

Predictive Engineering Sciences Overview

Harold (Hal Morgan)

Senior Manager, Computational Simulation Sciences
Engineering Sciences Center
Sandia National Laboratories, NM

Presentation to

Bob Keegan, CEO

The Goodyear Tire & Rubber Company
Visit to Sandia National Laboratories

October 22, 2007

*Sandia is a Multiprogram Laboratory Operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy Under Contract DE-ACO4-94AL85000.*

Sandia National Laboratories: Approaching 60 Years of National Service

- Born of the atomic age.
- Heritage of engineering and production.
- Science mobilized for national security.
- A legacy of industrial management.
- Six key mission areas:
 - Nuclear weapons
 - Nonproliferation
 - Assessments
 - Military technologies and applications
 - Homeland security
 - Energy and infrastructure assurance



*“you have ...an opportunity
to render an exceptional
service in the national interest.”
May 13, 1949 Letter from
President Truman to Mr. Wilson,
President of AT&T*



1949-1993



1993-Present

Our Highest Goal: become the laboratory that the United States turns to first for technology solutions to the most challenging problems that threaten peace and freedom.

Sandia National Laboratories is Distributed

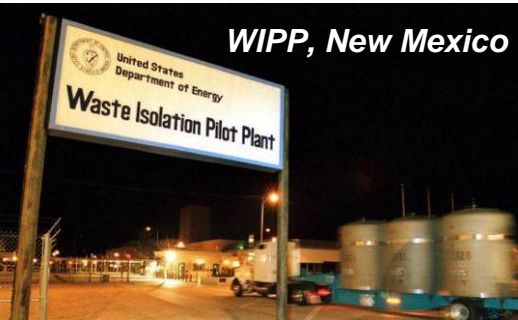
Tonopah, Nevada



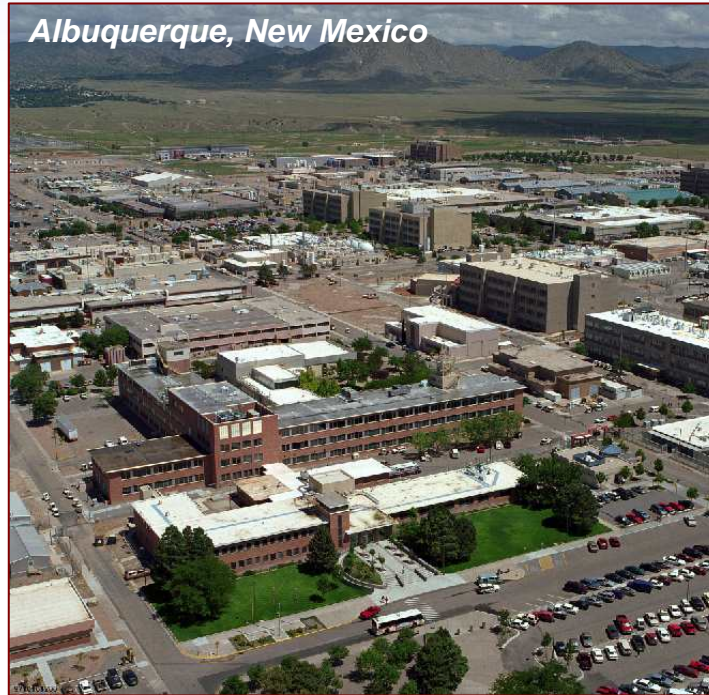
Pantex, Texas



WIPP, New Mexico



Albuquerque, New Mexico



Yucca Mountain, Nevada



Kodiak, Alaska



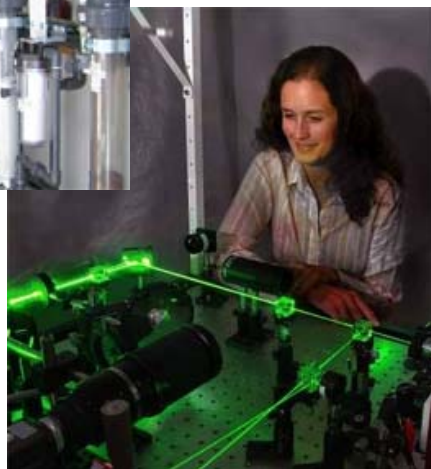
Kauai, Hawaii



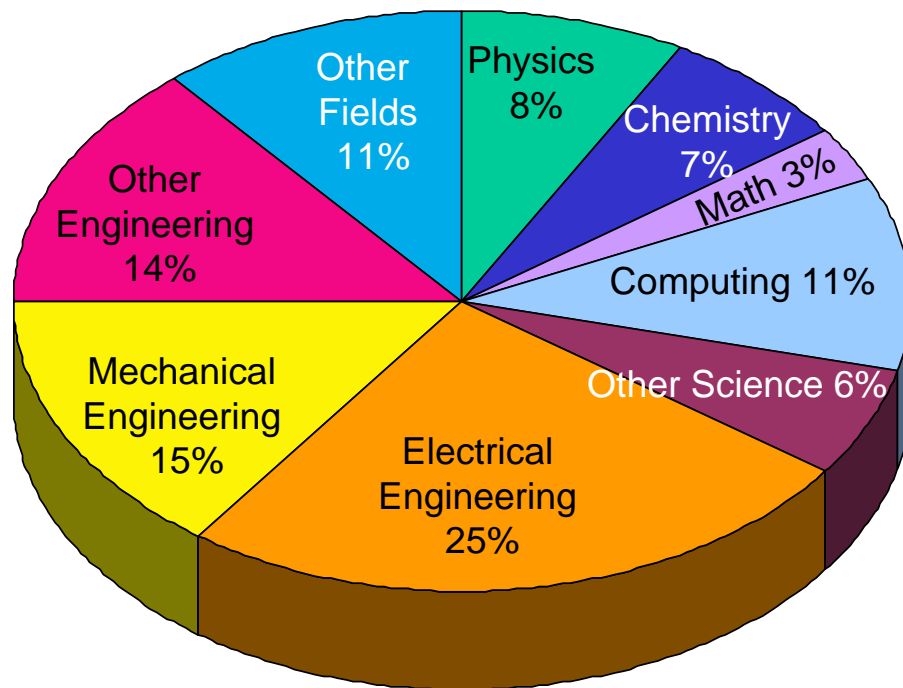
Livermore, California



Sandia Maintains a Highly Skilled Workforce



- Over 8,500 employees
- Over 1,500 PhDs; over 2,500 MS/MA
- Over 700 on-site contractors



\$2.3B budget in FY2006

Sandia's Programmatic Organization

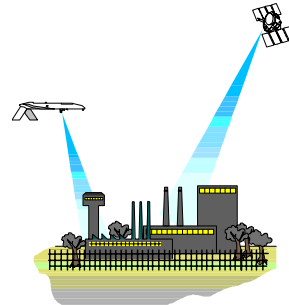
Nuclear Weapons One Management Unit:

- **Nuclear Weapons**



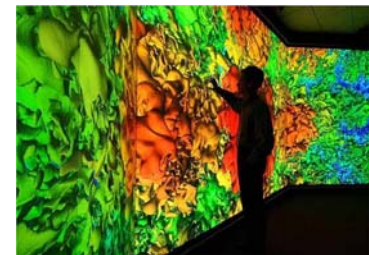
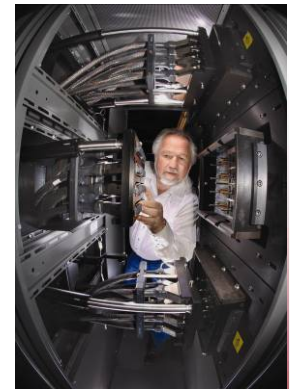
Integrated Technologies and Systems (ITS) Three Management Units:

