SAND2007-1839C

Engineering Modeling and Simulation at Sandia National Laboratories

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Multiphase Transport Processes
Engineering Sciences Center
Sandia National Laboratories

April 18, 2007

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

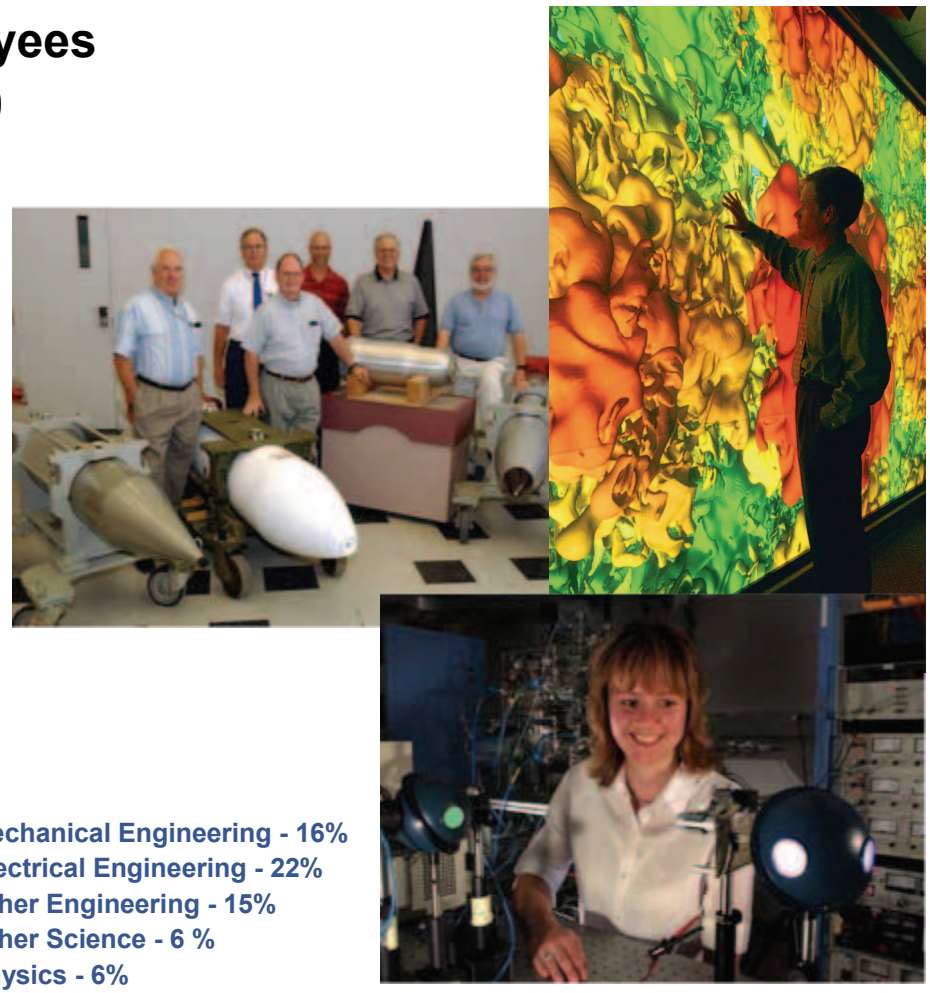
Sandia is a Mission-Driven Laboratory with Our Primary Business being National Security

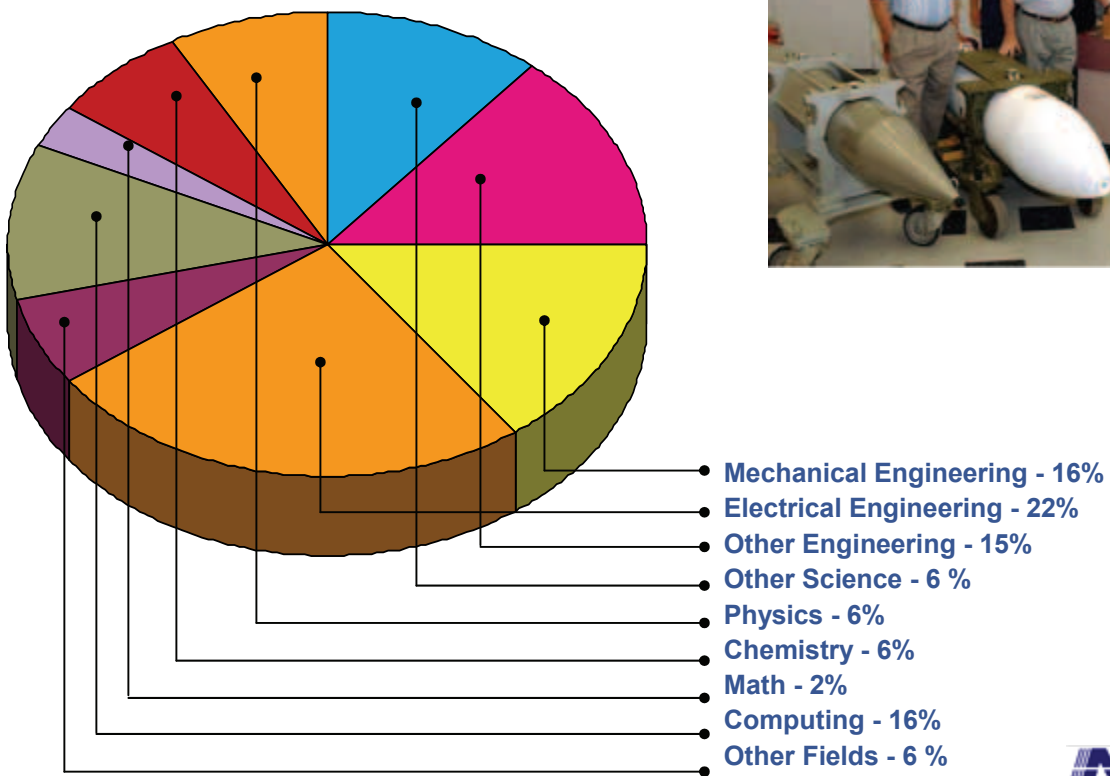
We serve many agencies of the US Government with:

- Design and development: nonnuclear portions of US nuclear weapons
- Production: advanced components
- Safety, security, use control
- Treaty verification, nonproliferation, counterproliferation
- Advanced military technologies
- Energy and environment
- Homeland security, countering weapons of mass destruction

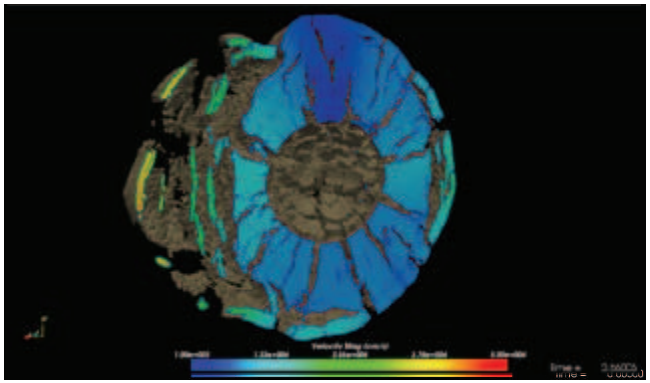
We Have A Highly Skilled Workforce

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

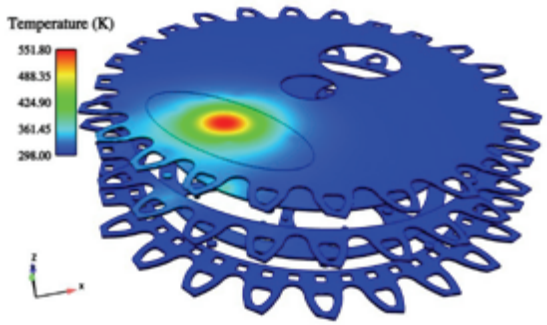




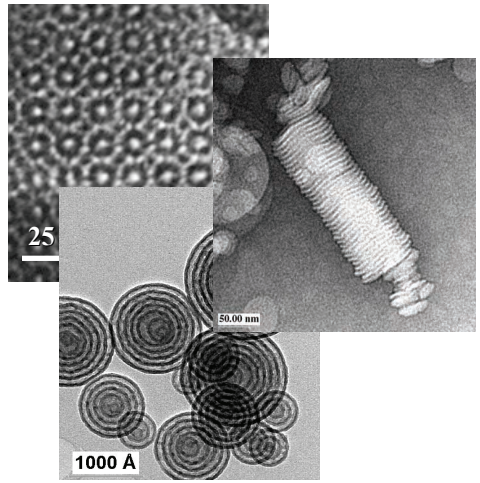
Our Mission Focus Relies on Strong Science, Technology and Engineering



