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Non-equilibrium Gas Modeling

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Thrust Panels Workshop
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NASA/LaRC, Norfolk, VA

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Sandia National Laboratories

Sandia Is a National-Security Laboratory

Design, development, and production of nonnuclear weapons components

Safety, security, use control

Treaty verification, nonproliferation, counterproliferation

Advanced military technologies

Energy and environment

Homeland security

Research, science, and technology

Sandia National Laboratories

Sandia Has Multiple Facilities to Meet National Needs

Albuquerque, New Mexico

Kauai Test Facility, Hawaii

Tonopah Test Range, Nevada

Yucca Mountain, Nevada

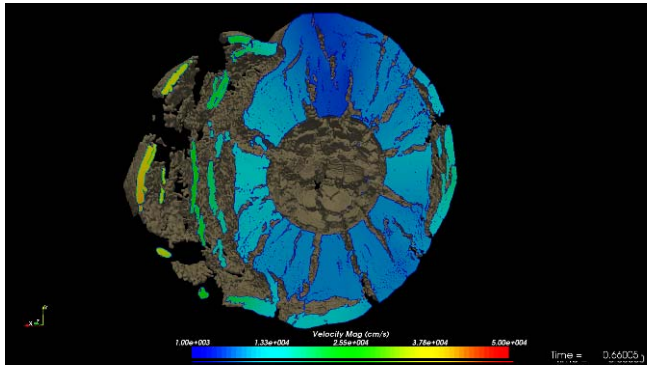
WIPP, New Mexico

Pantex, Texas

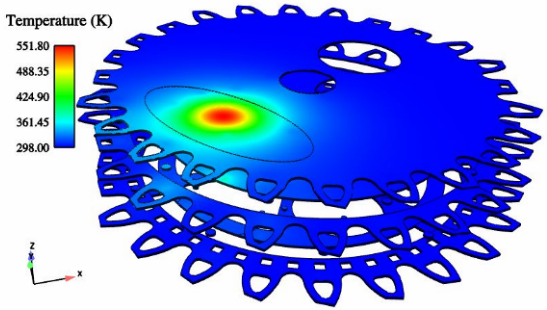
Livermore, California

Sandia National Laboratories

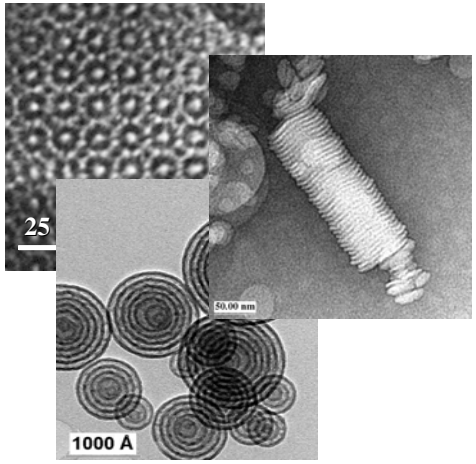
Sandia Relies on Strong Science and Engineering