- **Defense Systems & Assessments (DSA)**
- **Energy, Resources, & Nonproliferation (ERN)**
- **Homeland Security & Defense (HSD)**

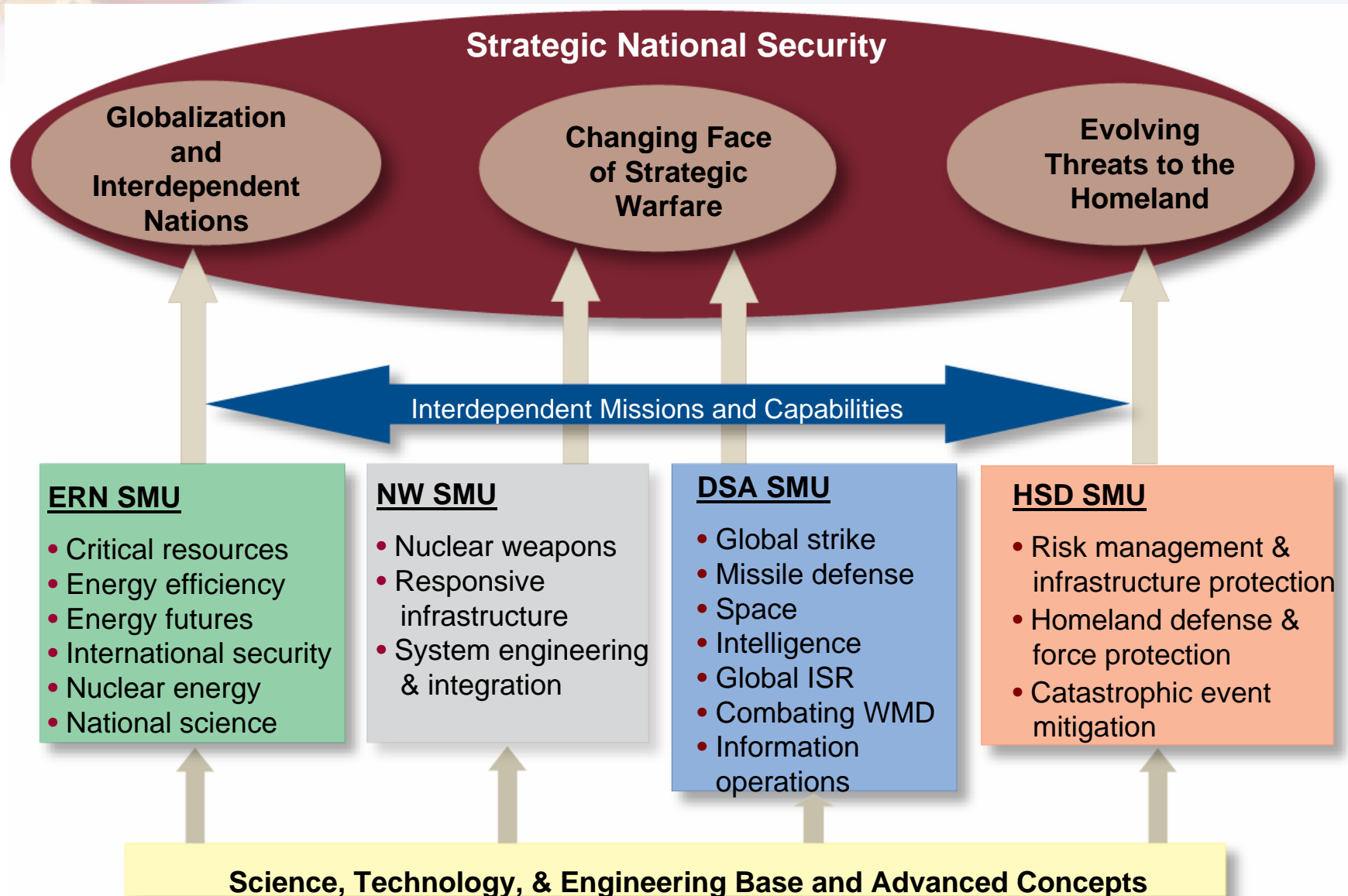


Laboratory Transformation Two Management Units:

- **Science, Technology, & Engineering**
- **Integrated Enabling Services**

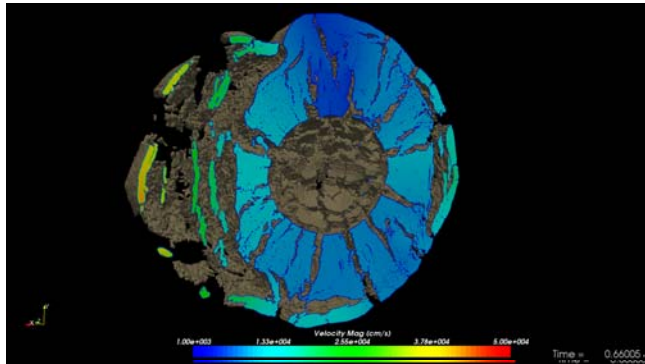


Sandia's Approach to Strategic National Security



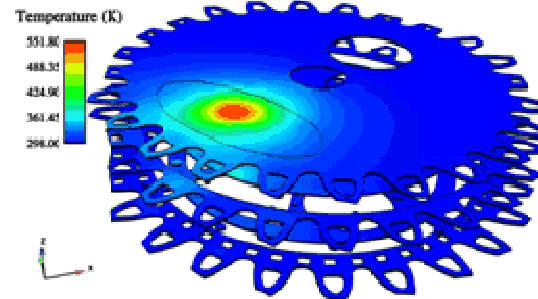
America's National Security Engineering Laboratory

