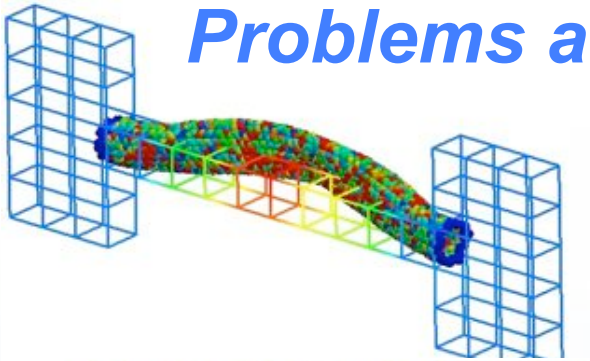
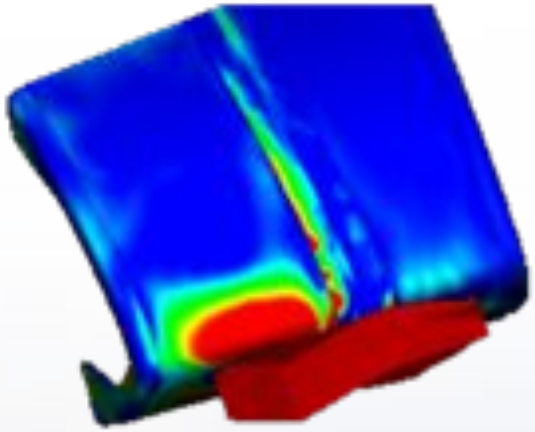
SAND2010-7525P

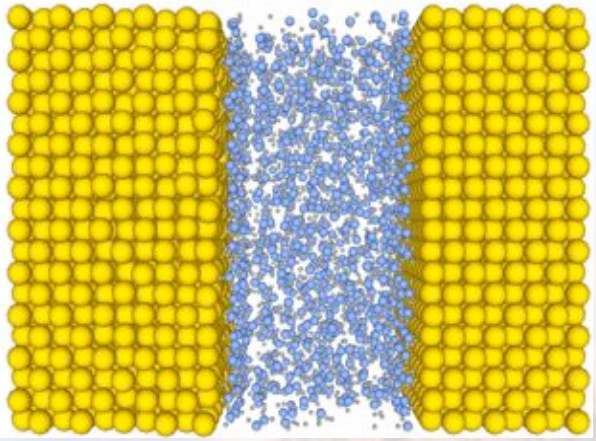
October 28, 2010

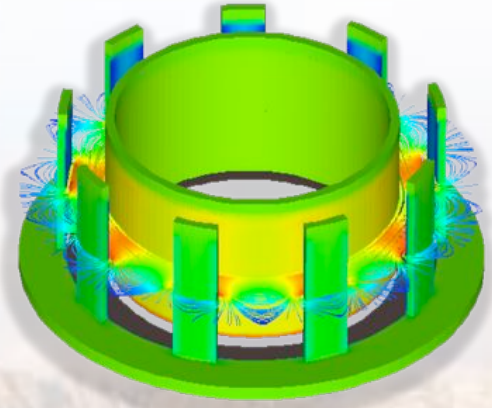
Modeling and Simulation of Engineering Problems at Sandia National Laboratories

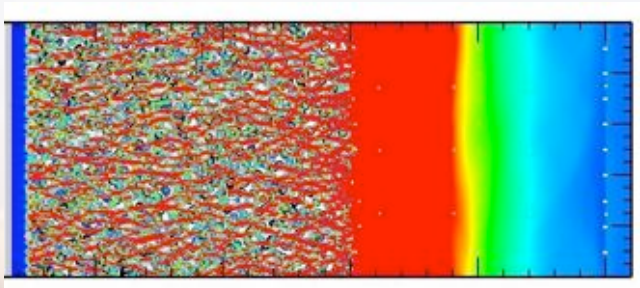


Jonathan A. Zimmerman
Mechanics of Materials Department









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Sandia National Laboratories

Our Business: National Security

- **We develop technologies to:**
  - Sustain, modernize and protect our nuclear arsenal
  - Prevent the spread of weapons of mass destruction
  - Provide new capabilities to our armed forces
  - Protect our national infrastructures
  - Ensure the stability of our nation's energy and water supplies.
  - Defend our nation against terrorist threats

Sandia National Laboratories

Sandia's Administration

- AT&T: 1949–1993
- Martin Marietta: 1993–1995
- Lockheed Martin: 1995–Present

Government-Owned Contractor-Operated

Federally Funded Research & Development Center

Sandia National Laboratories

Sandia's Sites

Albuquerque, New Mexico

Livermore, California

Kauai, Hawaii

Yucca Mountain, Nevada

WIPP, New Mexico

Pantex, Texas

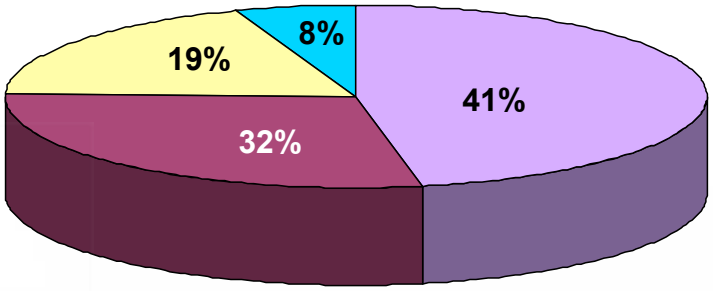
Tonopah, Nevada

Sandia National Laboratories

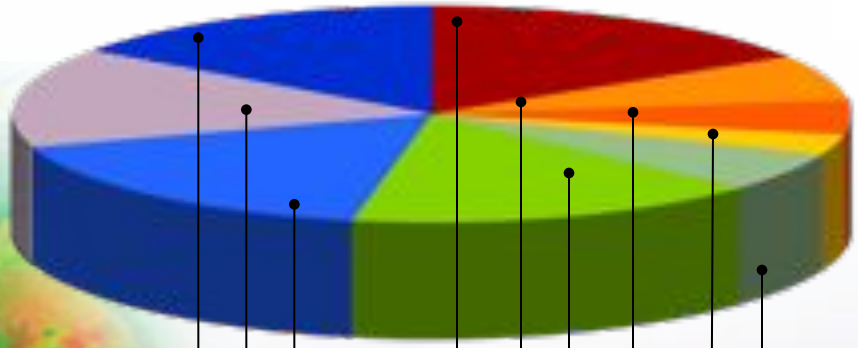
Sandia's People and Budget

- On-site workforce: 11,415
- Regular employees: 8225
- Gross payroll: ~$900 million

FY09 Operating Revenue
$2.2 billion

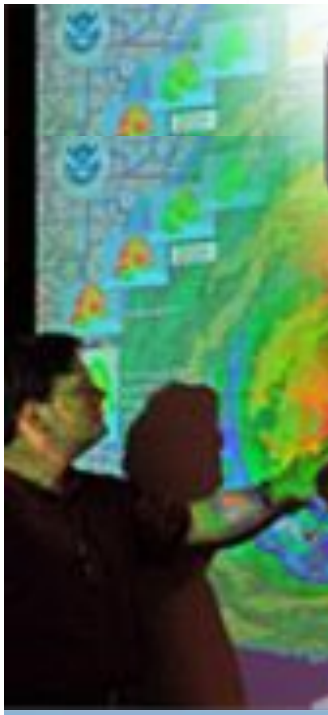


Technical staff (3,850) by discipline:



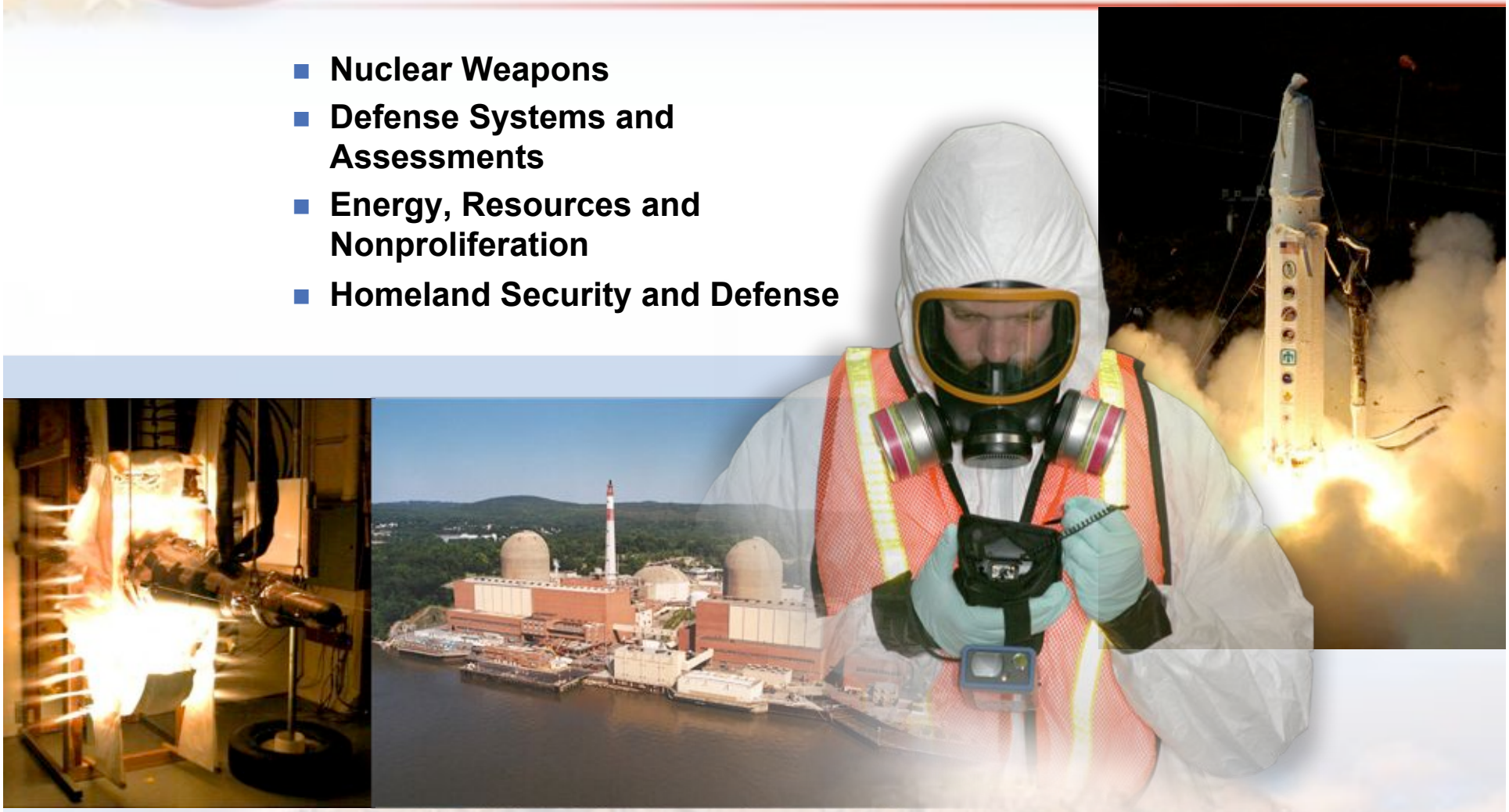
Physics 6%
Math 2%
Chemistry 4%
Computing 16%
Other Science 4%
Other Fields 17%

Electrical Engineering 19%
Mechanical Engineering 16%
Other Engineering 15%



Four Mission Areas

- Nuclear Weapons
- Defense Systems and Assessments
- Energy, Resources and Nonproliferation
- Homeland Security and Defense



Nuclear Deterrence for National Security

Defense Programs Mission

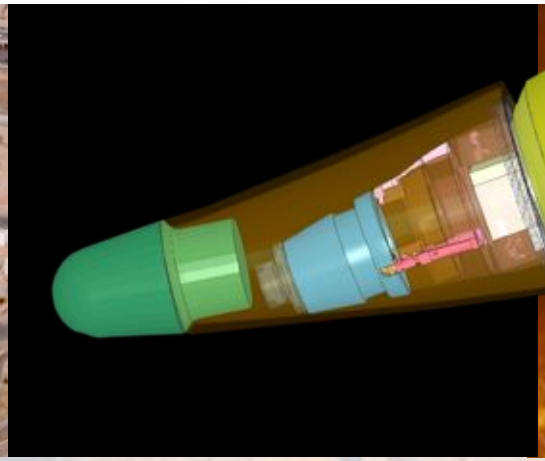
Credible deterrence built on

(1) a safe, secure and reliable nuclear weapons stockpile capable of meeting all military requirements now and in the future, and

(2) a science-based engineering infrastructure capable of responding to national security needs whenever they arise.

Microsystems and Engineering Sciences Applications (MESA) complex

AF&F impact simulation



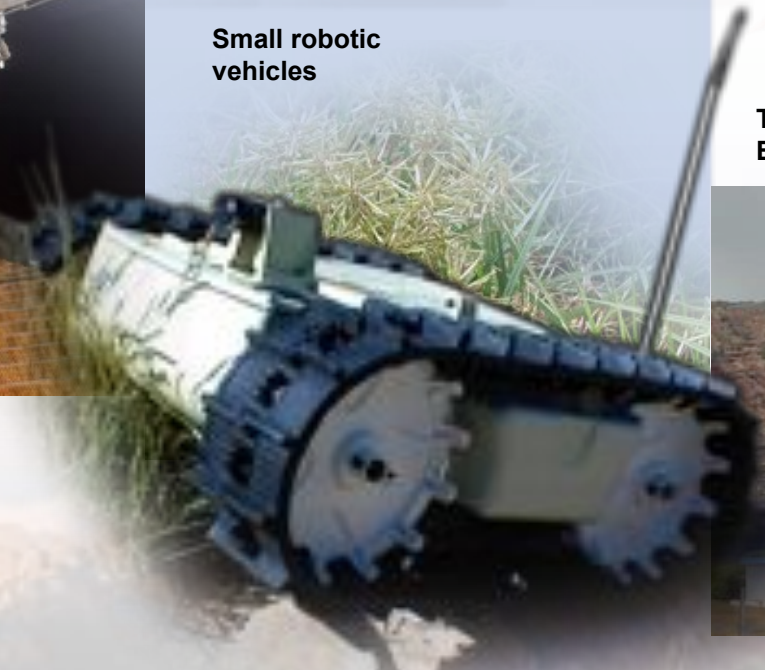
Pulsed power— Z Machine

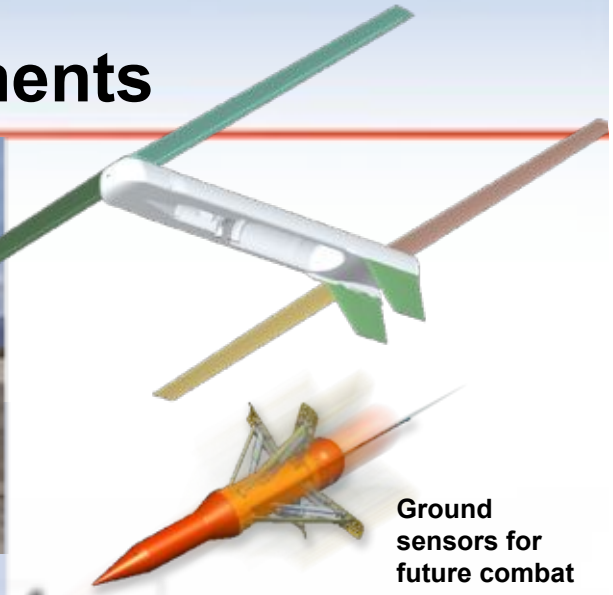
Defense Systems & Assessments

Predator UAV with SAR

Shuttle Orbital Inspection System

Small robotic vehicles





Ground sensors for future combat systems

Target launches for Ballistic Missile Defense

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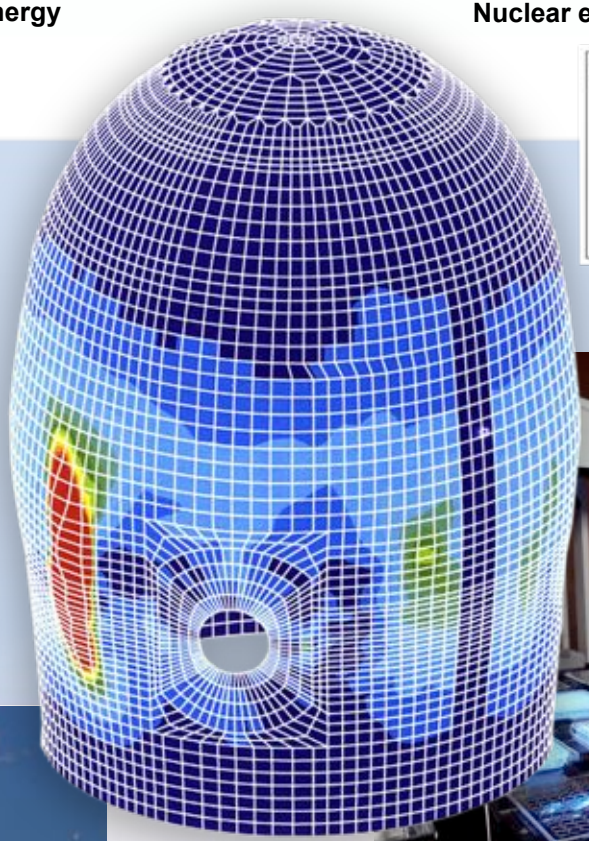
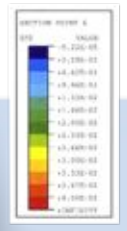
Energy, Resources & Nonproliferation