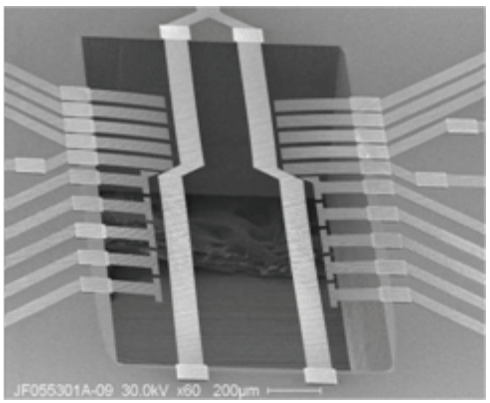
Computational and Information sciences



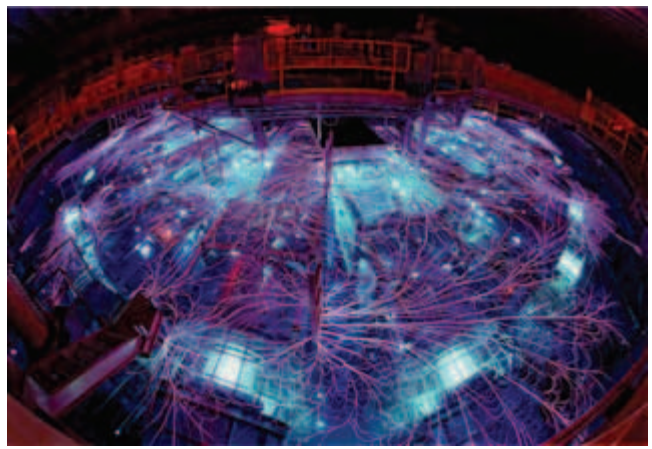
Engineering Sciences



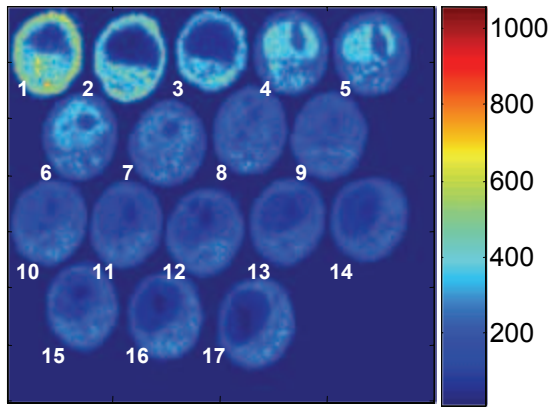
Materials Science and Technology



Microelectronics and Photonics



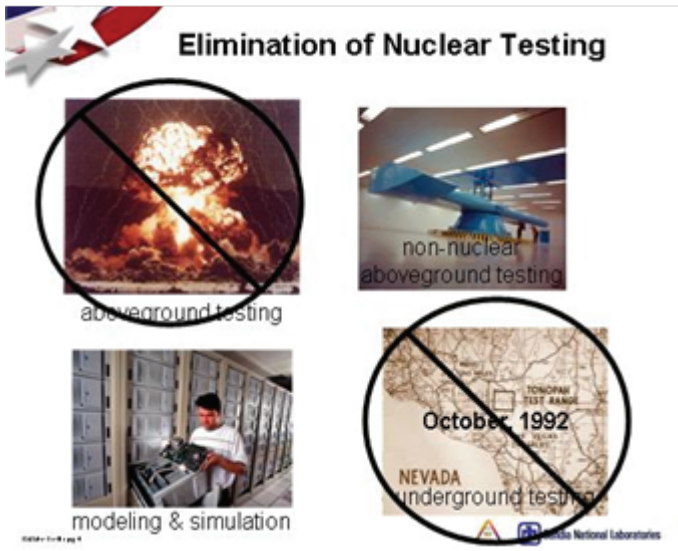
Pulsed Power

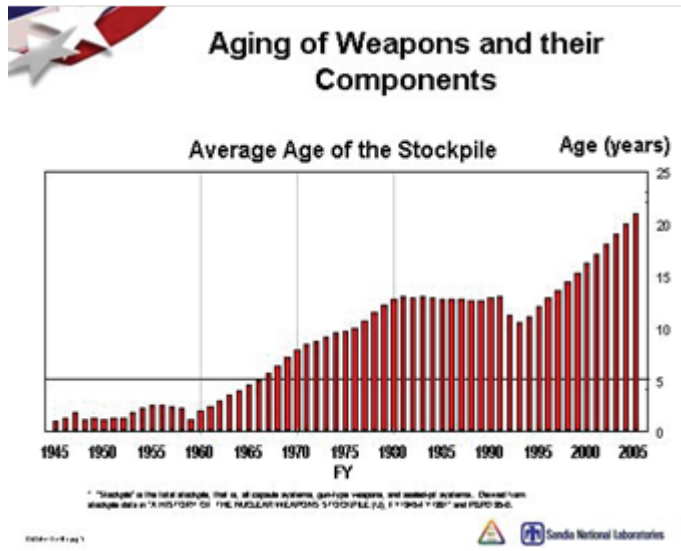


Bioscience

Modeling and Simulation Impact at Sandia National Laboratories

Sandia is changing the way we do our engineering business and system design qualification using modeling and simulation





Within the nuclear weapons program, qualification is the process of assessing system safety, reliability and performance, and of building the body of evidence that leads to system certification

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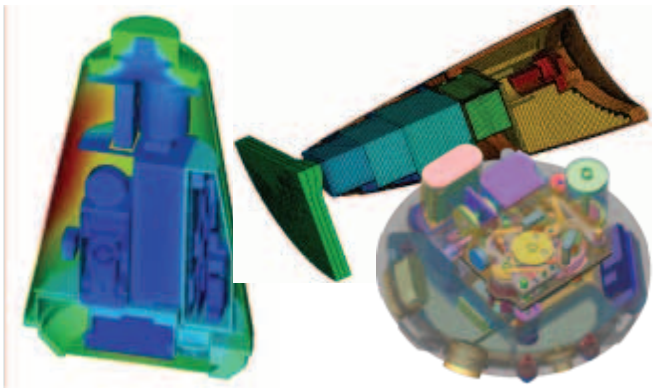
Engineering Sciences Capability Areas

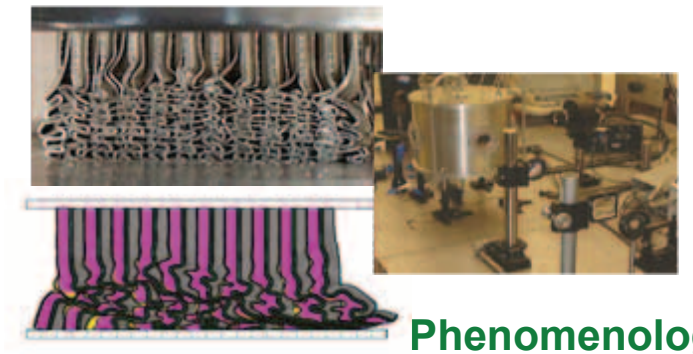
Engineering Modeling & Simulation



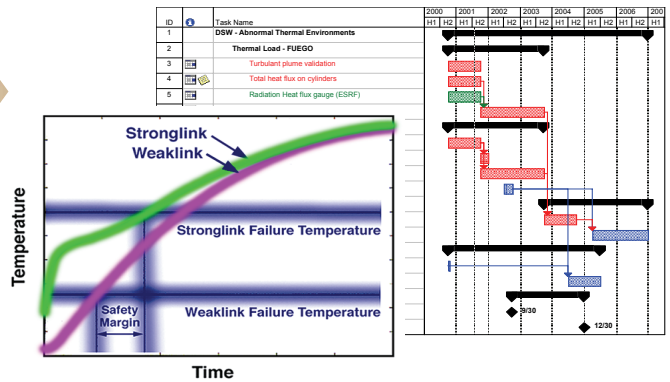
Large-Scale Test /Qualification

Code Development

Phenomenology & Model Development



Uncertainty Quantification/ Verification & Validation



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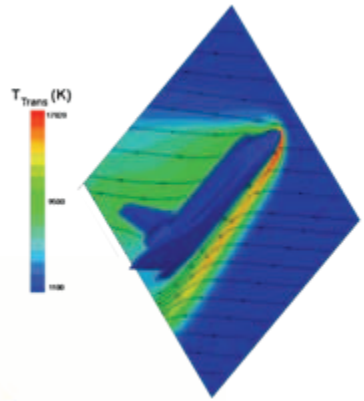
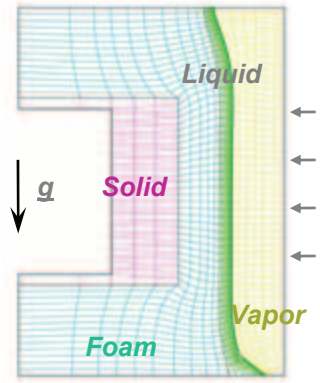
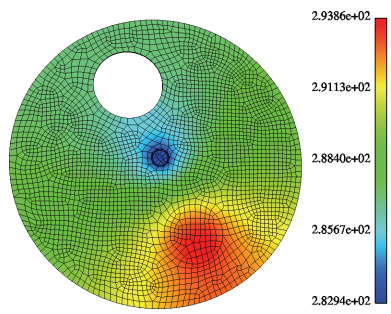
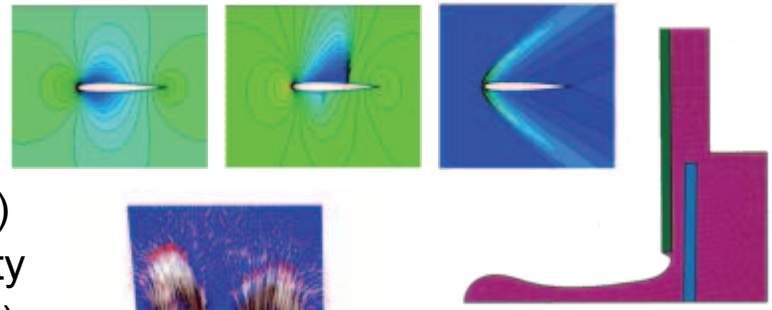
Computational Capabilities Address Broad Classes of Mechanics/Physics