Our Work is Supported by Our Science, Technology, and Engineering Capabilities

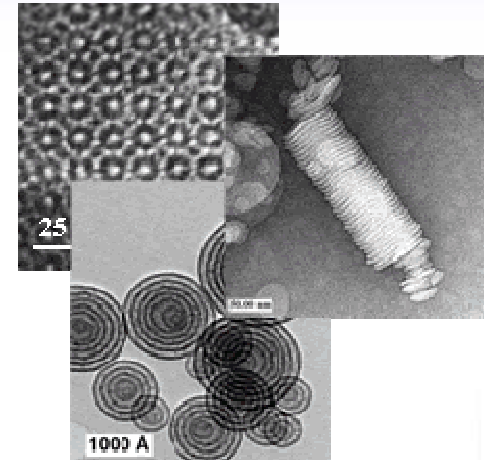


**Computational and
Information sciences**

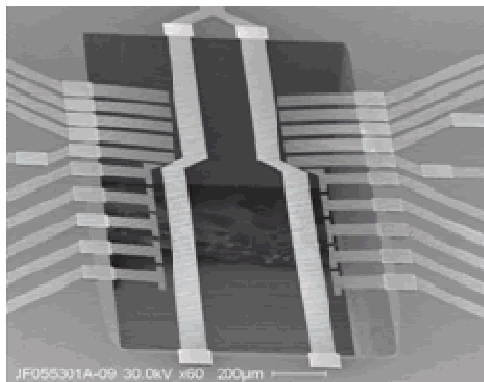
Bare Si; d-grain=0.5um



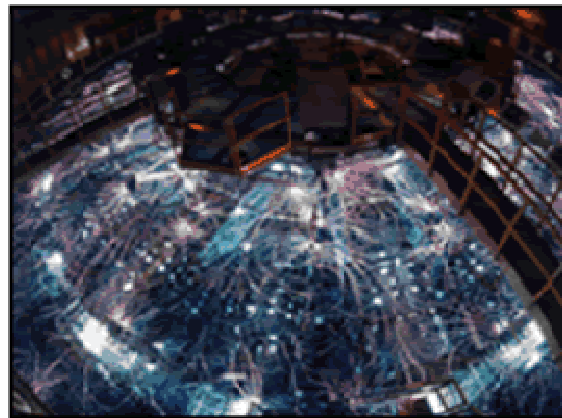
Engineering Sciences



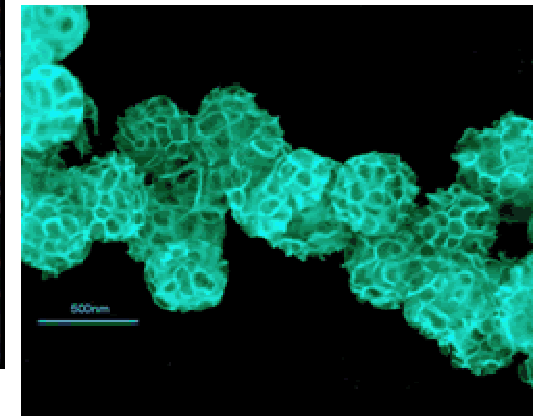
**Materials Science and
Technology**



**Microelectronics and
Photonics**



Pulsed Power

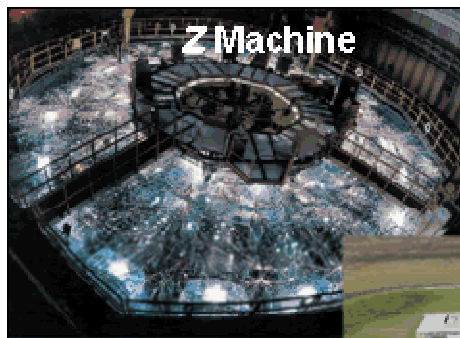


Biotechnology

Sandia has differentiating facilities



Microsystems and Engineering Sciences Applications (MESA)



Z Machine



Combustion Research Facility



Center for Integrated Nanotechnologies (CINT)

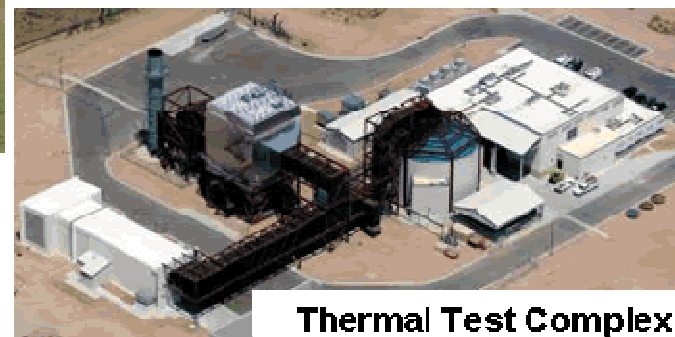
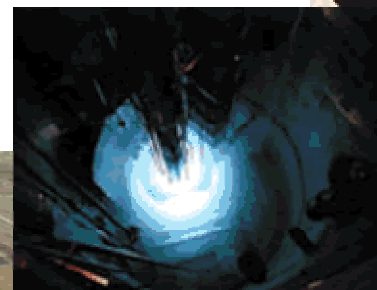


Red Storm

Sandia Pulsed Reactor III (SPR)



Annular Core Research Reactor (ACRR)



Thermal Test Complex

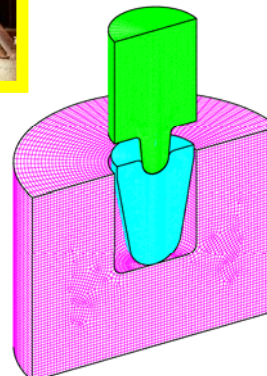
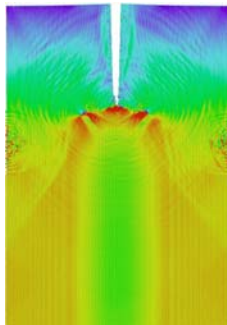
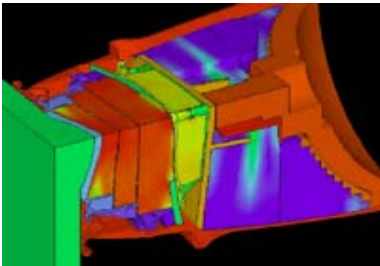
Engineering Sciences at Sandia National Laboratories

Mission:

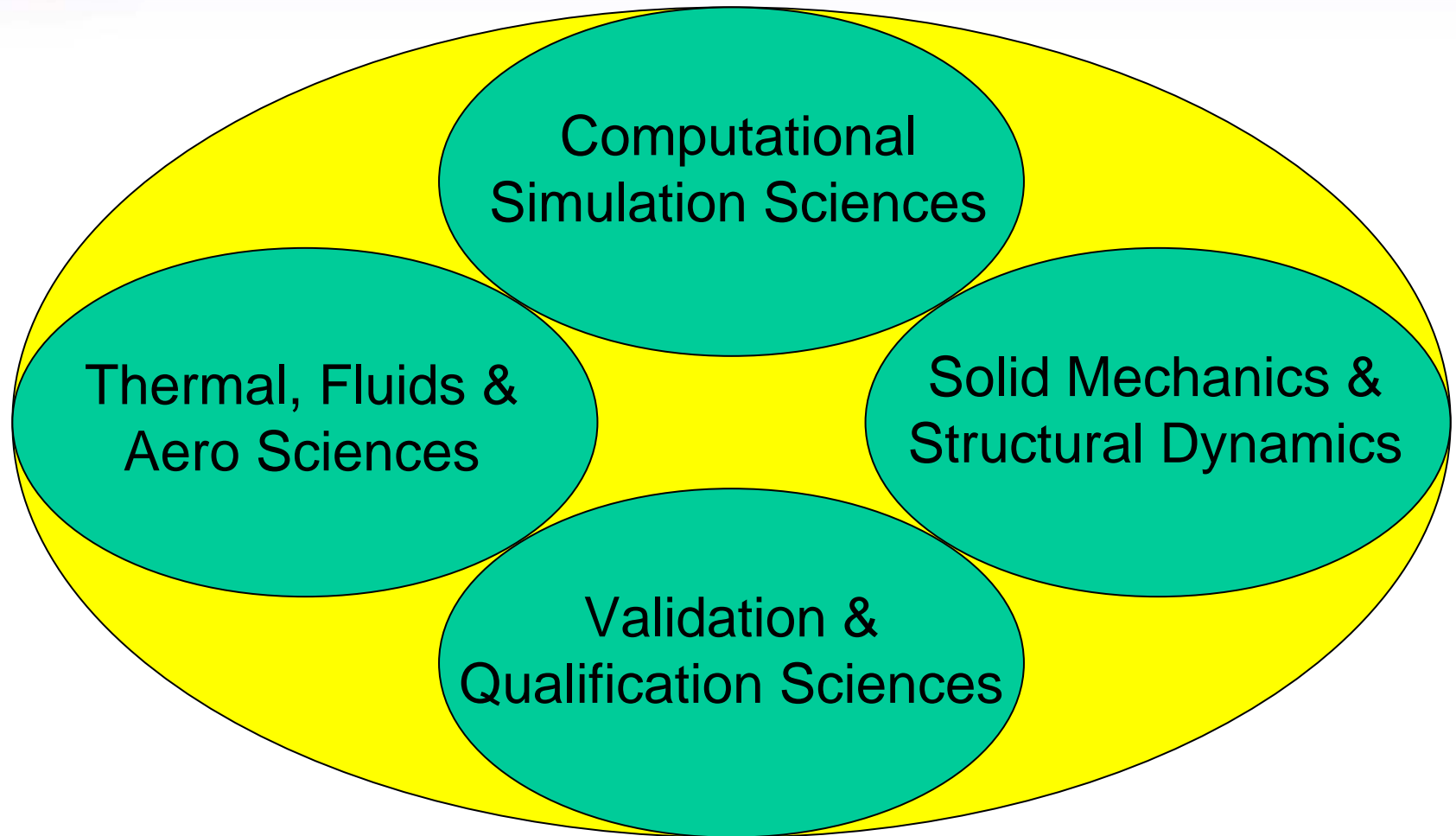
Provide Validated, Science-Based, Engineering Solutions Across The Product Life Cycle to Meet the Mission Needs of Sandia National Laboratories.