Renewable and alternative energy

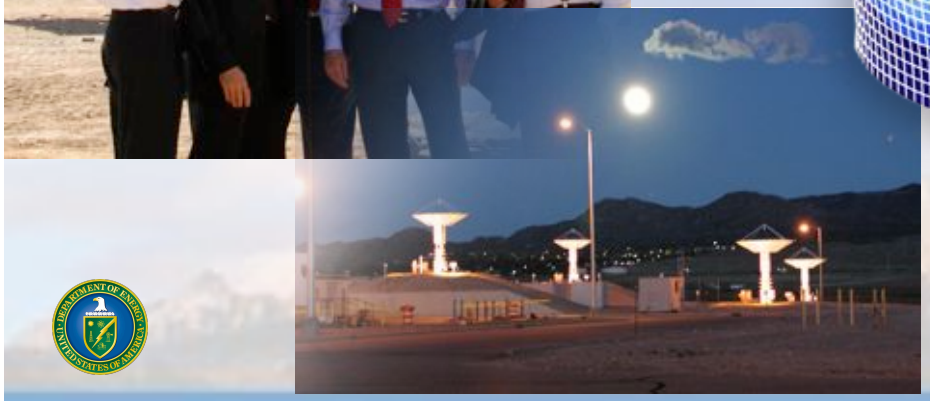
Nuclear energy





Fuel and water systems

Global security



Sandia National Laboratories

Homeland Security & Defense

Modeling catastrophic events

Infrastructure modeling and protection

Physical security and force protection

Maritime security

Sandia National Laboratories

Capabilities: Modeling and Simulation

- **What this brings us:**
  - Understanding of the underlying physics of material response
  - Ability to investigate design alternatives for improved performance
  - Predictive capability for investigating scenarios
  - Knowledge of the consequences of material aging
- **How do we do it:**
  - Fusion of multiple science and engineering disciplines

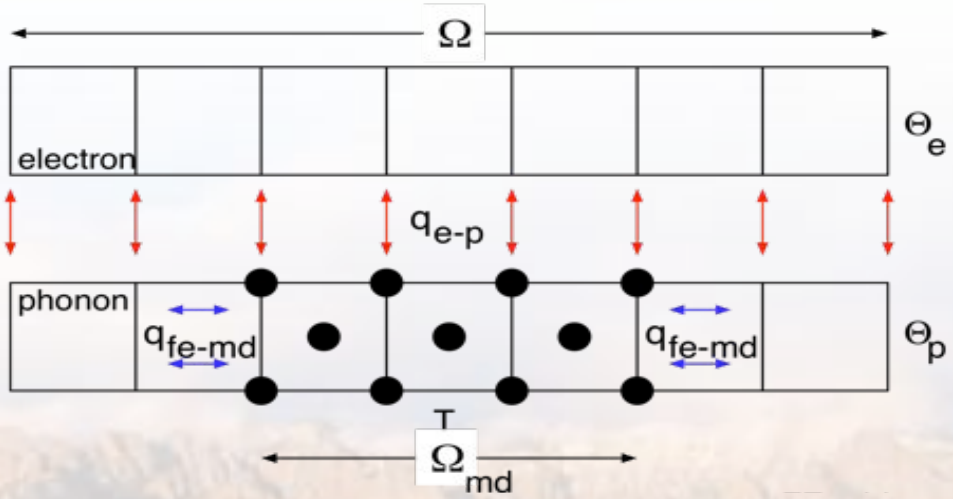
Mechanical Engineering	Electrical Engineering
Computer Science	Materials Science
Physics	Biology
Chemistry	Chemical Engineering

  - Examination of phenomena at all scales
    - Nano, Micro, Meso, Macro
- **Let me show you…**

Enhanced Molecular Dynamics for Simulating Thermal and Charge Transport

- **Problem**: Conventional molecular dynamics (MD) can emulate phonon energy transport, but not the electronic thermal and charge transport important in integrated circuits, thermoelectric materials, nanowire devices, etc.
- **Our solution**: Enhance MD with coupled and coincident finite element-based electron transport models.
  - Two temperature model couples electron and phonon temperatures
  - Drift-diffusion provides closure for power term

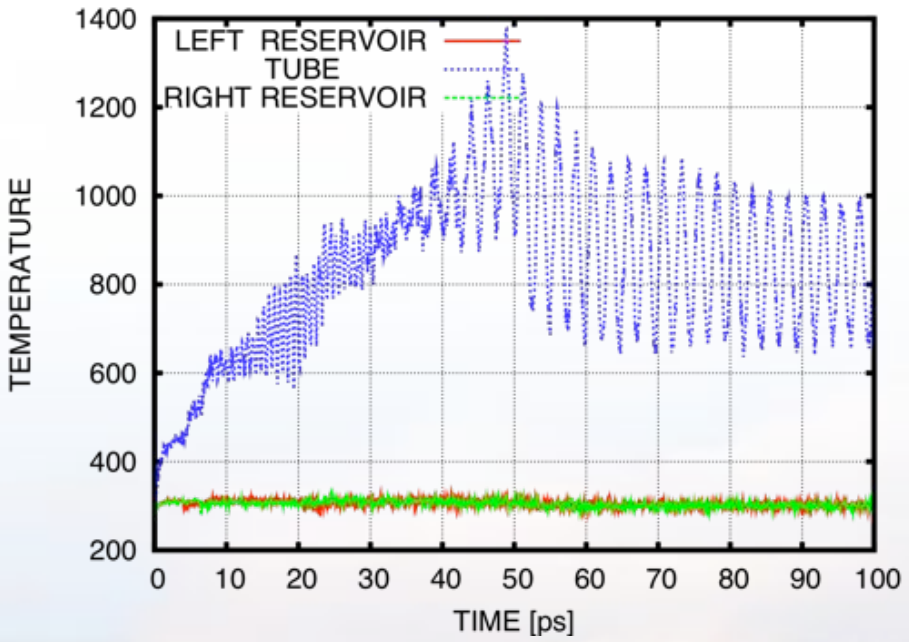
Researchers:
R. Jones
J. Templeton
G. Wagner
N. Modine
D. Olmstead