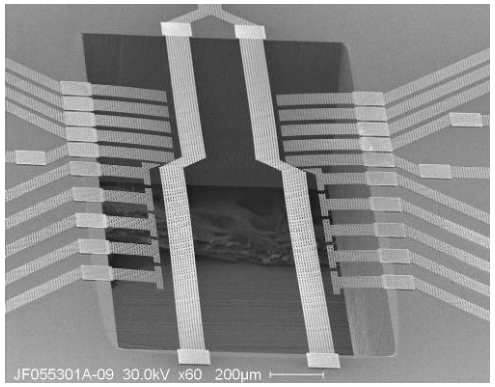
Computational and Information sciences



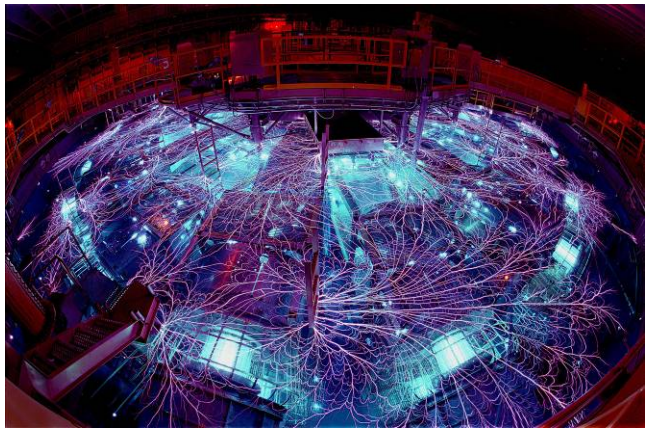
Engineering Sciences



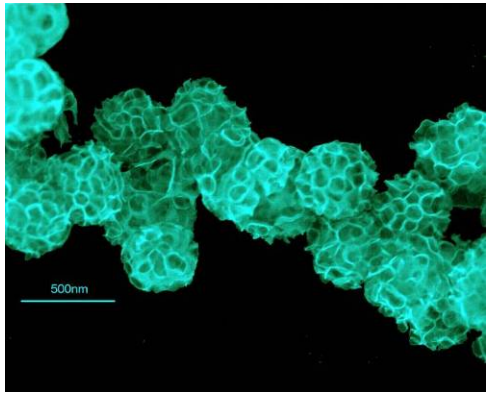
Materials Science and Technology



Microelectronics and Photonics



Pulsed Power



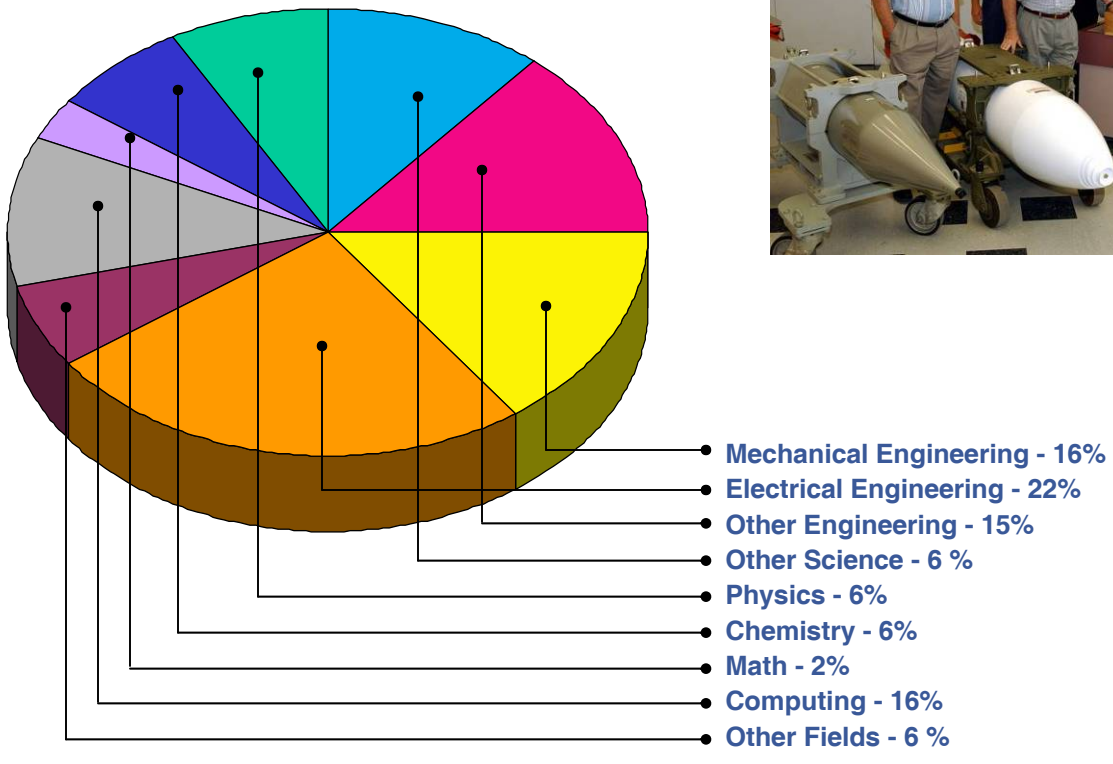
Biotechnology

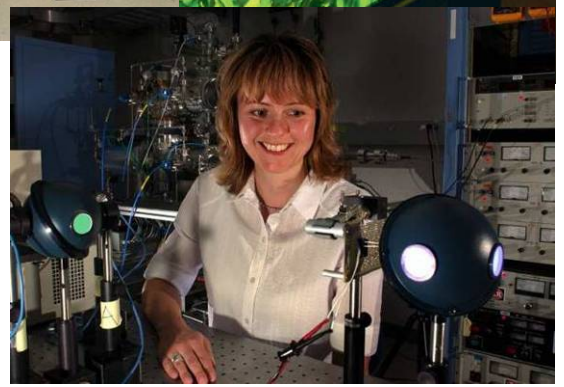
National Nuclear Security Administration