Strategic Intent:

Research to applications... the optimal Engineering Sciences solutions and capabilities, on time, every time.

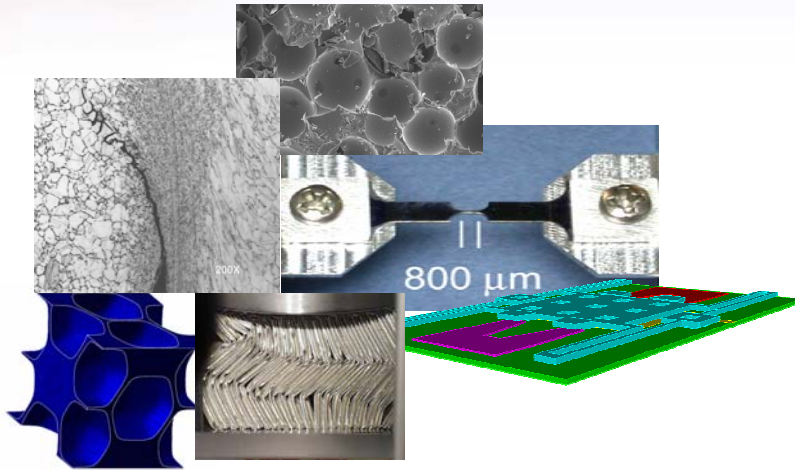


The Engineering Sciences Center in NM has as it's focus “engineering mechanics”



**Organization of 300+ staff and management:
structured to succeed through collaboration**

Engineering Sciences provides Sandia's stewardship of the engineering mechanics disciplines

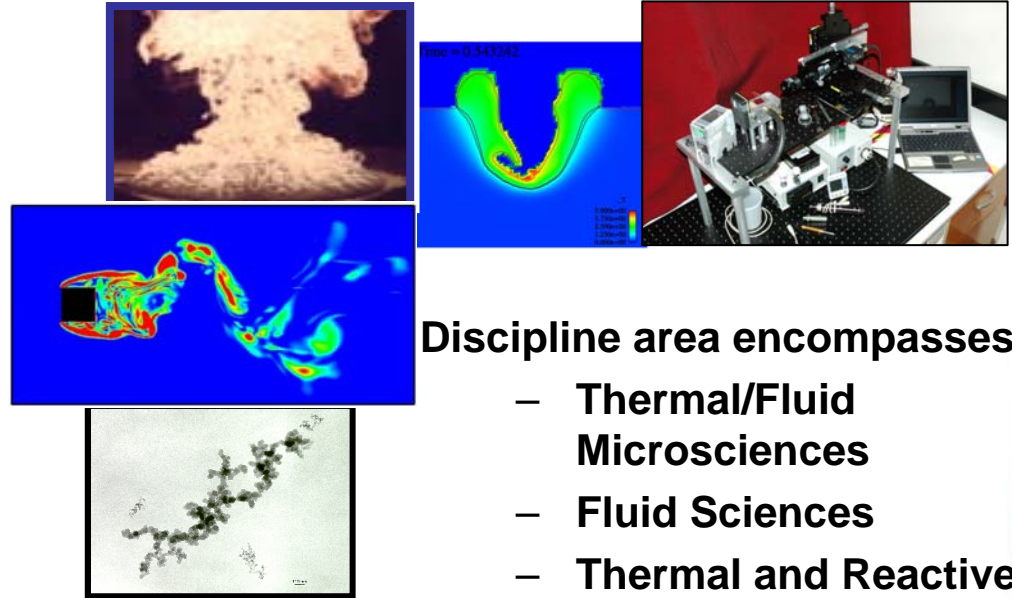


Solid/Material Mechanics & Structural Dynamics

Discipline area encompasses:

- Solid Mechanics
- Structural Dynamics
- Material Mechanics

Thermal, Fluids & Aero-sciences



Discipline area encompasses:

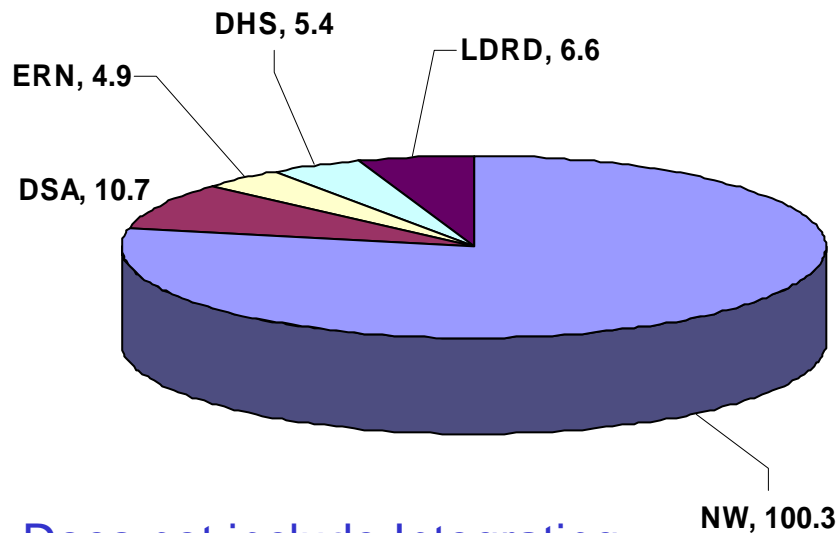
- Thermal/Fluid Microsciences
- Fluid Sciences
- Thermal and Reactive Processes
- Aero-sciences

Engineering Sciences Stewardship

- Assure a sound science-base to meet Sandia's mission goals of today
- Develop and nurture future science and technology that Sandia will depend upon to achieve its mission goals of tomorrow.
- Provide significant contributions to the leadership of engineering.