Jones et al., Intl. J. for Numerical Methods in Engineering, 2010

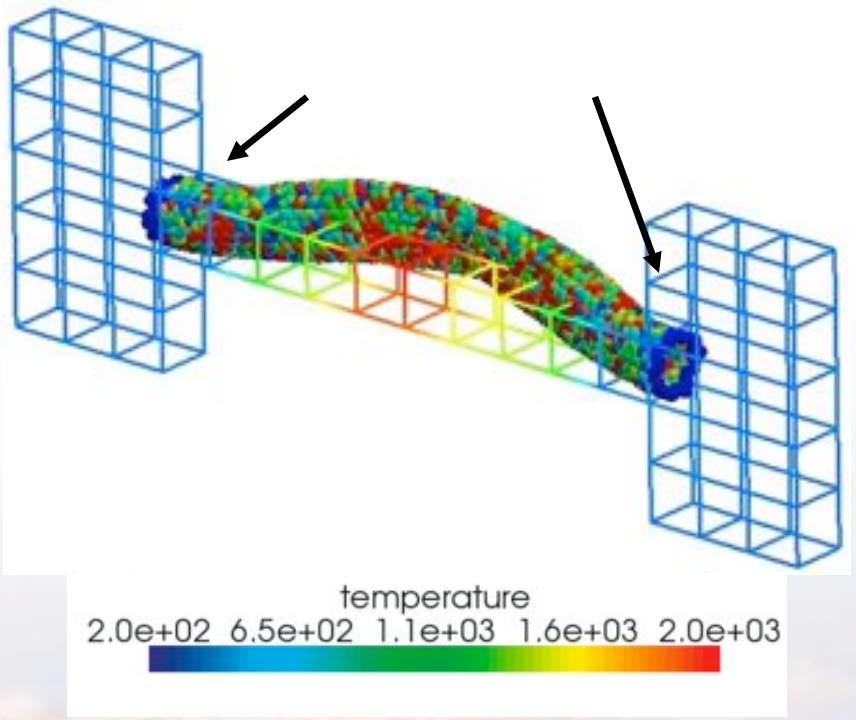
Laser heating of a metallic CNT

- **eMD can be used to model heating and thermal-induced vibration in nanostructures that possess a metallic character of thermal conduction, e.g. (8,8) armchair CNT.**



Evolution of average temperatures of CNT and reservoirs

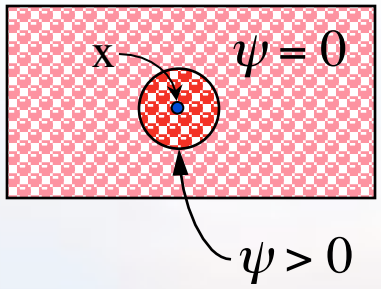
reservoirs of hot electrons



Atomistics-to-Continuum Field Estimation

Researchers:
R. Jones
J. Zimmerman
J. Templeton
X. Zhou
J. Lloyd

- **Problem:** How to connect atomistic simulation to continuum models so that engineering analysis can access detailed information on material deformation mechanisms.
  - Provide interface conditions between domains for coupled analysis
  - Construct constitutive models based on atomistic behavior
- **Our solution**: Using the Eulerian method by Hardy, and our Lagrangian method, we can extract information on stress and deformation fields that are consistent with continuum mechanics.



$$\boldsymbol{\sigma}(\mathbf{x},t) = -\left\{\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{x}^{\alpha\beta}\otimes\mathbf{f}^{\alpha\beta}B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^{N} m^{\alpha}\hat{\mathbf{v}}^{\alpha}\otimes\hat{\mathbf{v}}^{\alpha}\psi\left(\mathbf{x}^{\alpha}-\mathbf{x}\right)\right\}$$

$$\mathbf{P} = -\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta}\otimes\mathbf{X}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X})$$

Zimmerman, Jones and Templeton, J. Comp. Phys., 2010

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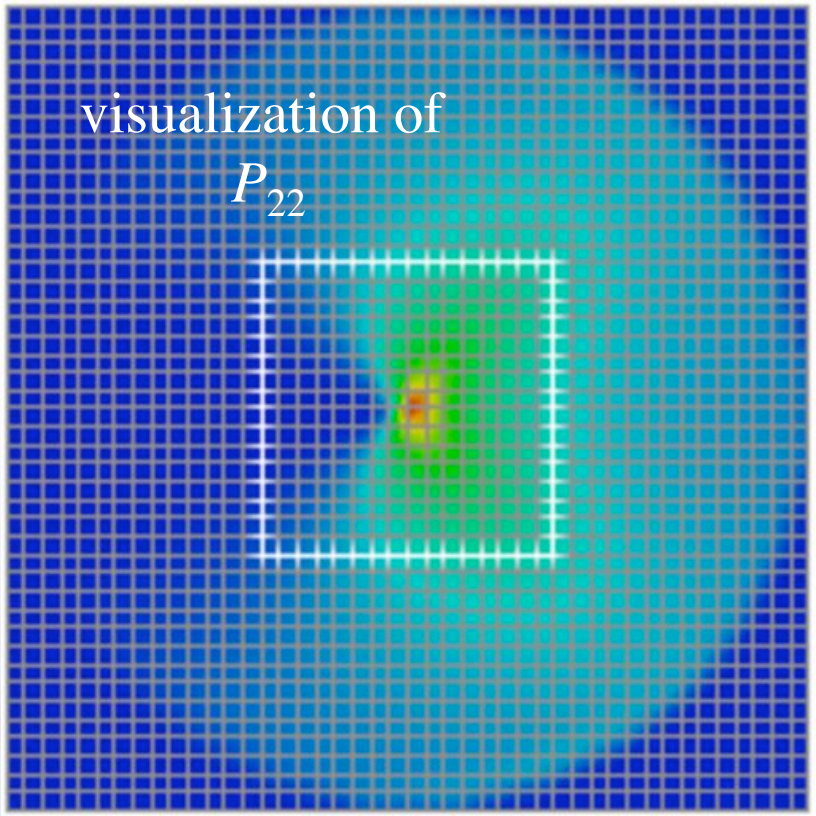
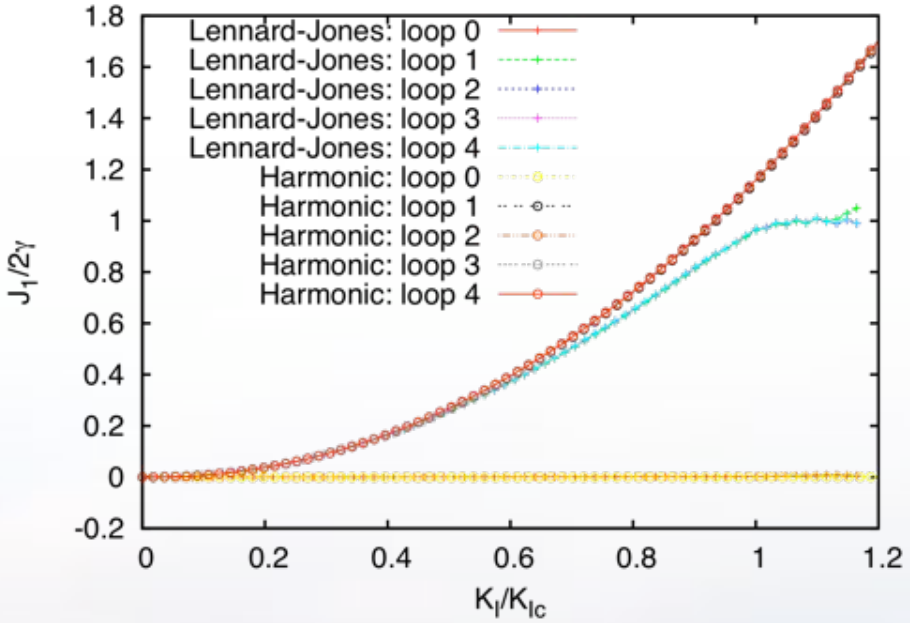
J-Integral estimation to predict crack growth

- **We can use this method to estimate the driving force for crack propagation, the J-Integral**

$$\mathbf{J} = \int_{\Gamma_0} \left(\Psi \mathbf{N} - \mathbf{F}^T \cdot \mathbf{P} \cdot \mathbf{N} \right) ds$$





Quasi-static and dynamic analyses show:

- path independency of J integral
- agreement with LEFM
- fracture occurs when J = 2γ