Sandia National Laboratories

Sandia Has a Highly Skilled Workforce

8,600 full-time employees
1,500 PhDs and 2,700 MS/MAs
2,200 on-site contractors
$2.33 billion FY06 total budget





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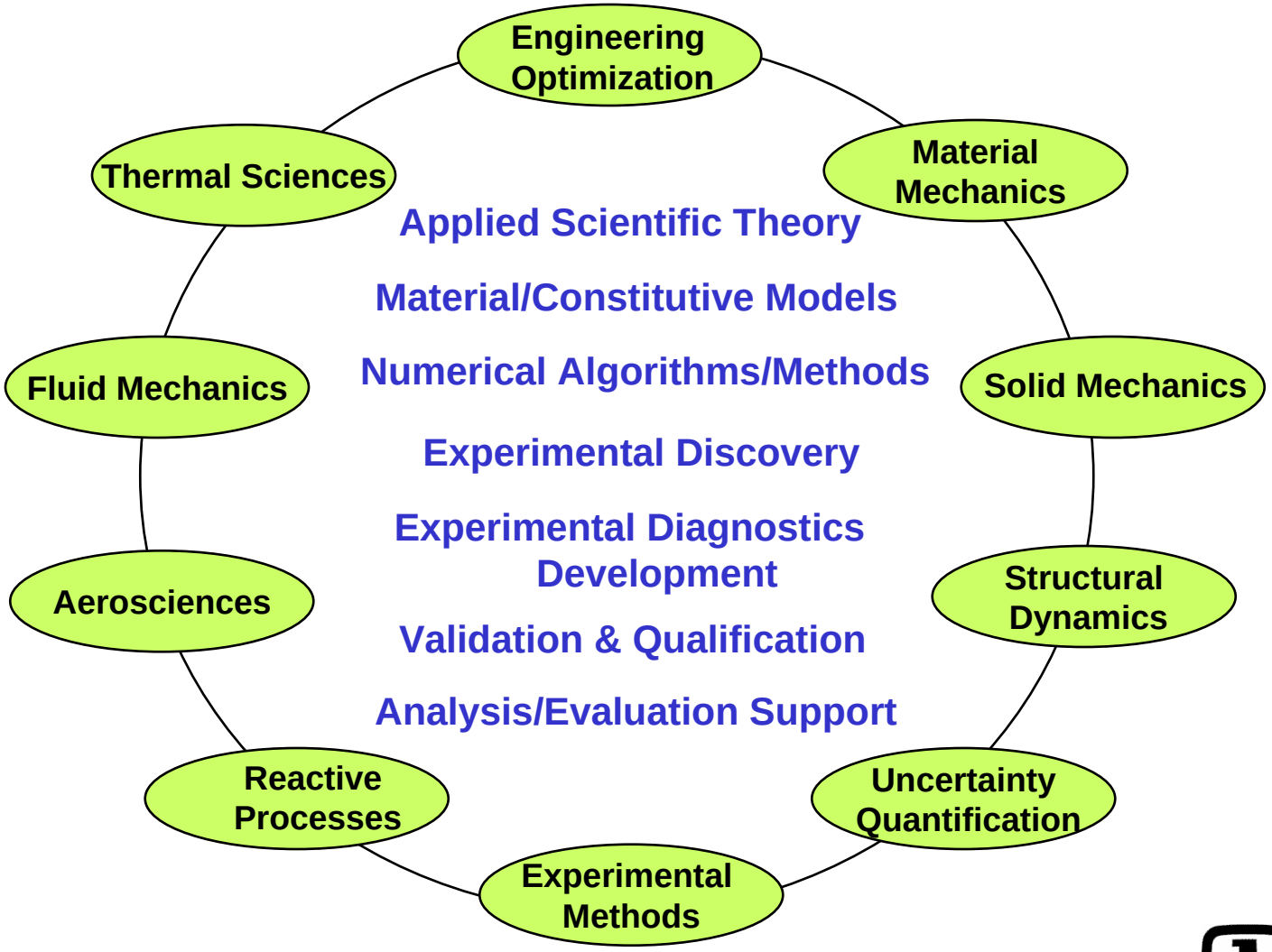
The Engineering Sciences Center Owns the Mechanics Disciplines