Engineering Sciences: People and Operating Budget

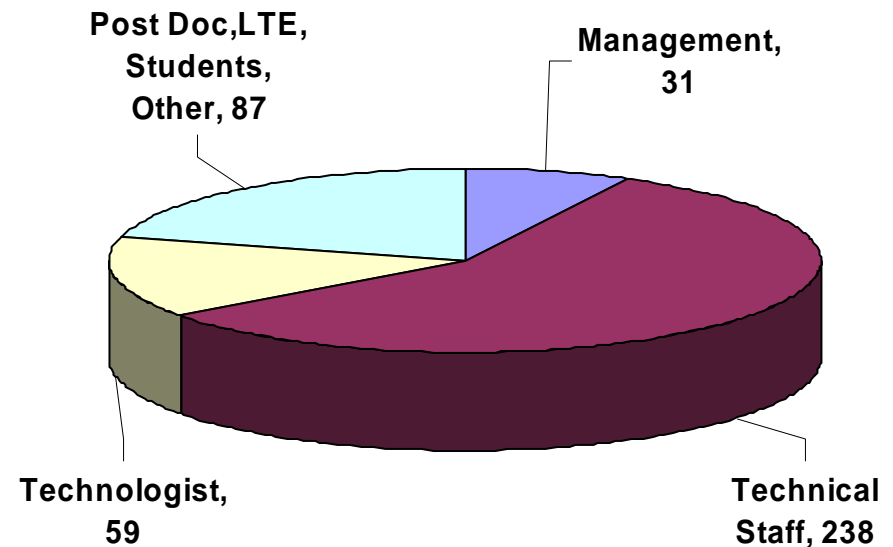
FY2006 Costs - \$127.9M



Does not include Integrating
Enabling Services Costs of ~\$9M+

NW – Nuclear Weapons
DSA – Defense Systems and Assessments
ERN – Energy Resources and Nonproliferation
DHS – Department of Homeland Security
LDRD – Laboratory Directed Research and Development

FY2006 Population - 415

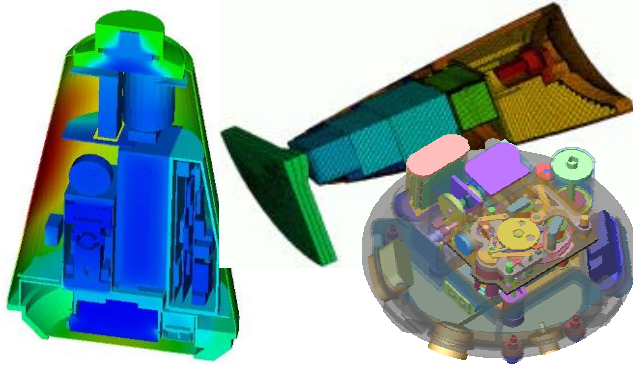


Technical Staff and Management

- 67% have Ph.D's and 27% have Master's Degrees
- 90% have advanced degrees in engineering
- 48% have degrees in Mechanical Engineering or Engineering Mechanics

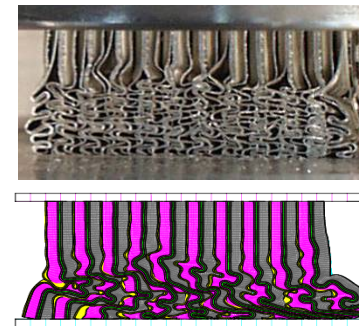
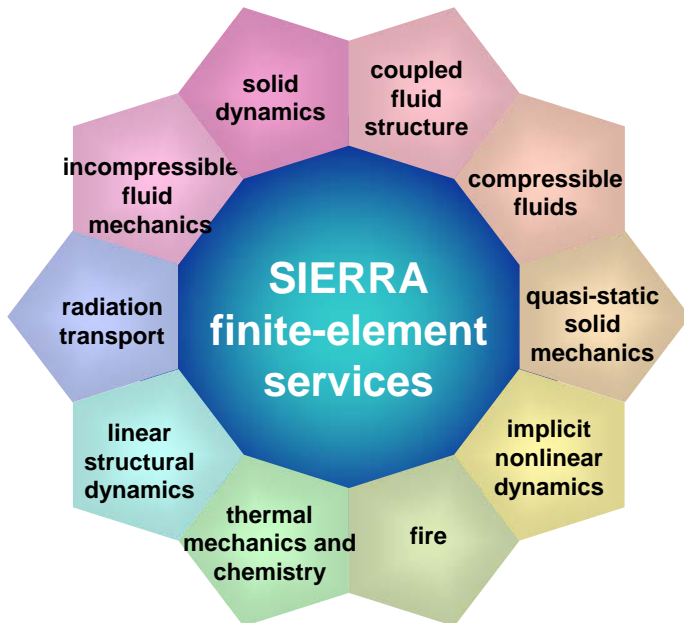
Engineering Sciences capabilities span research, development, and application

Engineering Modeling & Simulation

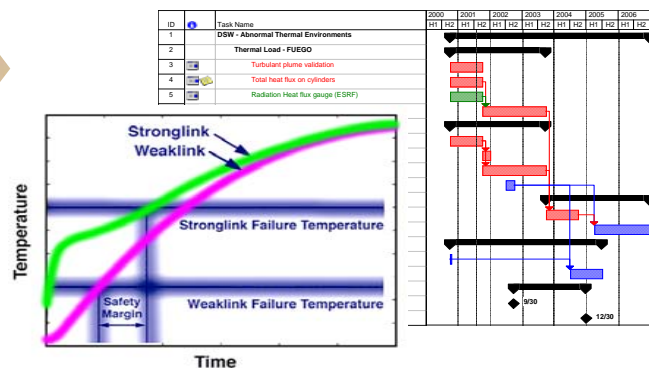


Large-Scale Test /Qualification

Code Development



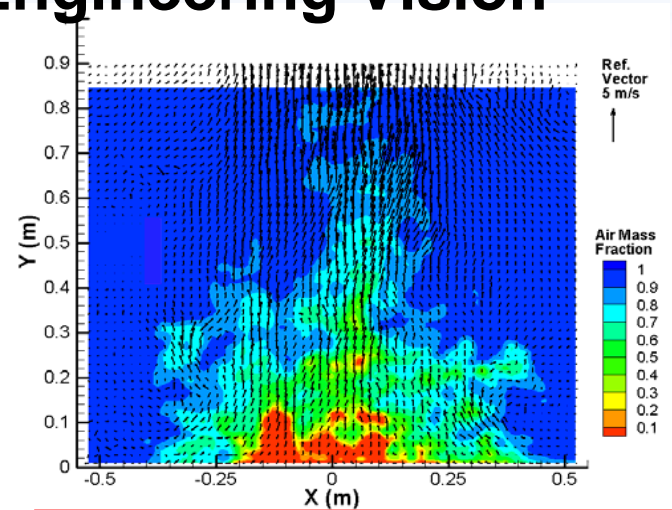
Phenomenology & Model Development



Uncertainty Quantification, Verification & Validation

Experimental Science is Critical to Meeting Our Simulation-Enabled Engineering Vision

- **Discovery**
 - **Identify (Observe)** and understand key phenomena
 - **Develop** advanced diagnostics that enable unprecedented spatial/temporal resolution
- **Validation**
 - **Build confidence** that theoretical & computational models represent reality
- **Integrated Tests**
 - **Build confidence** that integrated “system” level behavior is understood.
 - **Ensure** that all phenomena impacting behavior are adequately captured.
- **Enhance Understanding and Confidence**
- **Synergy with Modeling and Simulation**

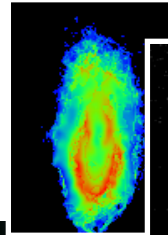


State-of-the-Art facilities and diagnostics for fire environment characterization