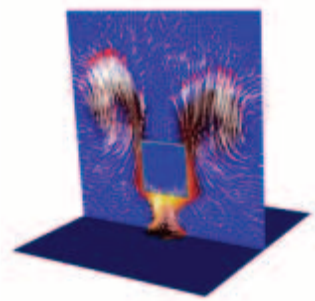
- Shock and Vibration
  - Salinas/Presto/Pronto3D (structural response)
- Motion, Friction, Wear, Material Failure
  - Adagio/Jas3D (quasi-statics)
  - Andante/Presto/Pronto3D (implicit dynamics)
- Thermal Response
  - Calore/Calagio/Coyote
  - Non-continuum thermal transport
- Electrical, Radiation, EM
  - Toro/Eiger-S (electrostatics)
  - Davinci (device behavior)
  - Xyce (circuit behavior)
  - CEPTRE (Coupled Electron-photon transport)
  - ITS (Integrated TIGER Series – Monte Carlo)
  - Emphasis (EM response)
- Fluid Response (liquid, gas and multiphase)
  - Aria/GOMA (capillary and electro-kinetic flows)
  - Faust/DSMC or other transitional flow capability
  - Fuego/Vulcan (subsonic variable density flows)
  - Premo/Saccara (transonic/supersonic flows)



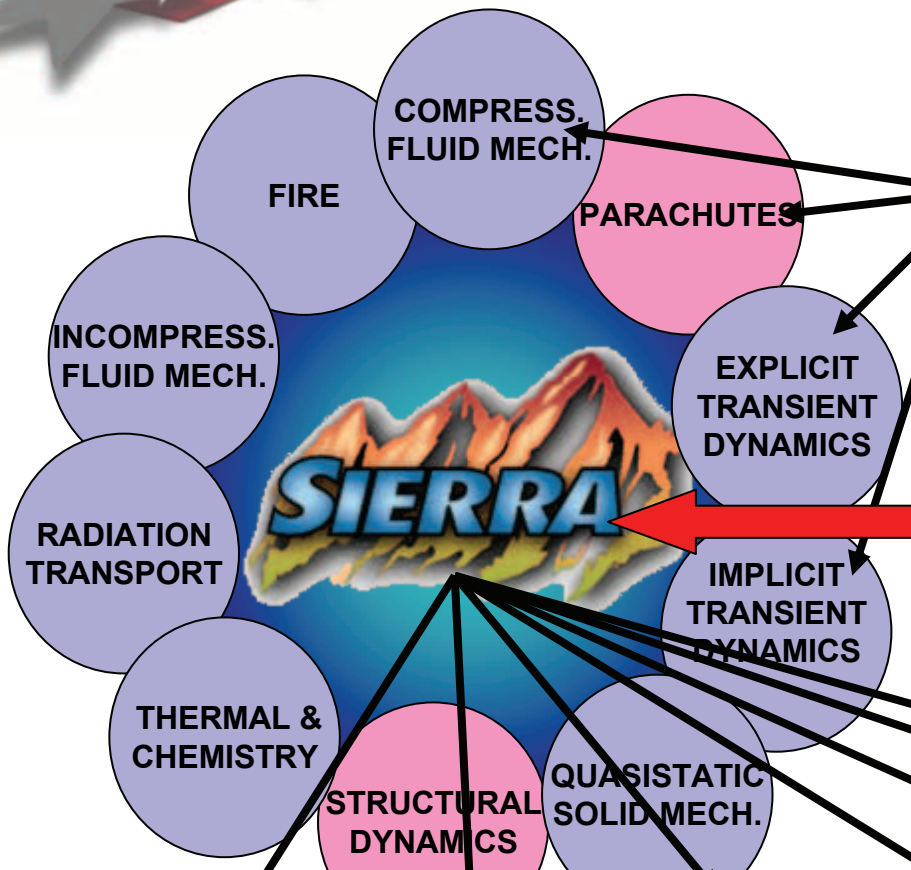








SIERRA Strategy: Minimize Cost to Develop, Maintain, and Port



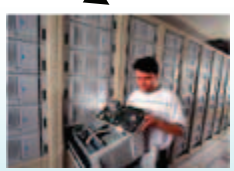
Physics dependent models and algorithms

Physics independent capabilities and algorithms


SNL Janus

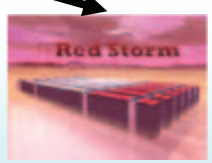

9100 Linux Rogue Cluster


SNL Linux NWCC


SNL Linux ICC


LLNL White


LANL Q



SNL Red Storm

National Nuclear Security Administration

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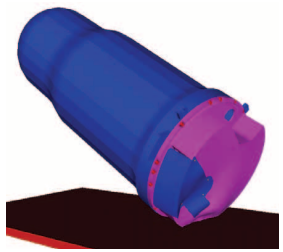
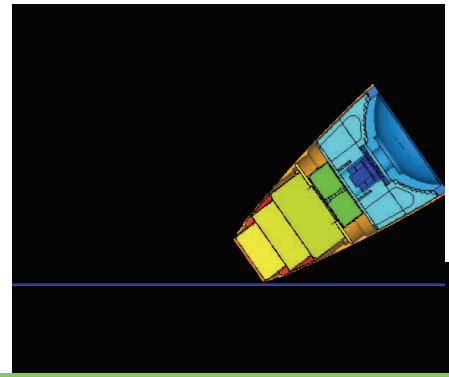
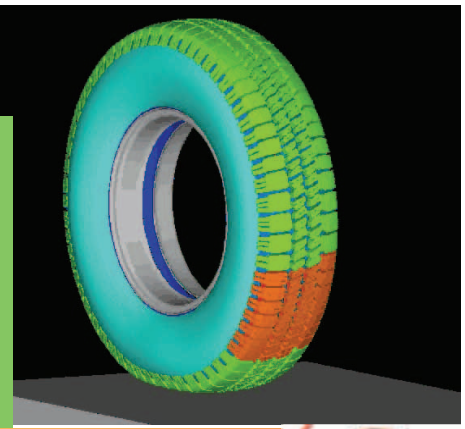
Computational Solid Mechanics and Structural Dynamics Tools







Presto
(Transient Dynamics)

Adagio/Andante
(Nonlinear Implicit Quasistatics/Dynamics)

Salinas
(Structural Dynamics)

Mechanics complexity

Failure/ fragmentation
Yielding
Contact
Large deformation
Shock
Vibration

nano-sec
micro-sec
milli-sec
secs
hours

Time Scale

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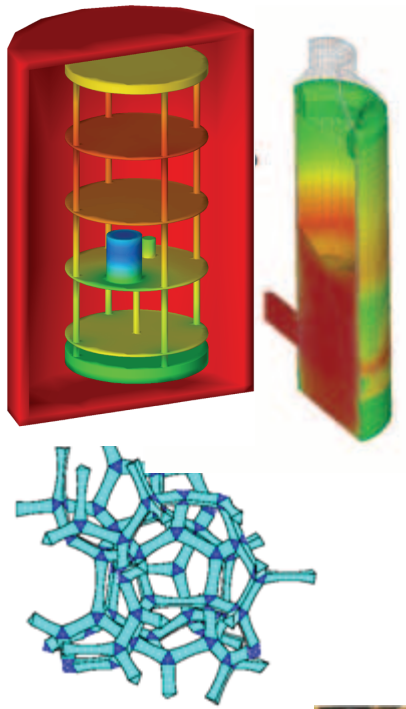
Thermal, Fluid and Aero Sciences

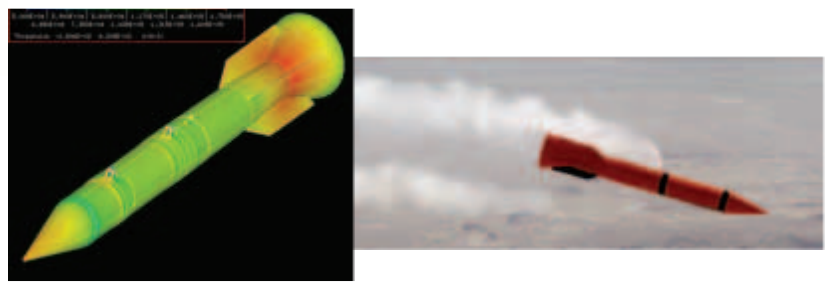
Fluid & Thermal Mechanics

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



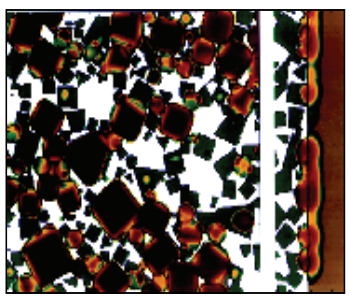
Aero Science & Technology

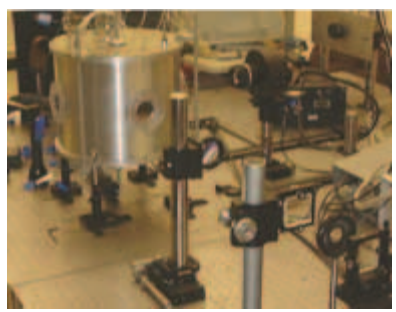
- Compressible Flows
- Aerothermodynamics
- Fluid/Structure Integration
- Aero & Flight Dynamics
- Parachute Technology



