

Summary and New Research Areas

Distribution A: Approved for public release; distribution is unlimited
From micro plasmas

Advantages of using Plasma Photonic Crystals:
- Tunability: variable Refractive Index and Band Gap
- Reconfigurable structure: variable crystal Geometry/Symmetry
- Inherent Nonlinearity: Harmonic Wave Generation

CHALLENGES:
- Can researchers achieve plasma crystal lattice scale to THz electromagnetic wavelength with a plasma frequency close to electromagnetic frequency?
- Can researchers generate and stabilize coherent organized microstructures from large otherwise uniform dense plasmas?
Recently, non-equilibrium plasmas have been formed in liquid water without formation of gas bubbles yielding propagation velocities of 5000 km/s for low energy nanosecond discharges (Starikovskiy et al., Plasma Sources Sci. and Technol. 20, 1, 2011).

Impact:

The formation of highly ionized channels in condensed media without void formation may create “liquid plasma” applications for ignition assistance, in-situ propellant modification, and accelerated combustion.

Challenge:

However, the roles of low energy non-equilibrium discharges with propellants and models for describing discharges in dense media are poorly understood.
**Borane-N,N diisopropyl ethylamine complex**

**Borane-triethylamine complex**

**Impact:** Low-toxicity and combustion instability control

**Challenges:**

- A fundamental study is needed to synthesize optimal amine-boranes and/or other borane molecules that are miscible in RP-1 with coupled simulation and feedback from small-scale characterization to develop optimal propellants and additives
- Applicable to ionic liquids?
Transformable Energetic Materials

Example: Co-Crystallization

Material A

Material B

co-crystallization

Material A

Material B

Application of “switching” energy (electro-magnetic, heat, light, etc.)
sensitized materials

Insensitive cocrystal of CL-20 and TNT

Heat activation


Challenges:

• Can we engineer green energetic materials that can transform (e.g. from propellant to explosive, or even in situ modification)?

• Can we model and predict transformations and necessary stimuli?
Quantum Lattice Algorithms for the Simulation of Multiphase/Multicomponent Fluid Phenomena

Classical computer bit: 0 or 1
Quantum qubit: \( |q\rangle = |0\rangle + |1\rangle \) (quantum state)
Quantum advantage: instantaneous result, noiseless, unconditionally stable, reversible

One or more qubits can be arranged on lattice sites (here 2-D)

System state at time \( t \) \[ (x_1, ..., x_n; t) \]

System evolves in time by
\[ |(x_1, ..., x_n; t + \tau)\rangle = \hat{S}\hat{C} |(x_1, ..., x_n; t)\rangle \]
where \( \hat{S} \) is a streaming operator (flow)
\( \hat{C} \) is a collision operator (fluid interactions)
both implemented via quantum gates

Algorithm can be run on quantum or classical computers

Shown by Yepez\(^1\) to reproduce the lattice Boltzmann equation, a popular CFD methodology.

BACK-UP SLIDES
Plasma Metamaterials and Plasma Optics

- plasma metamaterials, we can use the effects of $\text{Im}(\varepsilon)$

- Refractive index $N$ is imaginary -
  Bulk Electromagnetic waves cannot propagate
  But surface plasmons possible

- Refractive index $N > 0$
  Low density collisionless
  Plasmas – photonic crystals with tunable band gaps possible

- $N$ is negative -
  Metamaterial causes light to refract, or bend, differently
  than in more common positive refractive index materials

- $N$ is imaginary -
  Gyrotropic material (with imposed magnetic fields), leading to
  Faraday rotation and Optical Kerr effect, one-way waveguides

http://en.wikipedia.org/wiki/Negative_index_metamaterials

Distribution A: Approved for public release; distribution is unlimited
A plasma photonic crystal (PC) is an array of plasma structures which have the unique ability to control the propagation of EM waves.

Novel EM response can be obtained such as wave guiding, and spectral filtering.

O. Sakai and K. Tachibana (2012)
Plasma Photonic Crystals

State-of-the art PPC’s are designed for controlling several mm-wavelength radiation (tens of GHz)
- Plasma scales ~ several mm’s
- Plasma densities ~$10^{13}$ cm$^{-3}$

Propagation bands and bandgaps appear near cut-offs and resonances (e.g., plasma frequency)

Future trends and applications seek to control or manipulate higher frequencies – hence higher plasma densities and smaller plasma scales

Terahertz EM Wave Manipulation

$$n_e \approx 10^{15} - 10^{16} \text{ cm}^{-3}$$
$$a \approx d_p \approx 0.1 \text{ mm}$$
Plasma Photonic Crystals

Externally generating an array of microplasmas (using hollow anode discharge arrays, for example) will become increasingly difficult, particularly for the smaller scales and higher plasma densities needed for controlling THz and FIR waves.

Plasmas (and magnetized plasmas in particular) constitute highly non-linear and naturally unstable systems.