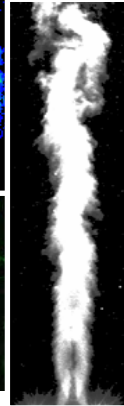
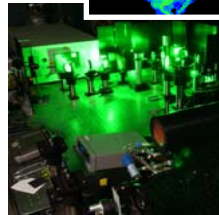
Engineering Sciences experimental facilities and capabilities are extensive



Trisonic & hypersonic flow characterization



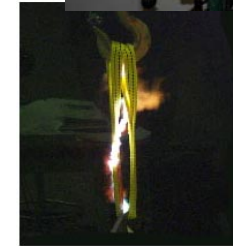
Noninvasive laser-based thermal/flow diagnostics



Sled Track, Blast Tube and Aerial Cable facilities



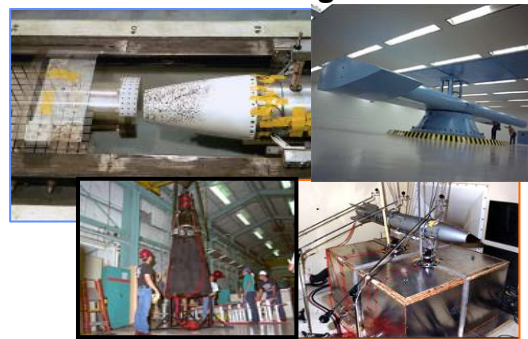
Electrical & EM Facilities



Thermal Test Complex – Radiant heat & fire testing



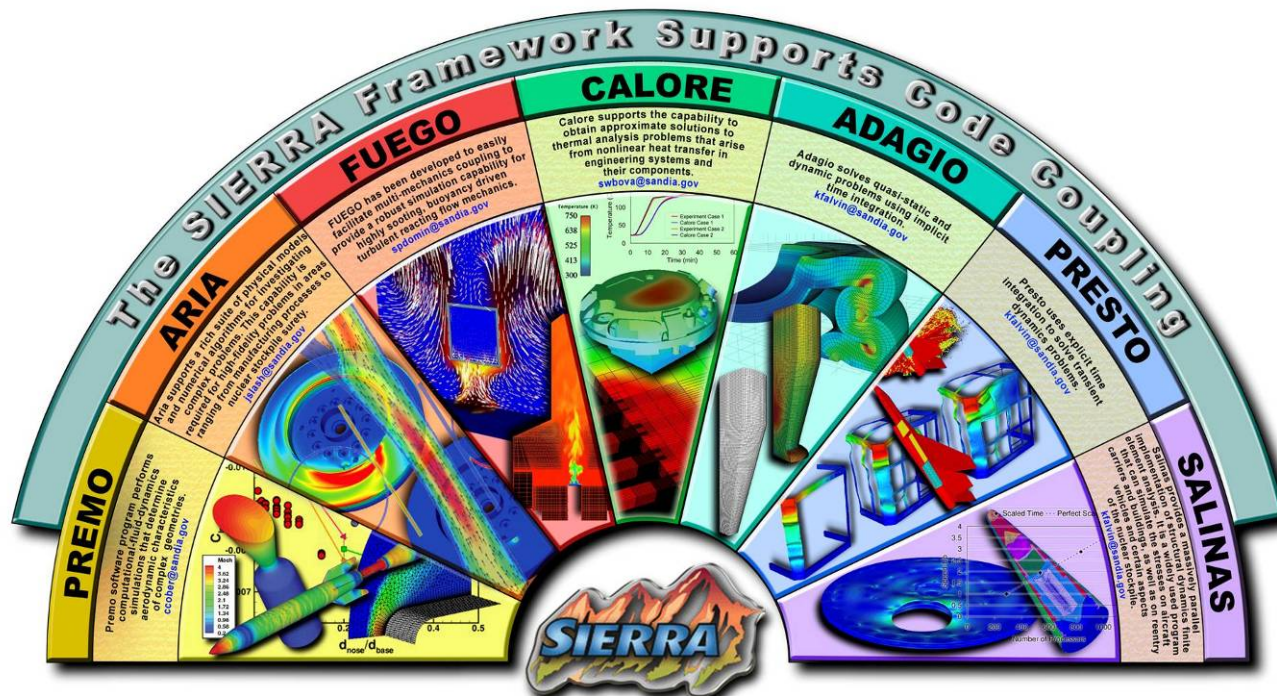
Modal, vibration, and mechanical shock & centrifuge facilities



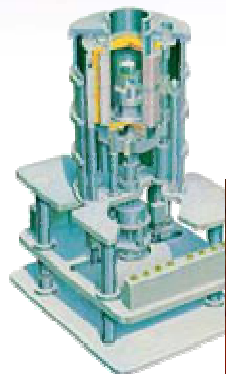
ES Laboratories

We steward significant lab-scale and large-scale testing capabilities where we perform research, development and applications work

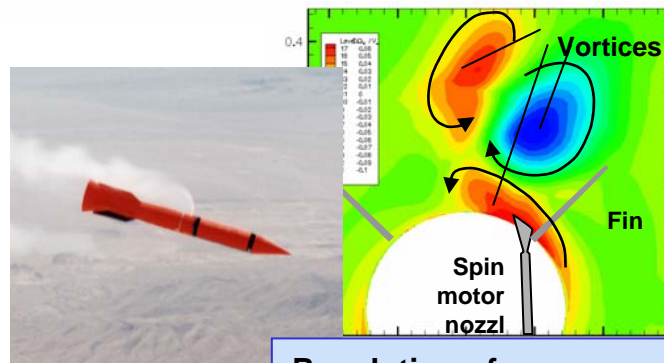
Engineering Sciences Computational Simulation



Computational simulation is the best way to address Sandia's diverse nuclear weapons challenges



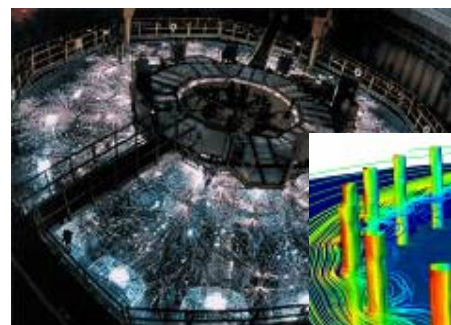
Modeling and simulation enhances and replaces test-based qualification



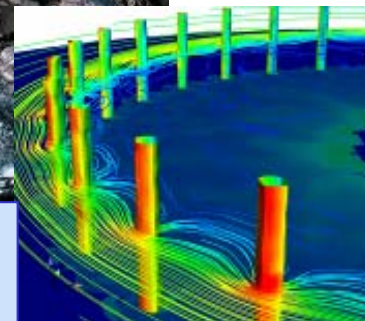
Resolution of weapon
Issues uncovered in
qualification and
surveillance



Modeling and simulation
allows probing broad
environments; too many
scenarios to test