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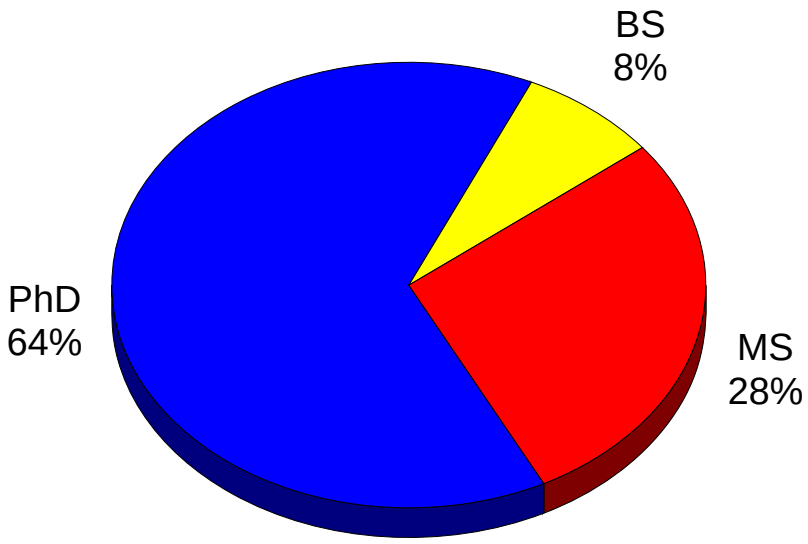
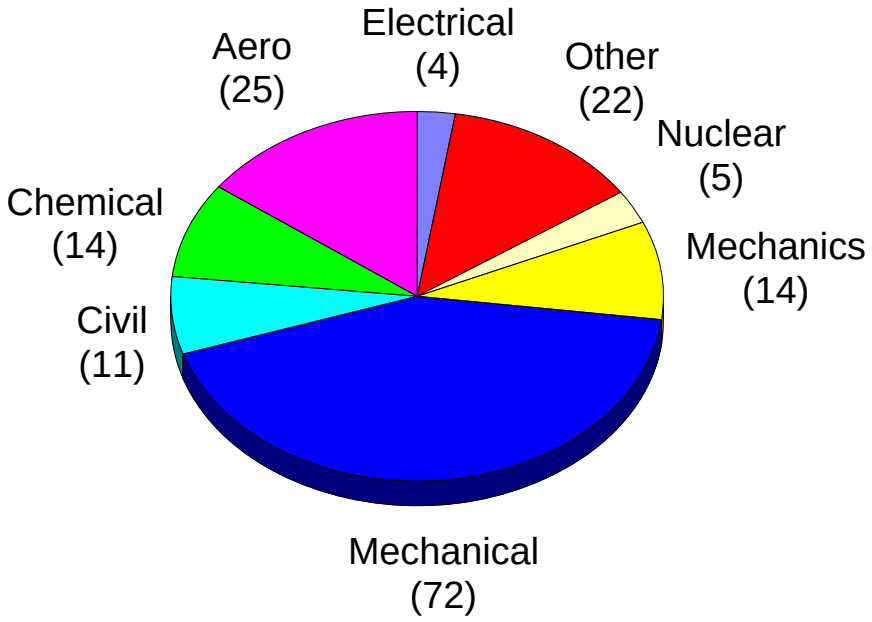
Engineering Sciences Center
Educational Background

Engineering Sciences comprises about 400 employees and contractors.

Degree Level



Engineering Degree



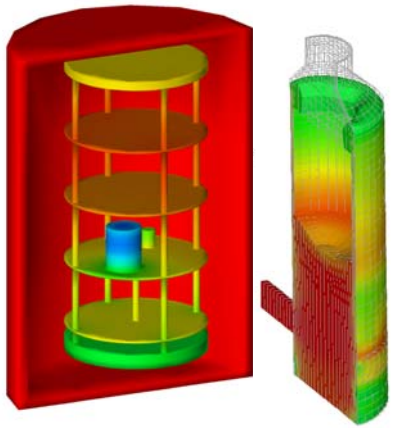
Our technical staff have experience across many engineering disciplines.