Jones and Zimmerman, J. Mech. Phys. Solids, 2010

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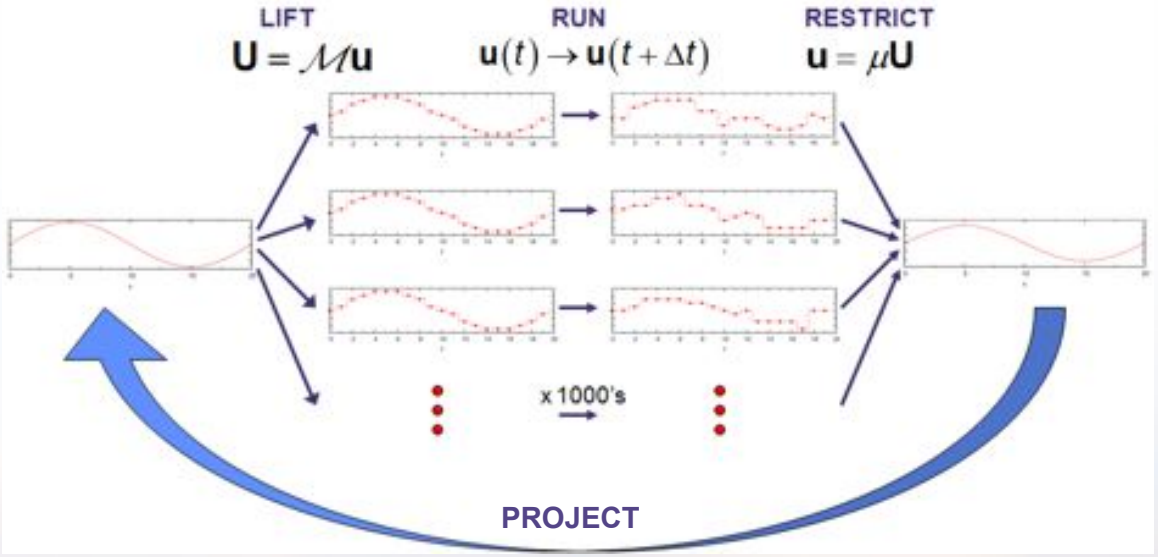
Equation-Free Simulation of Materials Aging

- **Problem:** How can we get the detailed physics of atomistic simulation for aging processes that occur over macro-timescales?
- **Our solution:** We are developing "equation-free" projective integration schemes to enable simulation of surface morphology evolution, bulk diffusion of vacancies, and interfacial diffusion.

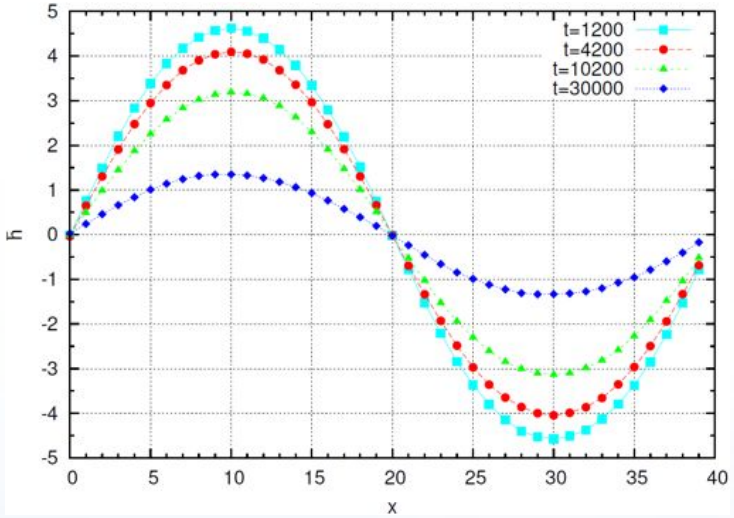
Researchers:
G. Wagner
X. Zhou
J. Zimmerman
A. Thompson
S. Plimpton



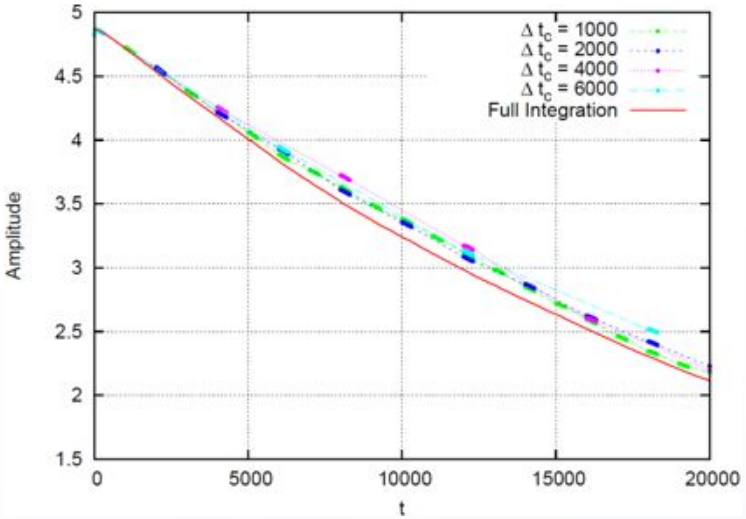
Lift/Restrict: Develop sufficiently accurate and efficient inter-scale operators
Run: Implement and improve accelerated atom-scale simulation techniques
Project: Understand identification and time integration of fast and slow modes

Equation-Free Surface Diffusion

- **We have used equation-free integration to accelerate kinetic Monte Carlo simulations of surface diffusion**



Surface profile decay using kMC



Accelerated decay simulations using increasing values of coarse projection time

Key finding: Parameterization of fine scale fluctuations (e.g. correlation functions) is needed to capture dynamics

Wagner, Zhou and Plimpton, Intl. J. for Multiscale Computational Engineering, 2010

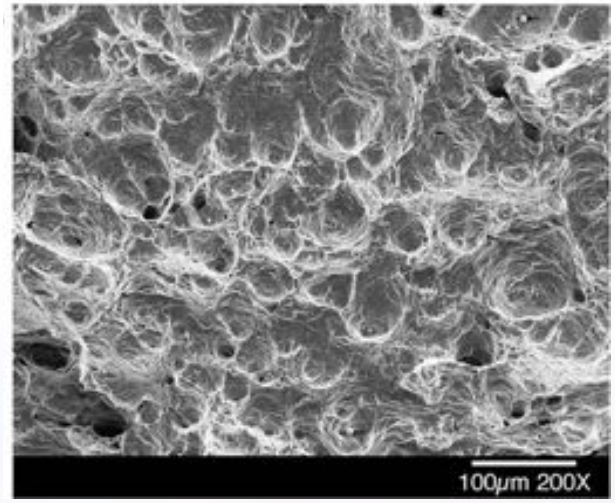
Sandia National Laboratories

Hydrogen: a troublemaker

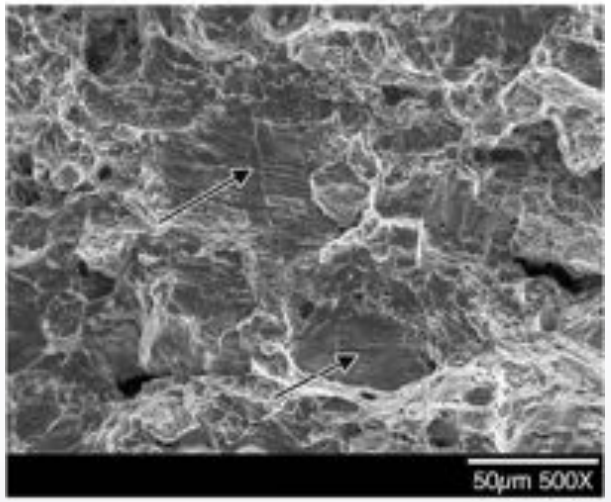
- **Problem:** Hydrogen in materials (e.g. 21Cr-6Ni-9Mn stainless steel) leads to localized deformation and crack propagation

Researchers:
J. Foulk
Y. Ohashi
A. Lindblad
P. Notz
P. Sofronis
D. Bammann

Nibur, Somerday, Balch, and San Marchi, Acta Materialia, 2009.