Seemingly uniform plasmas (see top left figure to the left) can be “coaxed” into self-organizing into regular patterns.

Challenge:
Can researchers generate and stabilize coherent organized microstructures from large otherwise uniform dense plasmas?
Plasma Photonic Crystals

Through self-organization of coherent periodic microstructures of high plasma density – several high bandwidth reconfigurable THz wave devices can be constructed:

Directional wave radiation through plasmon resonances

Directional wave guiding through mid-band defect wave localization
Pulsed lasers are transform-limited, cannot resolve distributions in moderately warm plasmas of relatively heavy species (e.g., argon, krypton, xenon).

Must use ultra-narrow continuous wave laser sources to resolve Doppler-broadened and shifted spectral lines in heavy ions!

- Mazouffre / CNRS used continuous wave laser source, was unsuccessful synchronize drifting phases in the coherent plasma fluctuations.

Cappelli / Stanford successfully synchronized continuous wave laser induced fluorescence to coherent structures in heavy ion plasmas

- Laser is chopped at frequency < coherent fluctuation frequency and individual sample-held signals are passed through digital lock-in amplifier to pull out time-synchronized LIF lineshapes as laser is scanned in wavelength.
When a single polarity is extracted in the pure ionic regime, counter ions accumulate in a double layer of charge and could produce corrosion of the emitter if its potential increases beyond the electrochemical window limit.

Voltage alternation incapable of removing electrochemical degradation at the tip apex, where the double layer potential grows faster than its upstream diffusion.

In addition to removing electrochemistry from the tip, this configuration allows for emitter manufacturing using dielectric materials.

Distribution A: Approved for public release; distribution is unlimited
• Ignition of aluminum particles may be assisted by design of coating. Examples are Ti/B and Ni/Al particles.
• **What is the influence of the core-shell design on ignition?**
  Molecular dynamics calculations are performed to investigate particle designs.

Ni coated Al Particle

Aluminum Core MP

Ni shell exerts cage-like effect and raises MP of core; ignition only after core melting

Al coated Ni Particle

Aluminum Shell MP

Surface pre-melting of Al shell implies lower ignition temperature of Al-coated Ni particles.

Distribution A: Approved for public release; distribution is unlimited
A Paradigm Shift in High Pressure Combustion Dynamics
Prediction and Control: Analytics and Dynamic Data Driven
Modeling and Validation

• Great Challenge Example: In a High Pressure/Temperature, Two-Phase, Turbulent, Acoustically–Excited Environment, investigate Amplification

Processes:
- Jet Break-up
- Atomization
- Vaporization
- Supercritical States
- Turbulence
- Compressibility
- Combustion
- Acoustic Field
- Boundary Interactions

• High amplitude and high frequency acoustic instabilities can lead to local burnout of the combustion chamber walls and injector plates

SCIENTIFIC CHALLENGE:
• Modeling and Simulations of highly complex, nonlinear, multi-physics, multi-scale stochastic phenomena
• Current state of the art methodologies are not adequate to address the challenges in this domain → new mathematics and computational methods are needed

Distribution A: Approved for public release; distribution is unlimited
Stochastic modeling is essential to capture the complex physical phenomena - a very challenging problem since current stochastic models only look at simplified problems.

The problem cannot be addressed using only simulations, or experiments.

Use of experimental data is essential to validate models and codes, but it should not be done *aposteriori* as it is done today.

Consistency of models with data is a major issue.

Hard to get data, either too much data, or too little — need a new mathematical framework to bring together data, experiments and simulations in a dynamic, feedback manner.

**Why these modeling efforts are not sufficient?**

- **Stochastic modeling** is essential to capture the complex physical phenomena — a very challenging problem since current stochastic models only look at simplified problems.
- The problem cannot be addressed using only simulations, or experiments.
- Use of experimental data is essential to validate models and codes, but it should not be done *aposteriori* as it is done today.
- Consistency of models with data is a major issue.
- Hard to get data, either too much data, or too little — need a new mathematical framework to bring together data, experiments and simulations in a dynamic, feedback manner.
Any model, by definition, involves stochastic behaviors

(PERTURBATION EXPANSION EXAMPLE)
classical wave equation for combustion instability:

$$L(P') = \frac{\partial P'^2}{\partial t^2} - \overline{C^2} \frac{\partial P'^2}{\partial x^2} = f(\overline{M}, Q, NL)$$

**model uncertainties** (the model has many approximations and assumptions) including intrinsic stochastic behaviors in the real physics

- **Parameter uncertainty**: random fluctuation of speed of sound due to temperature uniformity and fluctuation
- **Combustion noise**: turbulence-induced random combustion response, acoustic damping, shear-layer instability

**Source term uncertainty**

**Parametric Variability - Uncertainties at the Boundary Conditions**:

PROPER ORTHOGONAL DECOMPOSITION revealed that Kelvin-Helmholtz wave motion and the acoustic waves must be accounted as the boundary conditions for the chamber dynamics simulation

When the inlet flow condition fluctuates stochastically, the flame switches from one recirculation region to other (bifurcation)

Distribution A: Approved for public release; distribution is unlimited
Compressible LES Equations + Reduced Basis Model

Stochastic modeling requires many realizations. LES alone is too costly. So, a combined LES-Reduced Basis Model approach fits best.