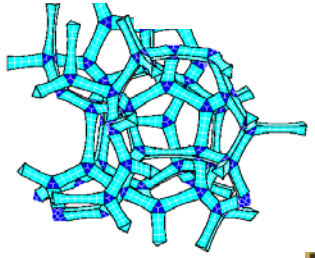
Sandia National Laboratories

Thermal, Fluid and Aero Sciences

Fluid & Thermal Mechanics

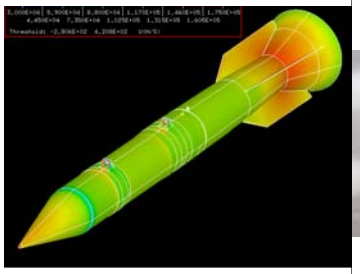
- •Multiphase Energy & Manufacturing Flows
- •Non-Newtonian Flow
- •Radiative/Conductive/ Convective Transport
- •Porous Flow
- •Noncontinuum transport processes
- •Aerosol Transport





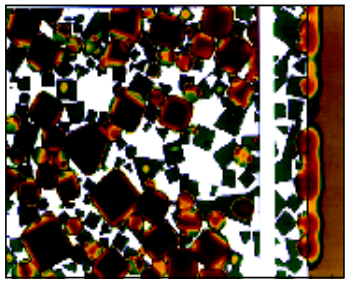
Aero Science & Technology

- •Compressible Flows
- •Aerothermodynamics
- •Fluid/Structure Integration
- •Aero & Flight Dynamics
- •Parachute Technology



Reactive Processes

- •Polymeric & Energetic Materials
- •Combustion
- •Corrosion & Electro- Chemistry



Experimental Technology

- •Advanced Diagnostics
- •Fundamental Expts
  - • Phenomenology
  - • Matls Charact.
- •Model Validation

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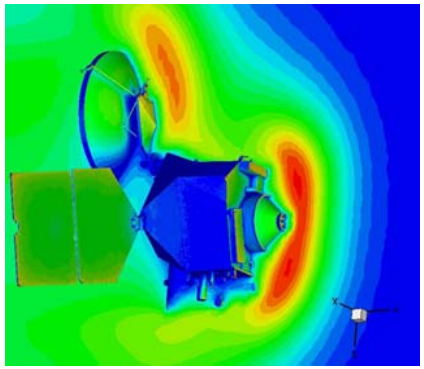
Non-equilibrium Gas Modeling Application Areas

Traditional

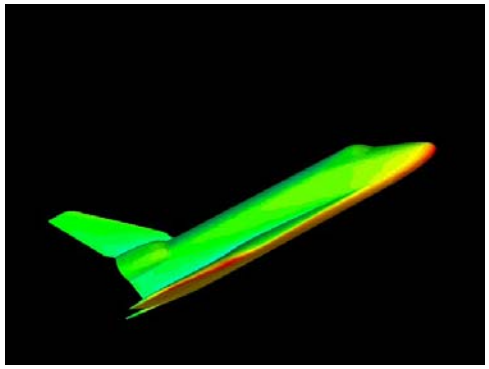
- Hypersonics and spacecraft
- Semiconductor equipment

Novel

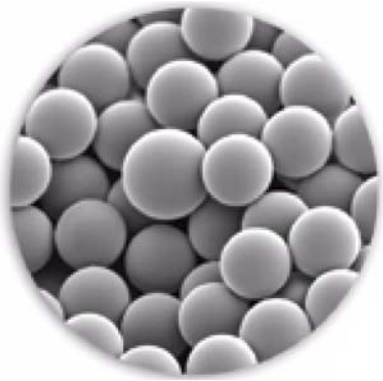
- MEMS damping, heat transfer
- Nanoparticle transport in gas