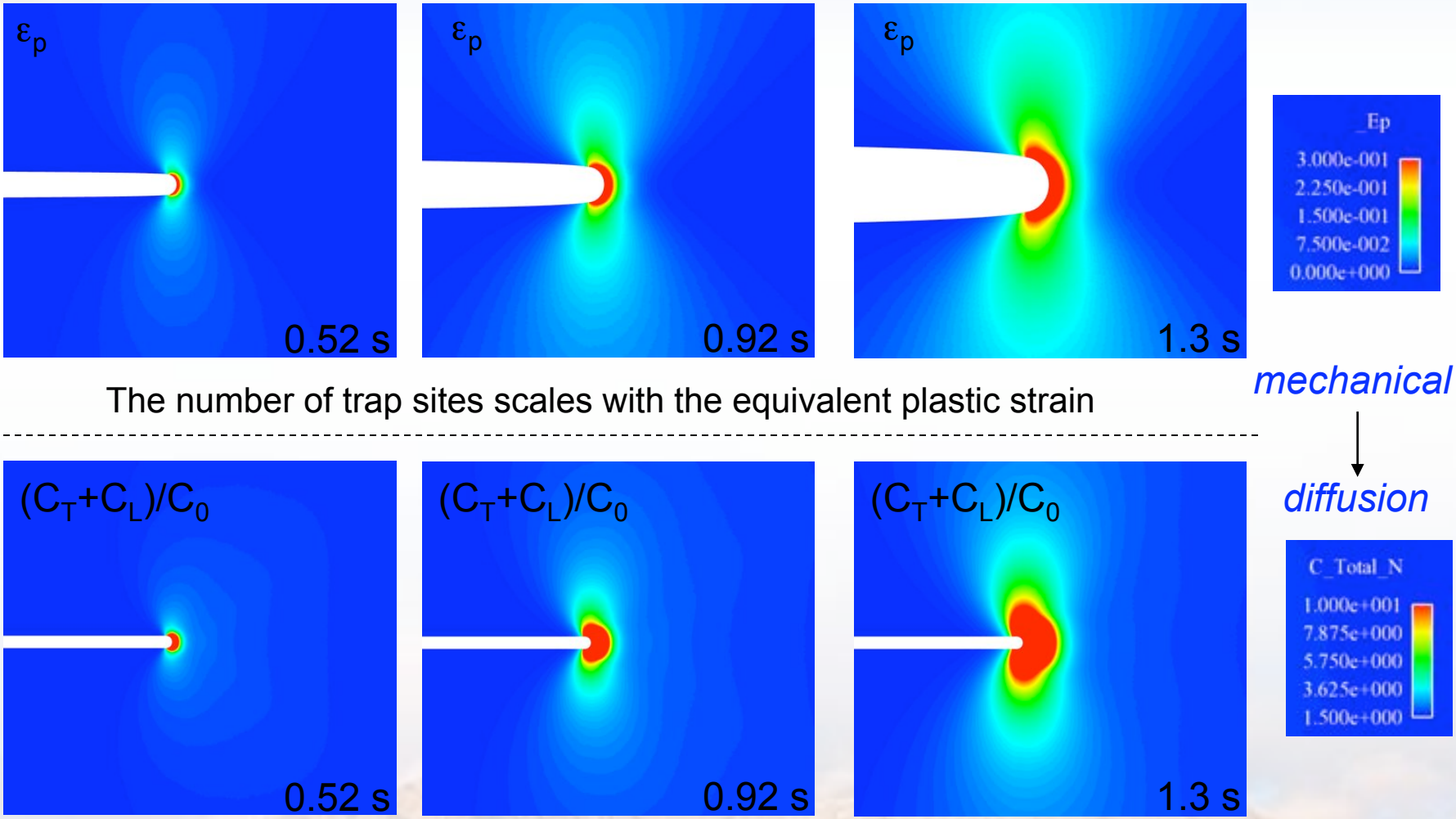
J_i = 816 kJ/m^2



J_{iH} = 129 kJ/m^2

- **Our solution:** Develop models that couple hydrogen trapping with enhanced localized plasticity (HELP) and embrittlement (HE) to predict material deformation and failure.

Evolution of Hydrogen Concentration



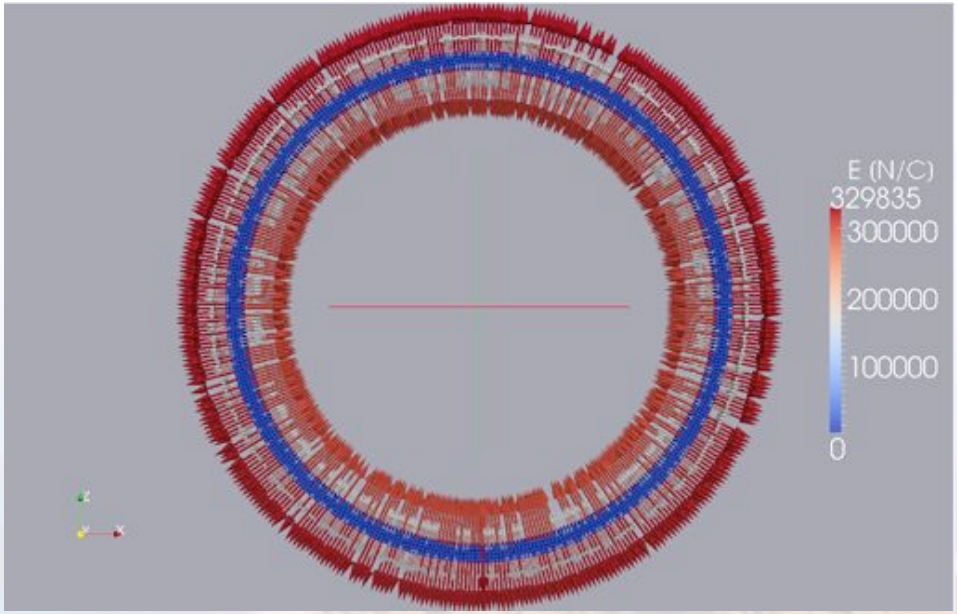
Total hydrogen concentration is dominated by trapping and evolves with plastic zone

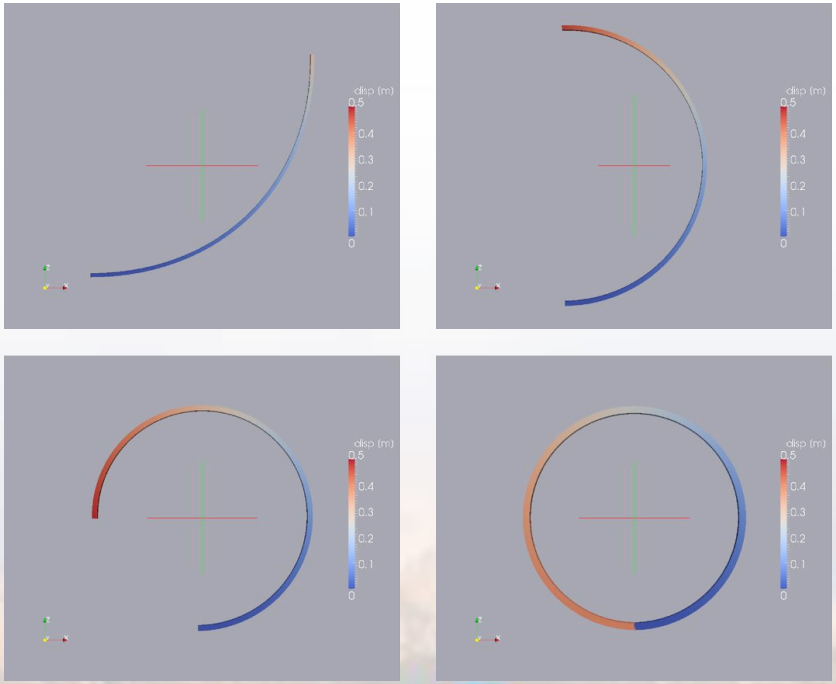
Large Deformation of Piezoelectric Materials

Researchers:
A. Mota
J. Zimmerman

Intl. J. Numer. Meth. Eng., 2010

- **Problem:** Some applications involve piezoelectric materials (coupled mechanical and electro-magnetic fields) subjected to large deformation. Existing methods are for small-strain regime.
- **Our solution:** We developed a finite element formulation (balance laws + constitutive relations) using reference frame-based variables.
- **Example:** Straight beam subjected to large deformations…