Reactive Processes

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





Experimental Technology

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

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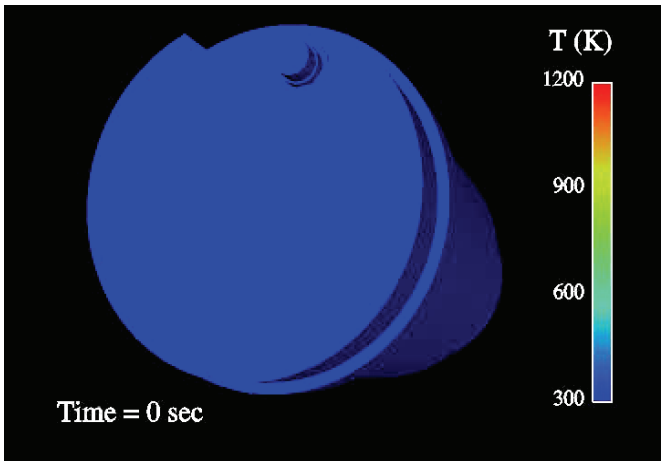
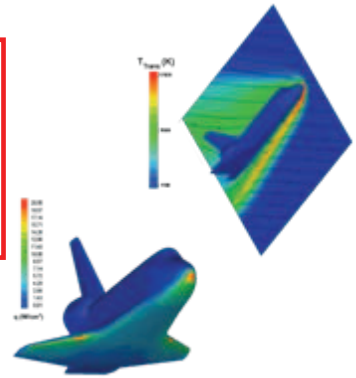
Thermal/Fluid Computational Tools

Calore
Thermal Analysis

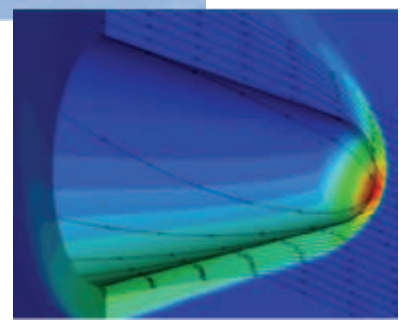


Fuego
Fire Environments

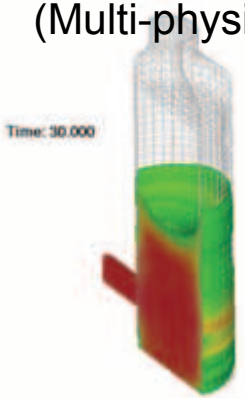
Faust
Sub-Continuum
Fluid Dynamics
and Heat Transfer

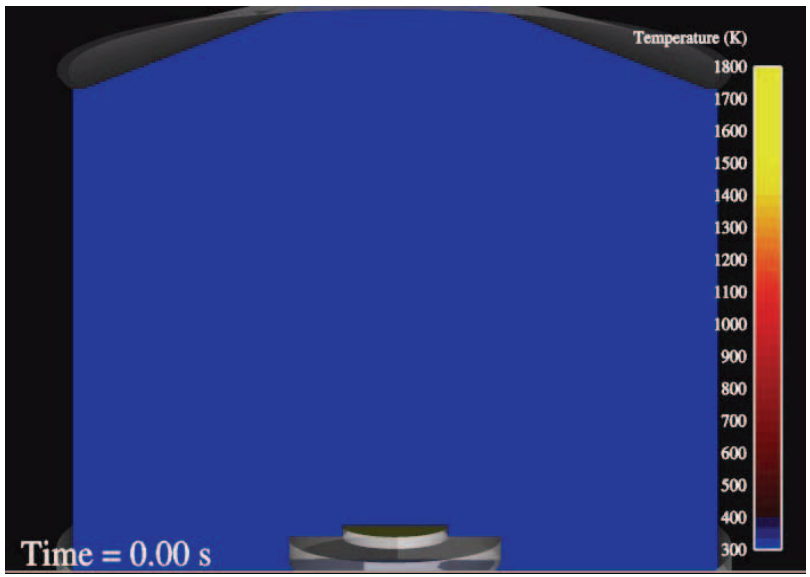


Premo
Compressible Fluid Dynamics



Aria
Non-Newtonian
Incompressible
Fluid Mechanics
(Multi-physics)





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Beyond the Codes: Critical Elements of a Simulation-Based Engineering Capability

- **Research experiments** - learning what we don't know about the salient physics underlying the problem
- **Validation experiments** - establishing the validity of the physical models used in computational predictions
- **Computational models** - developing a **predictive capability** using validated numerical simulations
- **New diagnostics** – may be needed in both research and validation experiments
- **Full-scale tests** - reality at the systems level, but not a design/development tool
- **Experienced, motivated people** - hard problems require the very best

The solution of complex engineering problems depends upon the successful integration of all of these capabilities

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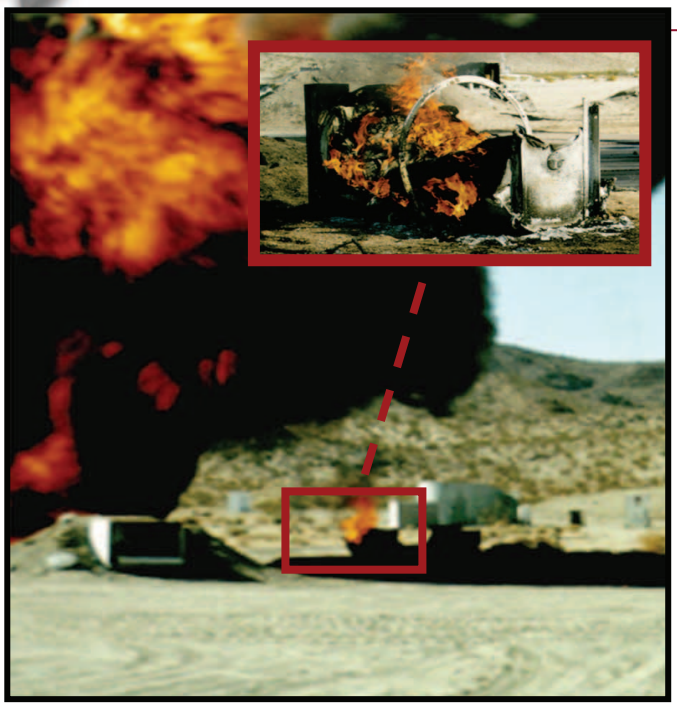
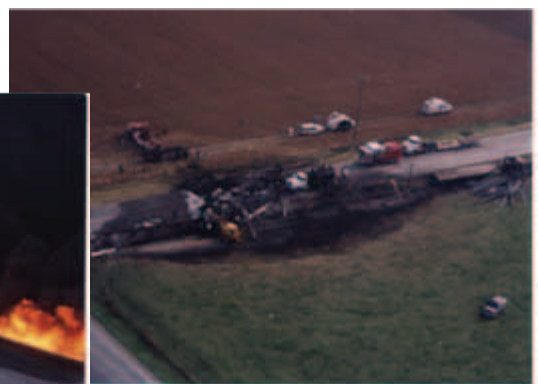
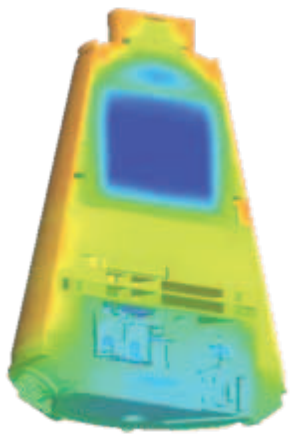
Weapon Response in a Fire



Nuclear Weapon Safety

- Assessments identify fire as a potential concern in the transportation & storage of nuclear weapons (DOE, DTRA)
- Qualification required for W76-1 Stockpile Life Extension – assert 1 in 10^6 probability of accidental detonation
- Limited testing opportunities and hardware availability demands high-fidelity modeling and simulation capability for assessing 'unknowns'.





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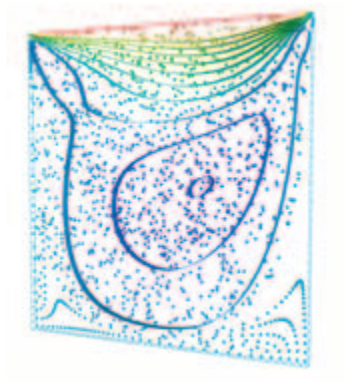
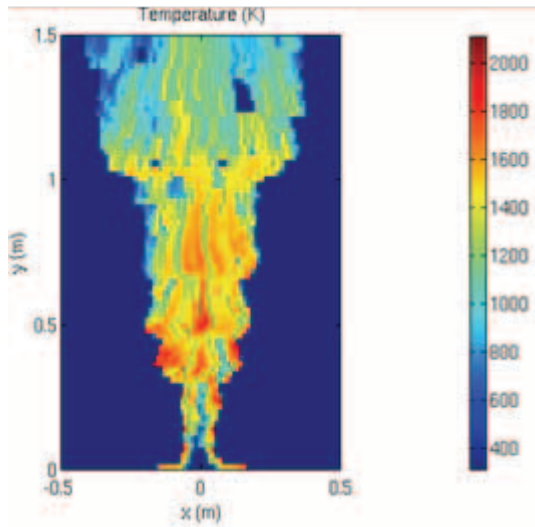
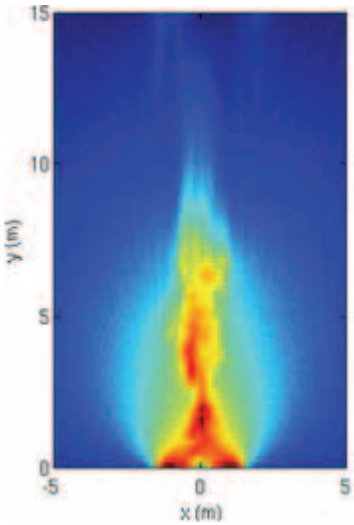
What is Needed for Simulating Fire?