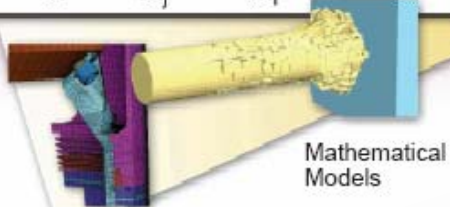


Breakthroughs in science
enabled by modeling and
simulation



The Advanced Simulation & Computing (ASC) Program has championed computational efforts

$$\frac{\partial \alpha^f \rho^f}{\partial t} + u_i^f \frac{\partial \alpha^f \rho^f}{\partial x_i} + \alpha^f \rho^f \frac{\partial u_i^f}{\partial x_i} = 0$$
$$\alpha^f \rho^f \frac{\partial u_i^f}{\partial t} + u_j^f \frac{\partial u_i^f}{\partial x_j} = -\alpha^f \partial \rho + K \Delta u_i + \frac{\partial \alpha^f \sigma_{ij}^f}{\partial x_j}$$



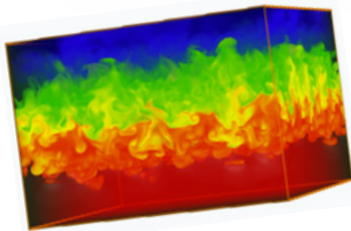
Design, Qualification,
Assessment, and Certification
of Nuclear Weapons



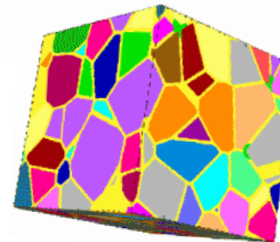
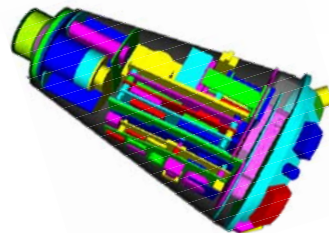
Limited Non-Nuclear
Testing



Massively Parallel
Computing



Red Storm Capability
High Performance Computer



ASC Mission: Provide the science-based simulation capability to assess and certify the safety, performance and reliability of nuclear weapons and their components without nuclear testing



ASC Strategic Alliances



Sandia has a Strong Computing Infrastructure – Critical in Full Utilization of Mod-Sim

Thunderbird

- More than 4480 nodes (8960 processors).
- Capacity machine for mid-sized tasks across hundreds of nodes.
- Nominally 60 teraflops

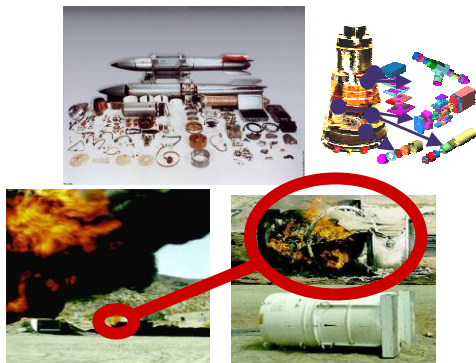


Red Storm

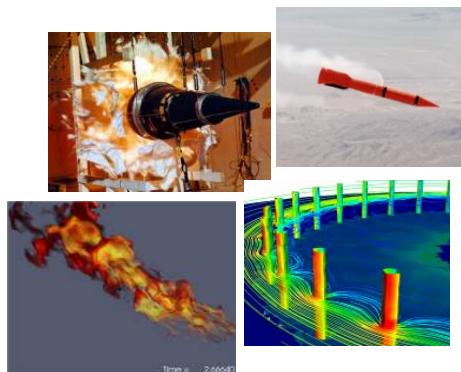
- Highly customized and tightly coupled system suited to perform large tasks across thousands of nodes.
- In excess of 120 teraflops; proposing expansion to ~500 teraflops

**Our Infrastructure supports both Capability
and Capacity Computing Needs**

ASC's investment in engineering codes enables simulation of a broad and diverse set of weapons applications



Complex Systems, Components, and Physics



Diverse Applications

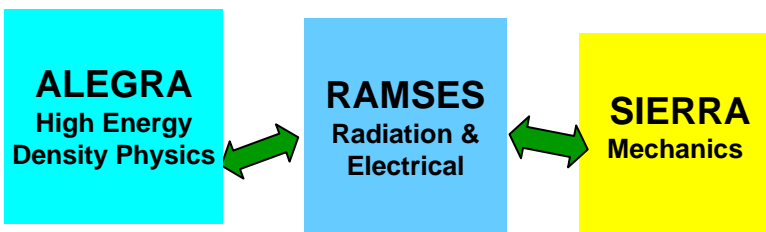
Code Suites in Three Different and Distinct Physics Areas

Distinct physics modules in each code suite

Many generic features for each code module that allow diverse single physics applications

Coupling between modules within a code suite

Coupling across modules



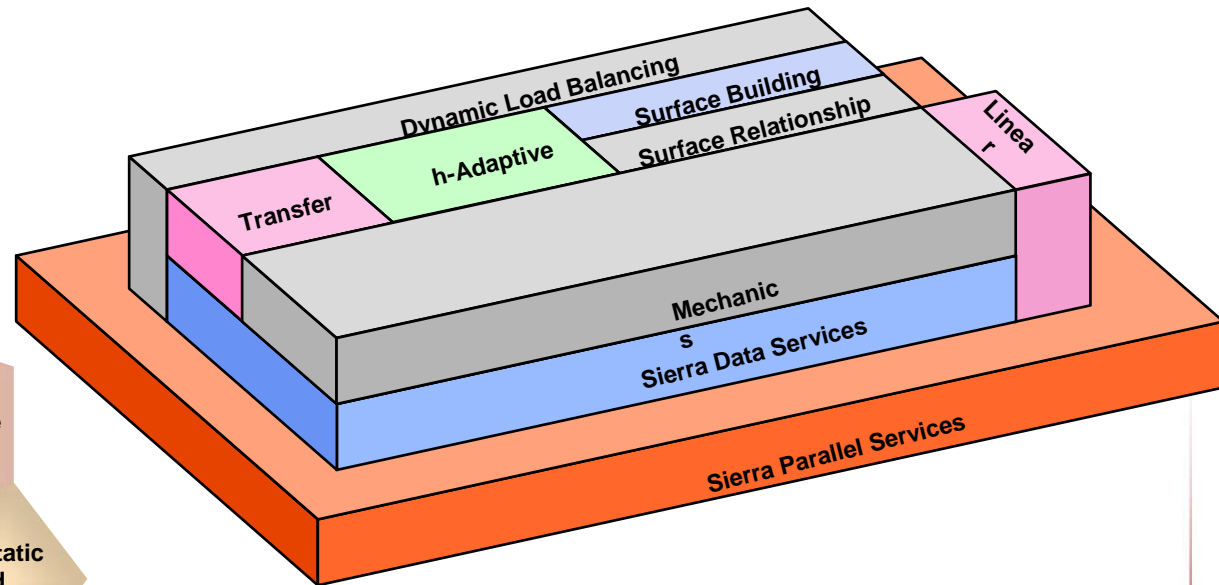
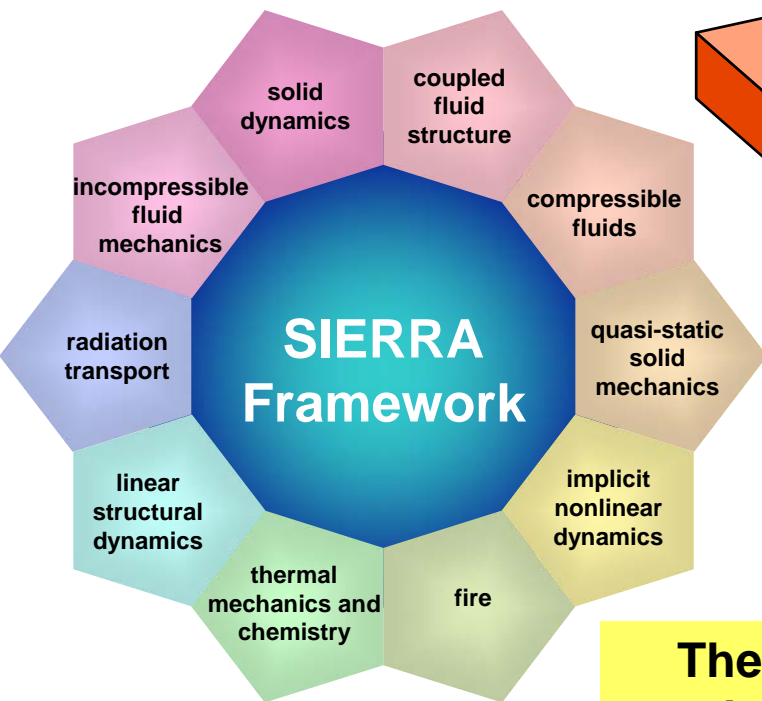
Sandia Code Suites