**Mass**
\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho \vec{u}_i}{\partial x_i} = 0
\]

**Momentum**
\[
\frac{\partial \rho \vec{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left( \rho \vec{u}_i \vec{u}_j + \vec{p} \delta_{ij} - \tau_{ij}^{sgs} \right) = 0
\]

**Energy**
\[
\frac{\partial \rho \vec{E}}{\partial t} + \frac{\partial}{\partial x_i} \left[ \vec{u}_i (\rho \vec{E} + \vec{p}) - \tau_{ij}^{sgs} \vec{u}_j + \vec{q}_i + H_i^{sgs} + \sigma_i^{sgs} \right] = 0
\]

**Species**
\[
\frac{\partial \rho \vec{Y}_k}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho \vec{u}_i \vec{Y}_k - \rho \vec{V}_{i,k} \vec{Y}_k + Y_i^{sgs} + \theta_i^{sgs} \right) = \vec{w}_k \quad \text{where} : k = 1, N_s
\]

**Subgrid Stress Flux**
\[
\tau_{ij}^{sgs} = \rho \left( \vec{u}_i \vec{u}_j - \vec{\tilde{u}}_i \vec{\tilde{u}}_j \right)
\]

**Subgrid Enthalpy Flux**
\[
H_i^{sgs} = \rho \left( \vec{E}_i \vec{u}_i - \vec{\tilde{E}} \vec{\tilde{u}}_i \right) + \left( \vec{u}_i \vec{P} - \vec{\tilde{u}}_i \vec{\tilde{P}} \right)
\]

**Subgrid Viscous Work**
\[
\sigma_i^{sgs} = \left( \vec{u}_j \tau_{ij} - \vec{\tilde{u}}_j \tau_{ij} \right)
\]

**Subgrid Species Flux**
\[
Y_i^{sgs} = \rho \left( \vec{u}_i \vec{Y}_k - \vec{\tilde{u}}_i \vec{\tilde{Y}}_k \right)
\]

**Subgrid Mass Diffusion Flux**
\[
\theta_i^{sgs} = \rho \left( \vec{V}_{i,k} \vec{Y}_k - \vec{V}_{i,k} \vec{\tilde{Y}}_k \right)
\]

**Arrhenius term**
\[
k = A e^{-E_a/RT}
\]
Stochastic at Every Scale

- **Molecular (atomistic) to micro scales (Angstrom-microns)**
  - Uncertainty in kinetics, transport properties
  - Kinetics interactions with fine-scale turbulence
- **Meso-scale (100 micron-mm)**
  - Small-scale turbulence-kinetics coupling
  - Uncertainty in coupling to large-scales
- **Macro-scale (cm-m)**
  - System level responses and nonlinear feedback effects
  - Uncertainty in boundary conditions
- Insufficient data will lead to uncertainty due to incomplete system characterization – Closures needs to include Uncertainty Quantification (UQ) in the model
- **Possible UQ Methods:**
  - Polynomial Chaos, Stochastic Collocation, Bayesian Approaches for Inverse Modeling and Data Assimilation, Sparse Sampling Methods, etc. The underlying problems are multiscale and high-dimensional. Dealing with the curse of dimensionality is a major challenge.
Dynamic Data Driven Strategic Simulation & Modeling

Dynamic Data (3D+Time) → analytics → Consistent data for LES, RBM

Boundary and Initial Conditions

Large Eddy Simulations for real gases with External stochastic terms

Uncertainty Quantification Process

Reduced Basis Model (RBM) With External Stochastic terms

Identification of triggering and driving mechanisms

Experimental domain

Computational domain = “Remainder” of engine

Validation

Distribution A: Approved for public release; distribution is unlimited
Self-consistent analytical theory used to optimize micro plasma source

- Critical research for in-space propulsion, plasma-enhanced combustion, plasma aerodynamics, small scale sensors, directed energy devices, plasma processing …

Goal: Develop efficient and stable cusp-confined micro discharge

- New “stream function” magnetic field analysis developed to predict plasma behavior throughout discharge

Micro-scale plasma source

Goal: Develop efficient and stable cusp-confined micro discharge

- New “stream function” magnetic field analysis developed to predict plasma behavior throughout discharge

Optimization using analytical theory yields 2X increase in plasma production over baseline

- Model trends experimentally validated

Distribution A: Approved for public release; distribution is unlimited