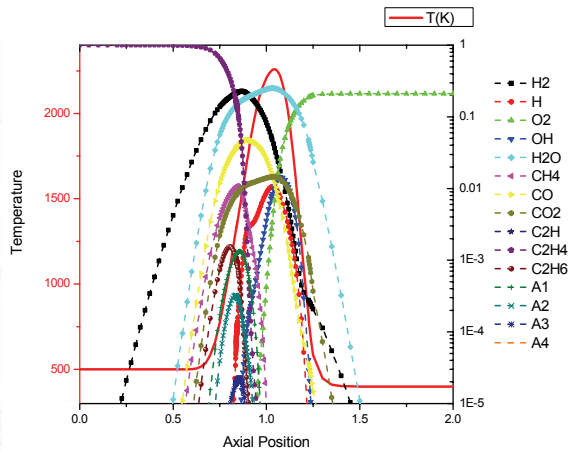
Required Physics

- Material decomposition
- Fluid dynamics
- Gas phase combustion
- Buoyancy effects
- Radiation transport
- Soot formation
- Particle combustion
- Conduction/convection
- Turbulence









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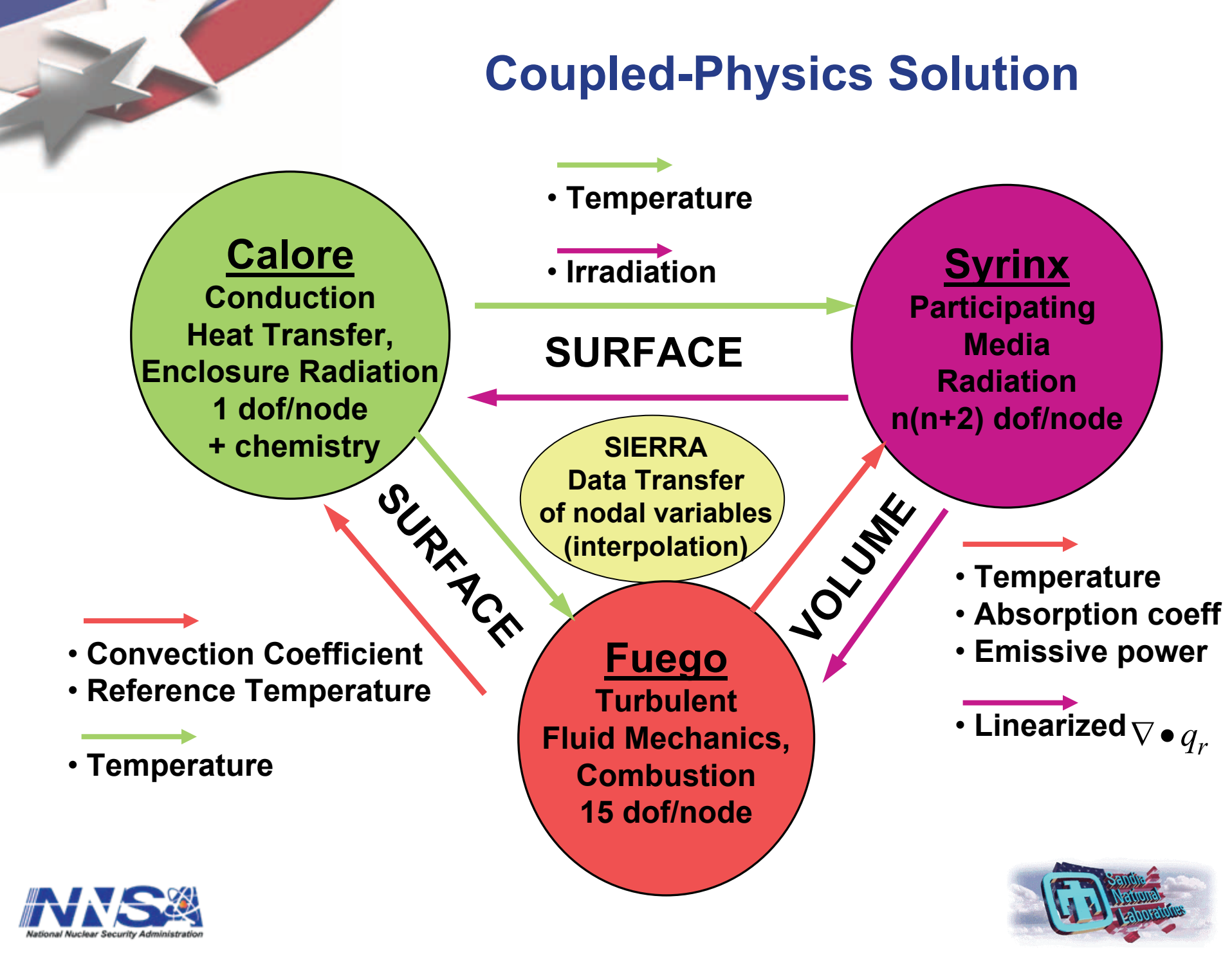
Coupled-Physics Solution



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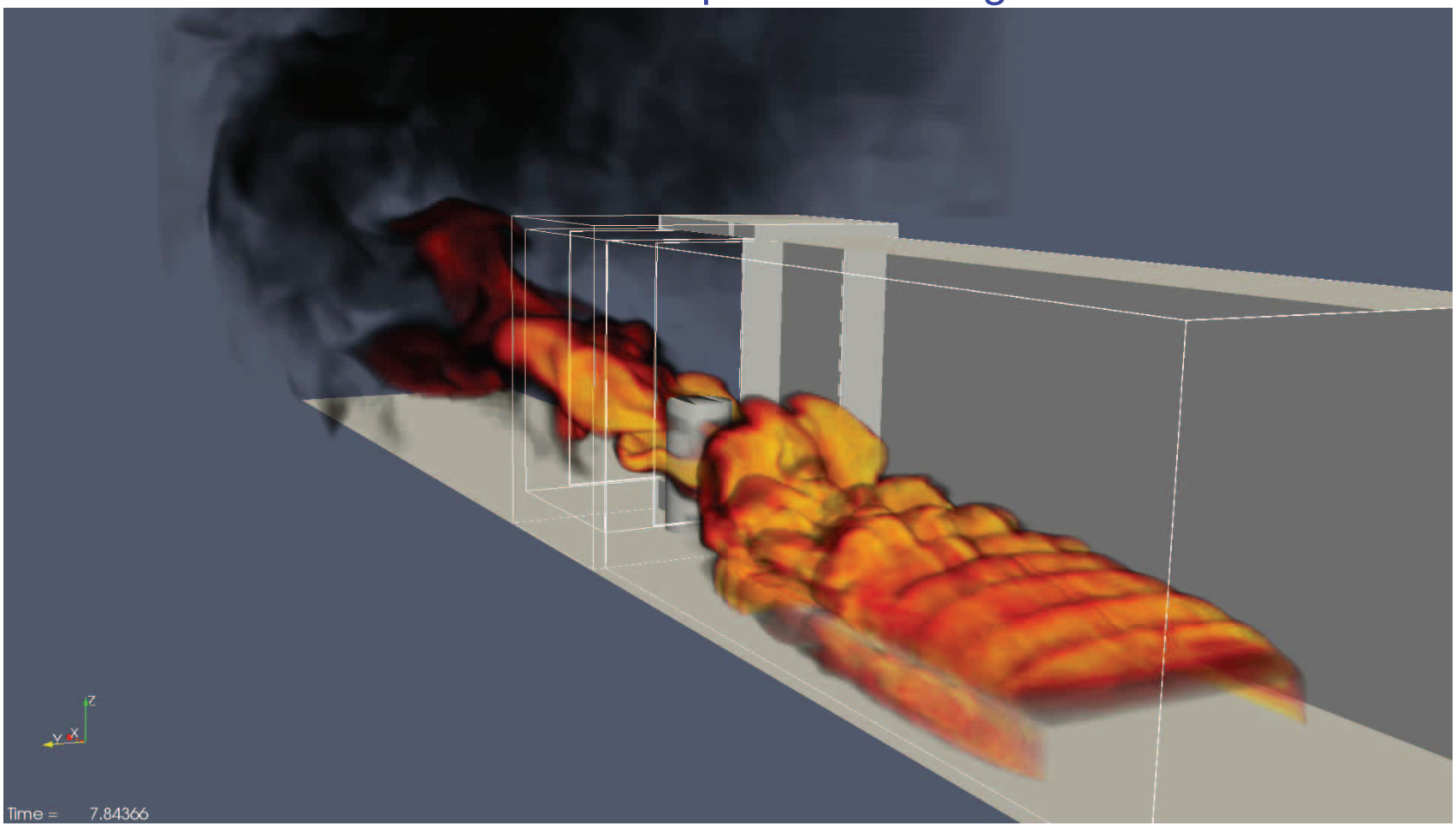
Example Simulation

Qualification Experiment Design



170M Degrees of Freedom, 2048 CPUs, 2 days

NNSA
National Nuclear Security Administration

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Laser Welding: Fluid/Thermal/Structural Coupling

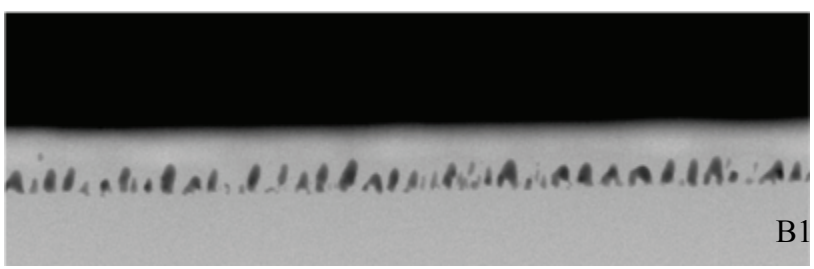
Laser Welding is used extensively in joining critical weapon system components