Theory: e=323.5 kN/C
Simulation: e=329.8 kN/C

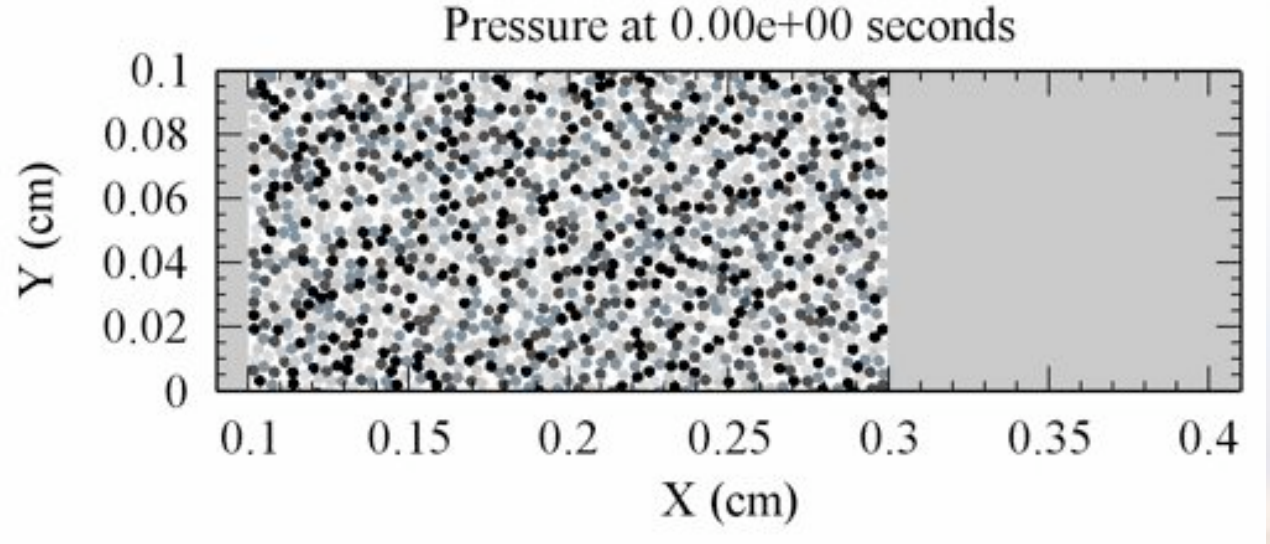
Sandia National Laboratories

Mesoscale Modeling of Granular Materials

Researchers:
J. Borg
T. Vogler

- **Problem:** We need understanding of (and the ability to model) compaction of granular materials
  - Materials processing
  - Penetration into earth and granular structured materials
  - Deformation-induced chemistry of explosive materials
- **Our solution:** Model as mesoscale particles governed by equations of state and (chemo-)mechanical constitutive models.

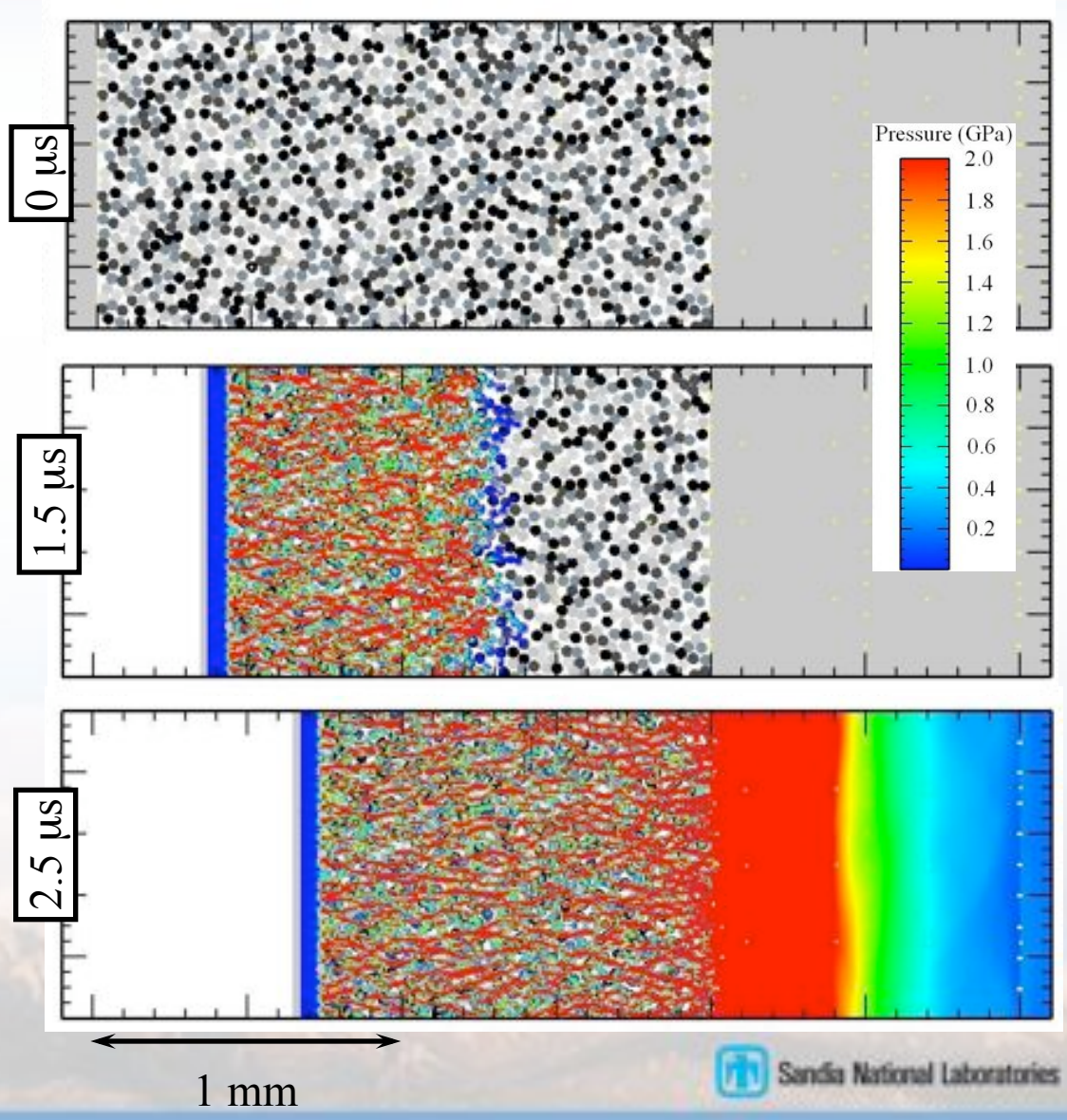
Dynamic Compaction of WC



Borg and Vogler, Modell. Sim. Mater. Sci. Eng., 2009

Computational Dynamic Compaction

- driver plate velocity u_p=300 m/s
- shock thickness on the order of ~2-5 particles
- strong force chains observed
- wave smooths in aluminum buffer



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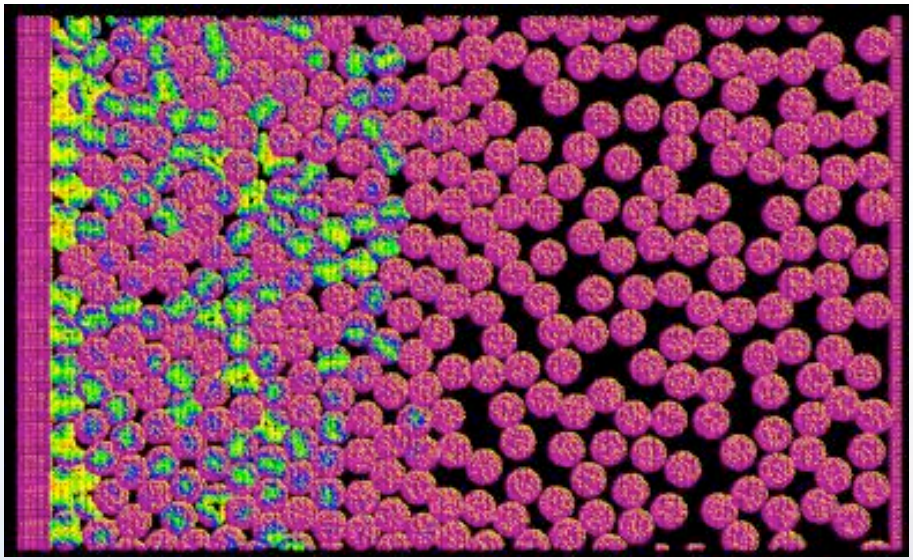
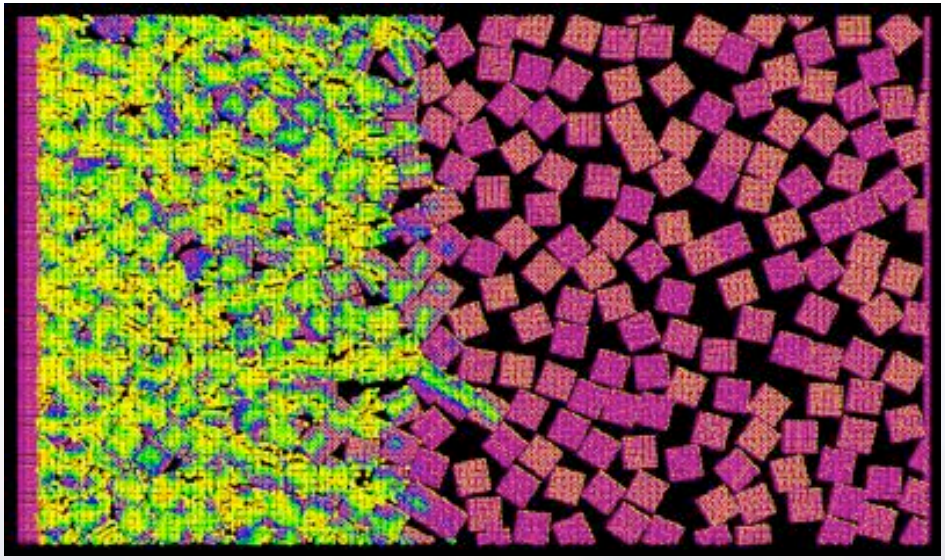
Mesoscale Calculations with Peridynamics