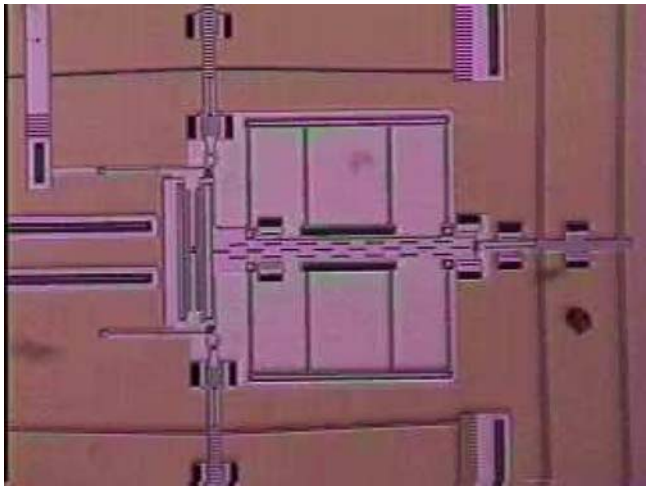
Mars Recon. Orbiter



Space Shuttle



PSL Nanoparticles



Thermal Actuators

EUVL Equipment

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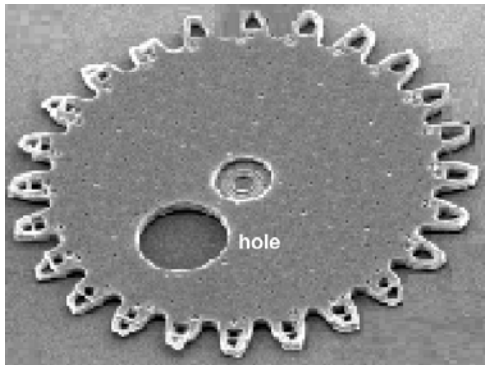
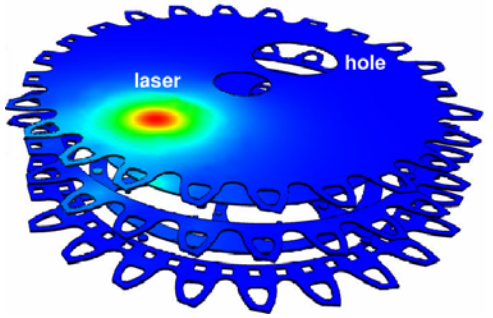
Non-equilibrium Gas Modeling

Major Technical Issues

- **Analysis**
  - Simulation *accuracy* for noncontinuum gas
  - Noncontinuum-gas *models* for engineering codes
  - Improved *understanding* of physical processes
  - Address *multi-discipline* problems
- **Codes**
  - Much faster *algorithms*
  - Efficient *massively parallel implementations*
  - New *computer technologies*
- **Data**
  - Accurate *physical properties* for gases and solids
  - Reliable, complete *validation* experimental results





Connectivity to Sandia Mission Needs

- MESA: Microsystems and Engineering Sciences Applications, $0.5B facility, completed summer 2007
- CINT: Center for Integrated Nanotechnologies
- NINE: National Institute for Nano Engineering, 1st center
- Hypersonics: space and upper-atmosphere systems

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Modeling and Simulation

High-consequence applications require high-fidelity analysis

Two main simulation methods

- Navier-Stokes plus slip-jump: *NSSJ*
- Direct Simulation Monte Carlo: *DSMC*

Important issues

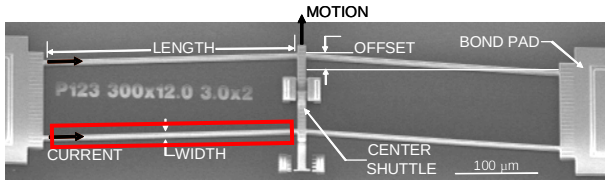
- How far can NSSJ approach be used
  - How do constitutive relations break down
  - Effect of thermo-chemical non-equilibrium
- Best accuracy/speed tradeoff for DSMC
- Transfer DSMC learning to NSSJ models
- Physical & chemical processes modeling