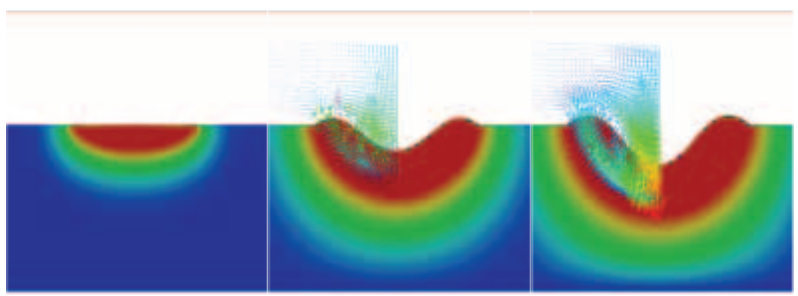
Many challenges exist in the creation of a successful laser weld

- Process Considerations (laser operation, joint requirements, materials, …)
- Weld Performance (strength, hermeticity, defects, nearby sensitive components, distortion, weld shape, …)

Needs/Goals:

1. Predictive capability for process & performance of weld
2. Understanding of process sensitivities on weld performance
3. Optimization capability for process & performance





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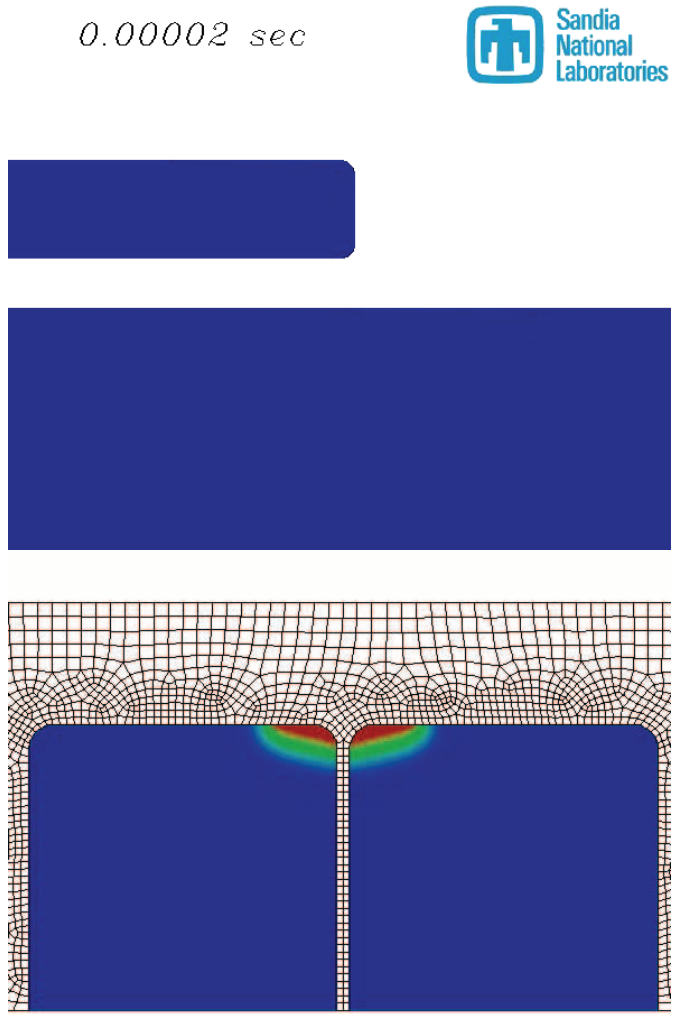
Dynamic Interface Example: LS Simulation of Laser Welding

Material joining by intense localized heating

- Extremely complex interfacial physics
  - Radially distributed laser heating
  - Vapor recoil pressure
  - Vaporization heat loss
  - Radiation and convection heat loss
  - Critical role of surface tension
- ALE simulations require frequent remeshing
  - Expensive analyst time, introduces inaccuracy
- Level set simulations under active development
  - Complete set of interfacial conditions applied along level set interface cutting through elements



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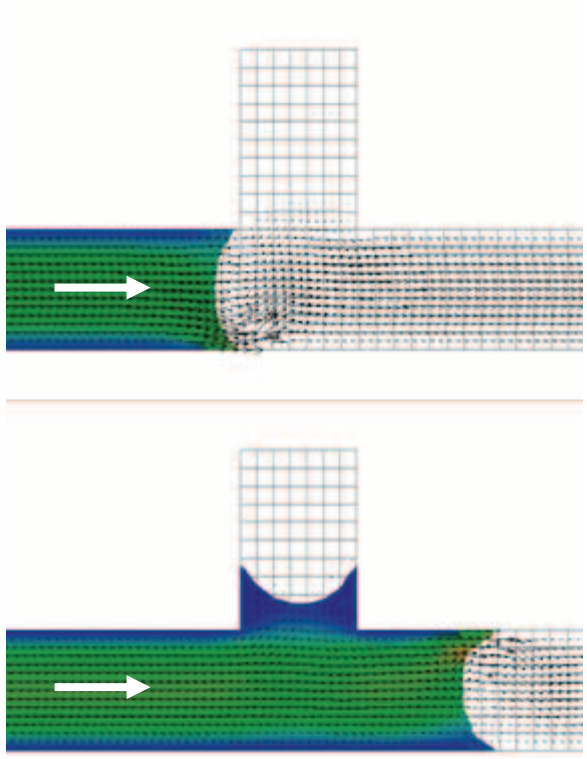
Rapid Turnaround Potting Analysis

- Problem: understand process parameter influence on complete filling of a channel.
- Customer needed this information in 4 weeks
- Utilized our state-of-the-art M&S capability for fluid flow and engineering experience to meet deliverables within budget and deadline.

Polymer channel filling



Guidance: reduce channel aspect ratio, reduce flow viscosity, reduce flow velocity and do not add a surfactant.

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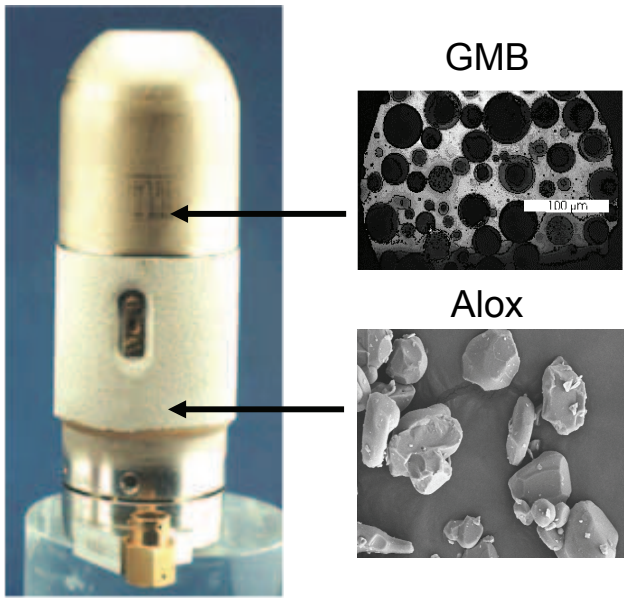
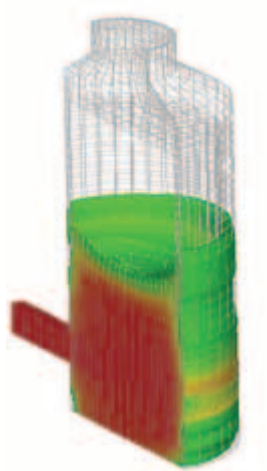
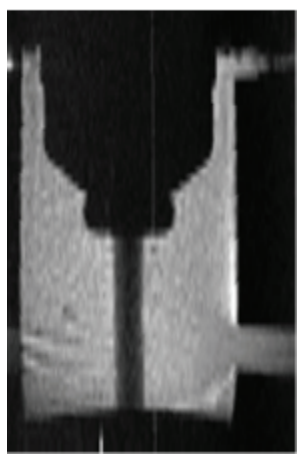
Predictive Modeling Capability for Encapsulation Processing



- **Encapsulation defects, e.g. voids, fracture, delamination and property inhomogeneities, can lead to component failure.**
- **Need predictive models to help design encapsulants, optimize cure schedule, improve manufacturing processes and provide material properties for shock/solid modeling/dielectric breakdown/failure**

- **Encapsulants are epoxies filled with solid particles to provide performance enhancements, e.g. structural integrity, voltage isolation, stress wave media**
- **These processes are usually the last operations and highly value-added processes**