- Peridynamics: Non-local particle simulation method that includes fracture of particles and contact forces
- Results so far: Mechanical response insensitive to particle shape despite large differences in particle fracture (dissipation due to fracture is small)

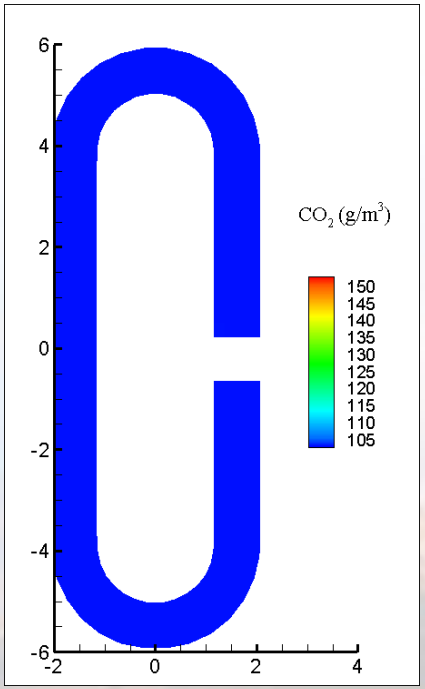


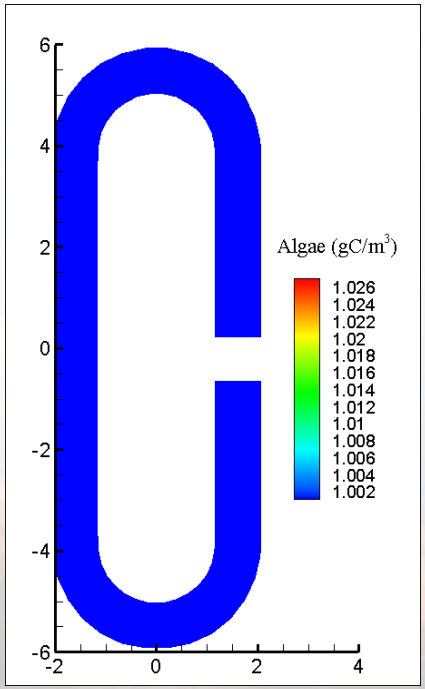


Modeling Algae Growth in Open-Channel Raceways

Researchers:
S. James
A. August

- **Problem:** The need for alternative fuels has led to an interest in microalgae as a biomass useful for solar energy conversion. How do we design containment structures that optimize the amount and distribution of algae?
- **Our solution:** Use models that couple nutrient and algae kinetics with Computational Fluid Dynamics. Include effects such as non-optimal illumination and temperature.





Plastic-lined, concrete raceway

Sandia National Laboratories

Modeling and Simulation Tools to Design Future Complex Hydride Storage Systems

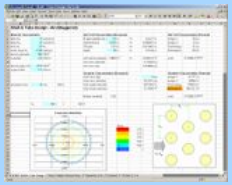
Engineering Characterization

$$R_1 = A_1 e^{-E_1/RT}\left(p^{n_1} - p_1^{*n_1}\right)s_1$$

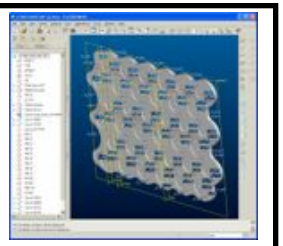
Kinetics Model

Simulation Tool

GM

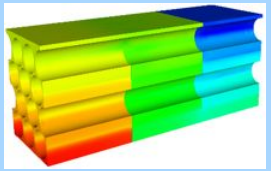


Desktop Analysis



CAD Design

Iterative Design Process



FEA Models

Combination of commercial software (Comsol) and Sandia codes used on parallel computing platforms

Final System Design

Sandia National Laboratories

Opportunities for You at Sandia

- Internships
- Fellowship programs
- Post-doctoral research
- Limited Term Employment (LTE)
- Full Time Employment (FTE)

Internships

- **Sandia has many programs for summer and year-round internships**
  - Center for Cyber Defenders (CCD)
  - Computer Science Research Institute (CSRI)
  - Enabling Predictive Simulation Research Institute (EPSRI)
  - National Engineering Research Institute (NSEI)
  - Physical Science Institute (PSI)
  - Sandia Institute for Modeling and Simulation (SIMS)
  - Science of Extreme Environments Research Institute (SEERI)

- **For more info:**
  http://sandia.gov/careers/intern-institutes.html

Fellowship Programs for New BS Graduates

MASTERS FELLOWSHIP PROGRAM (MFP)

- **Top minority BS students get tuition, stipend and benefits to go earn a MS degree.**

CRITICAL SKILLS MASTERS PROGRAM (CSMP)

- **Top BS students get tuition, stipend and benefits to go earn a MS degree in an area critical to Sandia.**

Requirements include GPA minimum (3.2), 2 months working at Sandia, and U.S Citizenship.

Sandia National Laboratories

Post-Doctoral Research at Sandia

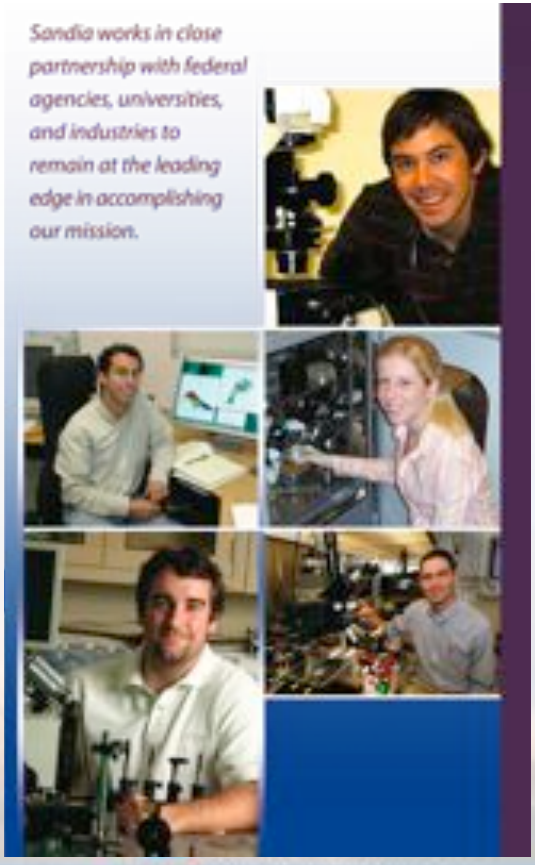
- **We offer post-doctoral employment for a period of 2-3 years in a variety of science and engineering disciplines.**
- **Sandia has minimum GPA requirement (3.5)**
- **Foreign Nationals (non-U.S. Citizens) are welcome.**

- **Truman Fellowship**

SANDIA NATIONAL LABORATORIES
President Harry S. Truman Fellowship in
National Security Science and Engineering

- U.S Citizenship
- Ability to get Security Clearance
- Minimum GPA of 3.7
- Received Ph.D. within last 3 years

- Yearly salary over $110K



Employment

- **Opportunities for MS and PhD graduates in many science and engineering disciplines**
- **Limited Term Employment (LTE)**
- **Full Time Employment (FTE)**
- **Positions for Foreign Nationals and U.S. Citizens**
- **For a complete listing of available positions at NM and CA locations:**

  http://www.sandia.gov/careers/search-openings.html
- **For information on all opportunities:**

  http://www.sandia.gov/careers/index.html
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