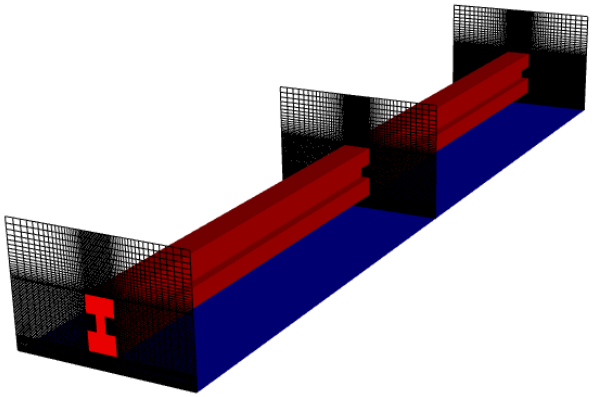
Detailed validation is required

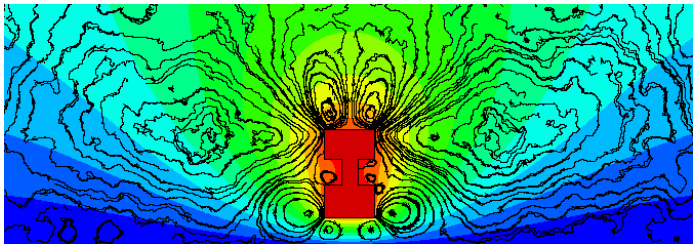
- Flight data
- Code comparisons

Better methods are needed

- Evolutionary improvements
- Revolutionary advances







temperature (color) and streamlines

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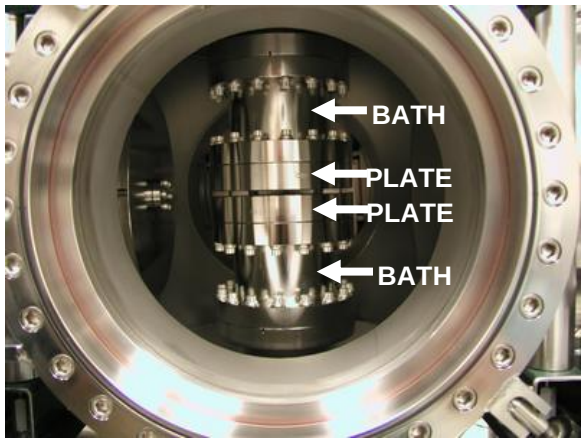
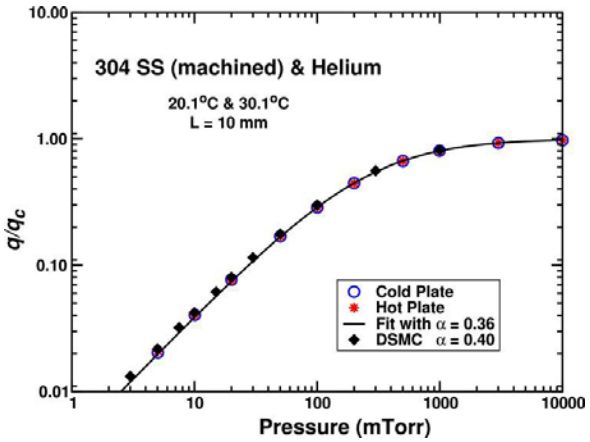
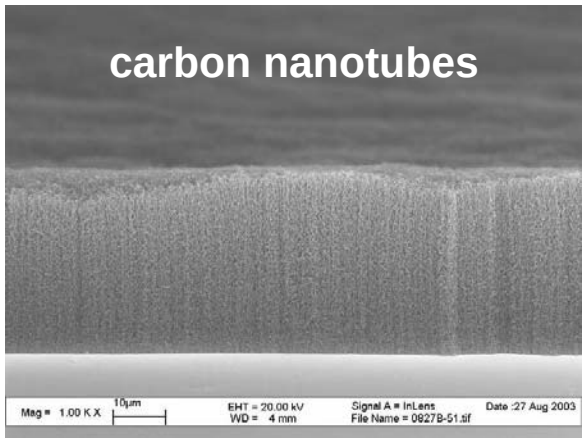
Thermophysical Properties







Critical modeling inputs are often not well quantified

Accommodation values

- "Known" surface properties need to be revisited
- New surfaces may offer significant advantages

Chemical reaction data

- Energy-dependent cross sections, rate data
- Earth atmosphere chemical reaction data
- Ionization and radiation cross sections

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Sandia Hosts Int'l DSMC Workshops

DSMC: Theory, Methods, and Applications (DSMC07)
Santa Fe, New Mexico; September 30-October 3, 2007

Sandia is advancing state-of-the-art by hosting DSMC workshops

- Hosted first workshop (DSMC05) two years ago
  - Highly successful: 60 participants, 10 countries, 40 talks
- Hosting second workshop (DSMC07) this fall
  - Graeme Bird short course on "Sophisticated DSMC Algorithm"
  - Berni Alder plenary talk on "Hydrodynamics by DSMC"
- Website: http://www.esc.sandia.gov/dsmc07/dsmc07.html

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Non-equilibrium Gas Modeling
Future Directions for Research

To address problems of national importance, research must focus on major technical issues

- **Analysis**
  - Simulation *accuracy* for noncontinuum gas
  - Noncontinuum-gas *models* for engineering codes
  - Improved *understanding* of physical processes
  - Address *multi-discipline* problems
- **Codes**
  - Much faster *algorithms*
  - Efficient *massively parallel implementations*
  - New *computer technologies*
- **Data**
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NASA CLV

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