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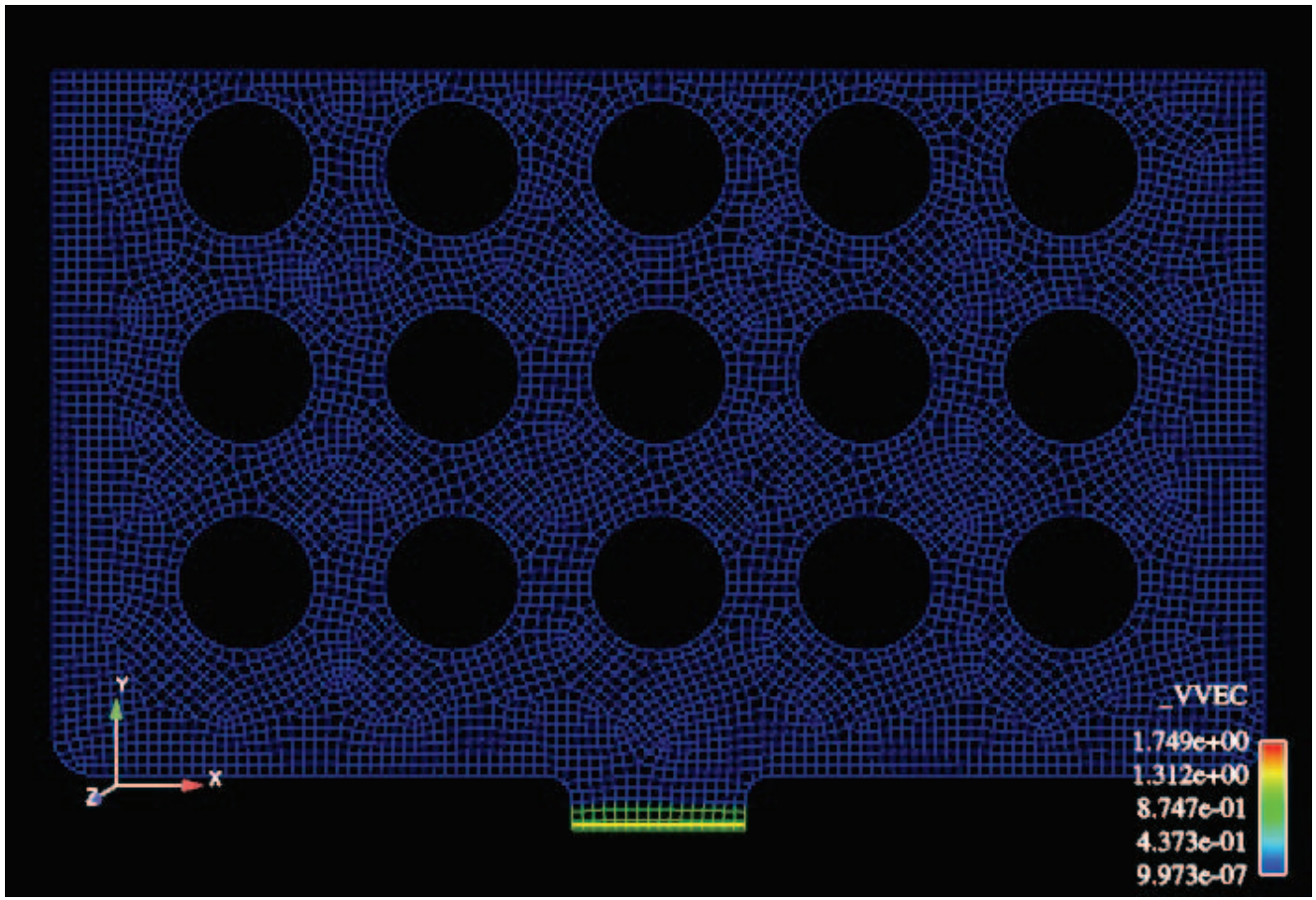
Simulation of Complex Structure Flow



Questions: Where do voids form? Can overfilling remove them? What is the optimal flow rate or pressure? Change viscosity?

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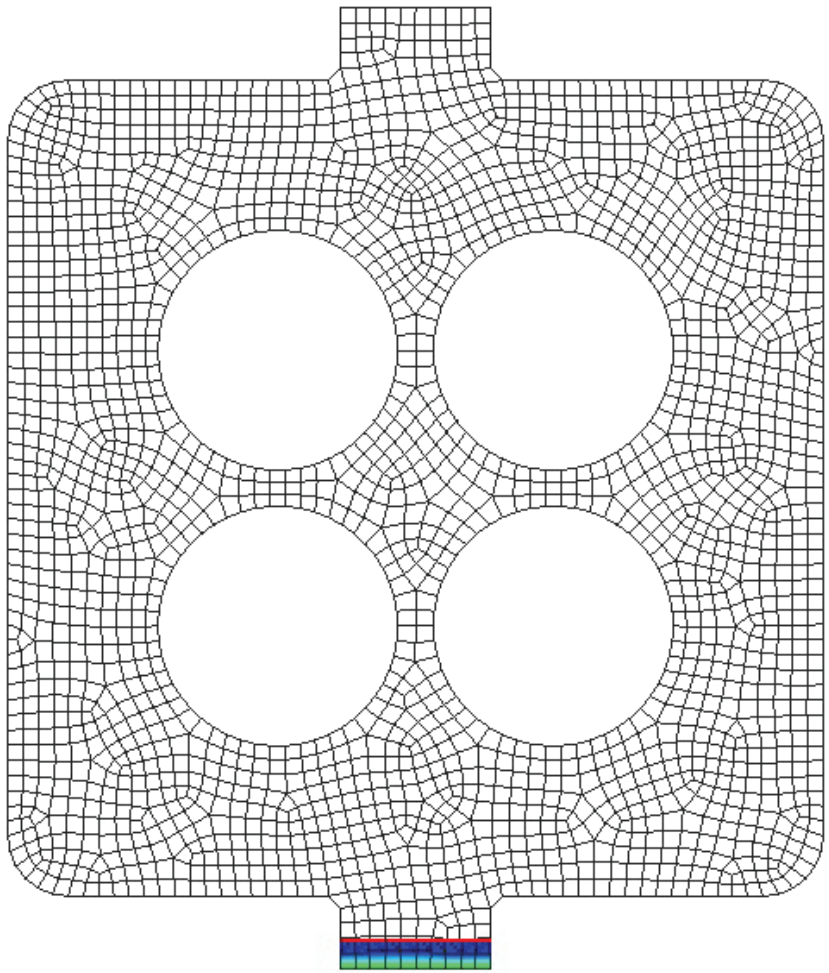
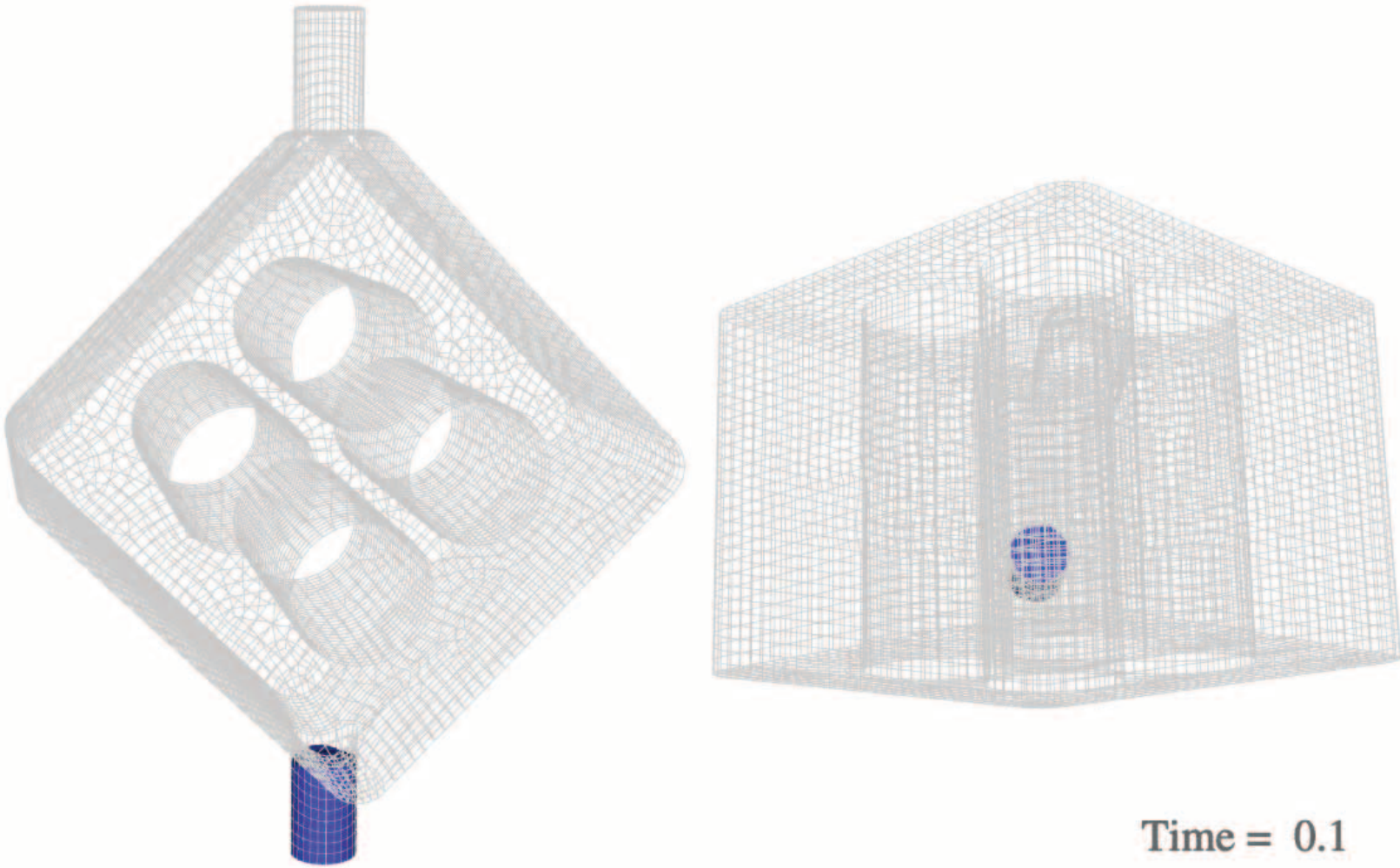
Current State-of-the-art Incorporates Level Sets with Adaptivity



Current Work is Focused on Full 3D



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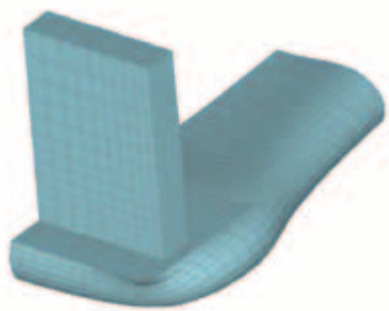
CRMPC CRADA History

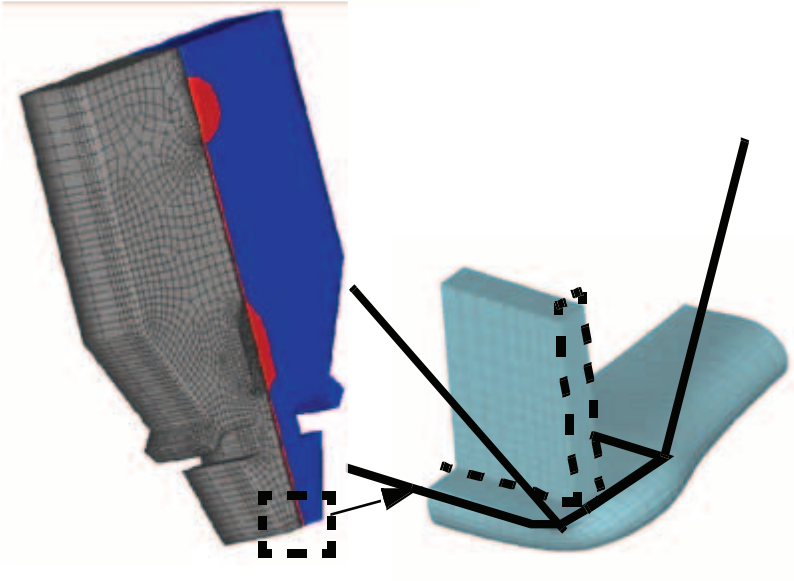
- CRMPC initiated in 1994-1996 timeframe
- Started with seven companies, dues were $50,000/year with matching dollars from Sandia.
- CRMPC contract funded research and development of Goma an incompressible, multiphysics code in the following areas:
  - Research of free and boundaries
  - 3D Die Design with Solid-fluid interactions
  - Wetting on Deformable Substrates
  - Coating Window Predictions (slot coating)
  - Extensive Porous Media Capability
  - Automated Geometry, 3D Meshing
  - Issue Tracking, QA Testing, Software Distribution, etc.



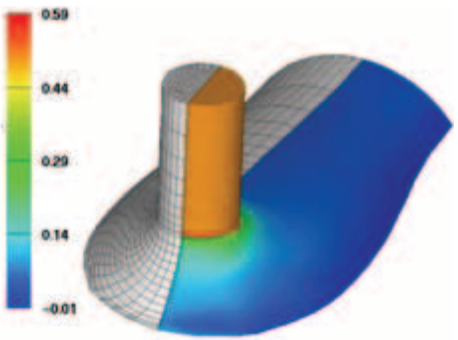
- Work on Goma development through the CRMPC occurred over a five year period.
- Upon completion of these core capabilities (2002) within Goma, subset of the CRMPC companies invested in a three year extension that shifted the focus to Eulerian Front Tracking Algorithms. Currently in Extension III.

Thin Continuous Liquid Film Coatings and Structures

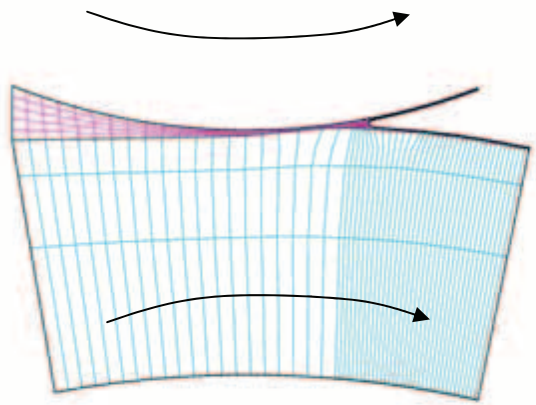
Extrusion Coating

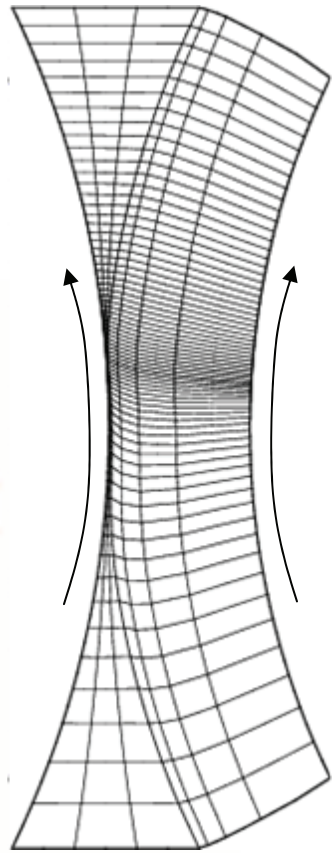


Micropen Lithography



Deformable Roll Liquid Metering and Laminating.





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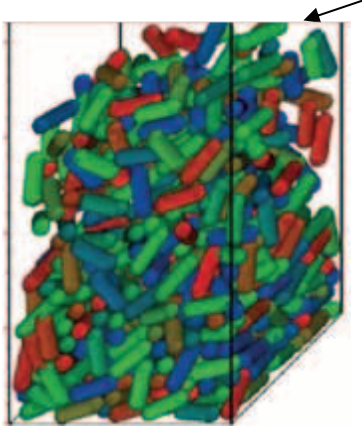
Enabling Nanoengineering

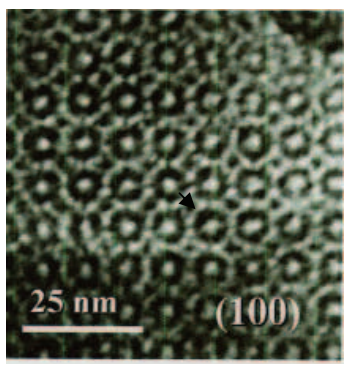
Coupled Particle and Flow Solver – LAAMPS/ARIA/ACME

- **Disperse nanoparticles in materials to engineer functional nanocomposites**
- **Fluidization in liquid is the preferred processing and handling method**
- **Modeling and simulation of dense suspensions to build process understanding and control**
- **Combine continuum simulations of fluids, MD and DEM simulations of particulate systems**

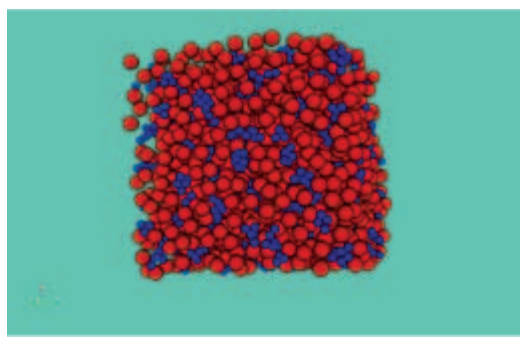
Fluidization/Processing - e.g. coating, casting…
-Rheology, Microstructure, self-assembly, bulk stability



Rheology



Surface self-assembly



Dispersion stability

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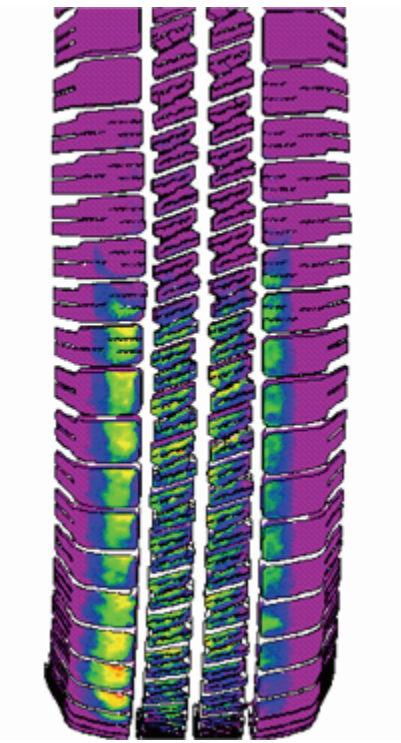
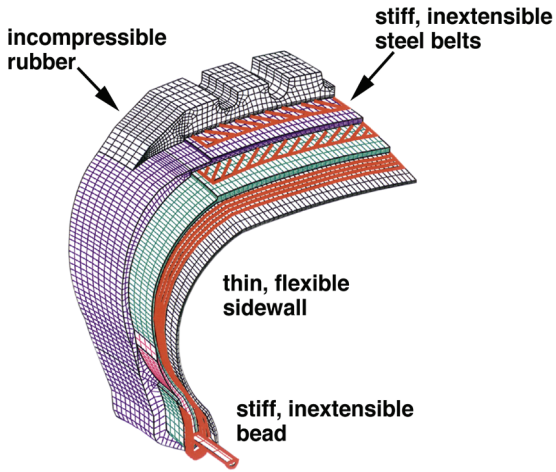
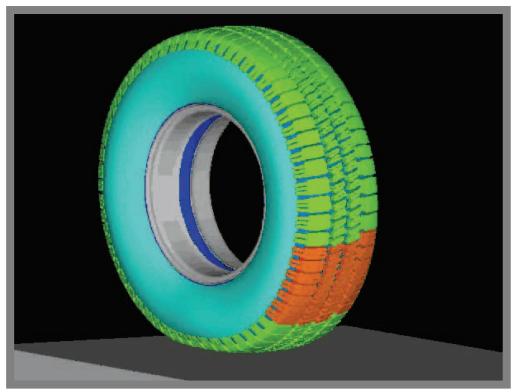
Goodyear/Sandia Interaction



- Increase Model Complexity by Several Orders of Magnitude
- Decrease Computational Run Times by 2 Orders of Magnitude (day)
- Automatic Coupling between Solid Geometry, Meshing, Mechanics Codes, and Visualization of Results
- Reduce Prototype Tire Builds from 3 – 4 to 1
- Reduced yearly R&D Costs by $100M!
- M&S investment led to best sales quarter in 7 years and 3rd best in company history





The Goodyear/Sandia interaction is mutually beneficial. Goodyear gets "rocket science" applied to tires. Sandia gets real-world development and testing of simulation technology.

National Nuclear Security Administration

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