SIERRA Mechanics

We have developed unprecedented coupled mechanics simulation capabilities using the SIERRA framework

Engineering Mechanics
Loosely or tightly coupled
physics



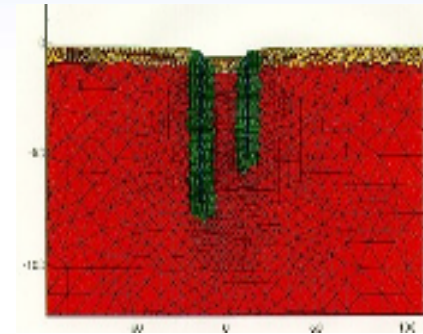
SIERRA Framework Building Blocks are intended to separate “Mechanics” and “Computer Science”

These engineering mechanics tools are being deployed across the Sandia program areas

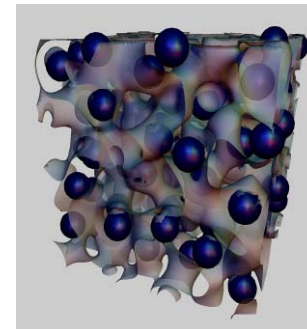
But... We are not finished!

We are developing a comprehensive strategy for the next decade to achieve predictive computational simulation

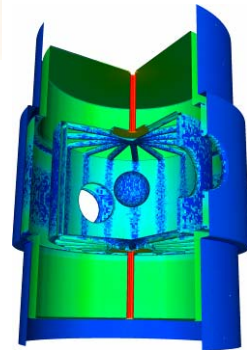
- New codes/mechanics modules meeting mission needs
- Improved physics insertion
- Enhanced algorithmic and framework development
- Increased code usability, reliability, robustness and performance
- Enhancements to computing environment to reduce time to analysis
- New computational capabilities for Uncertainty Quantification (UQ) & Quantification of Margins (QMU)



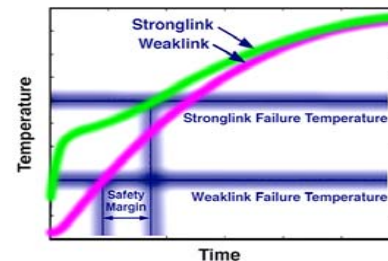
Multi-scale Algorithms



Computational Materials



Enhanced Physics

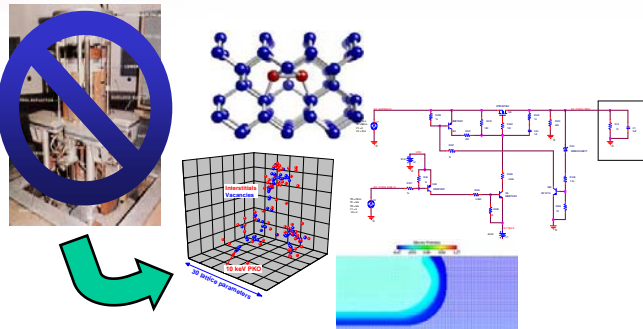


UQ/QMU Tool Development

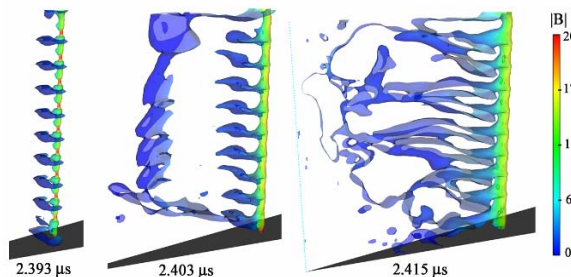


New Codes

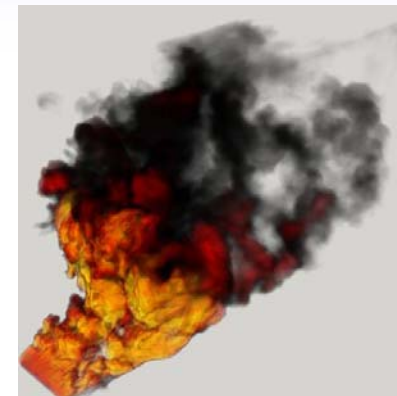
Computational simulation is impacting the Nuclear Weapons program



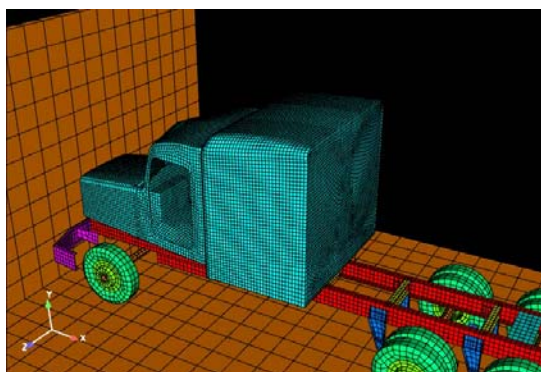
Qualification Alternative to SPR (QASPR)



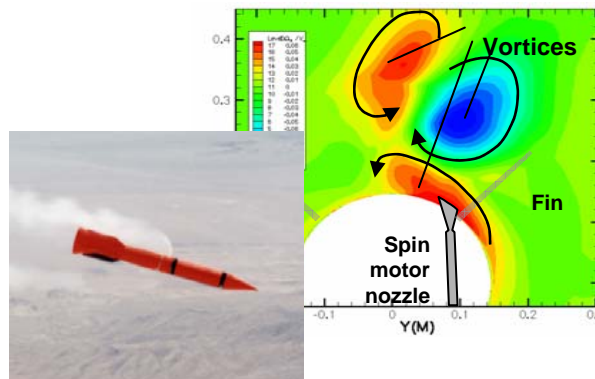
Science Resolution: High Energy Density Physics Phenomena for Weapons physics



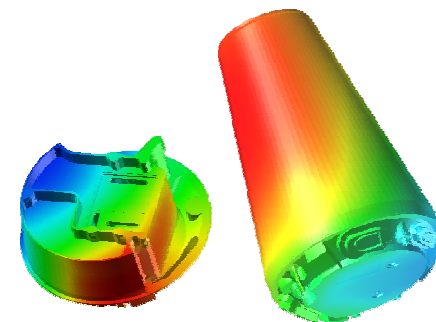
System Qualification: Abnormal Thermal Environment Characterization



Vulnerability Assessment: SGT Transportation Accidents

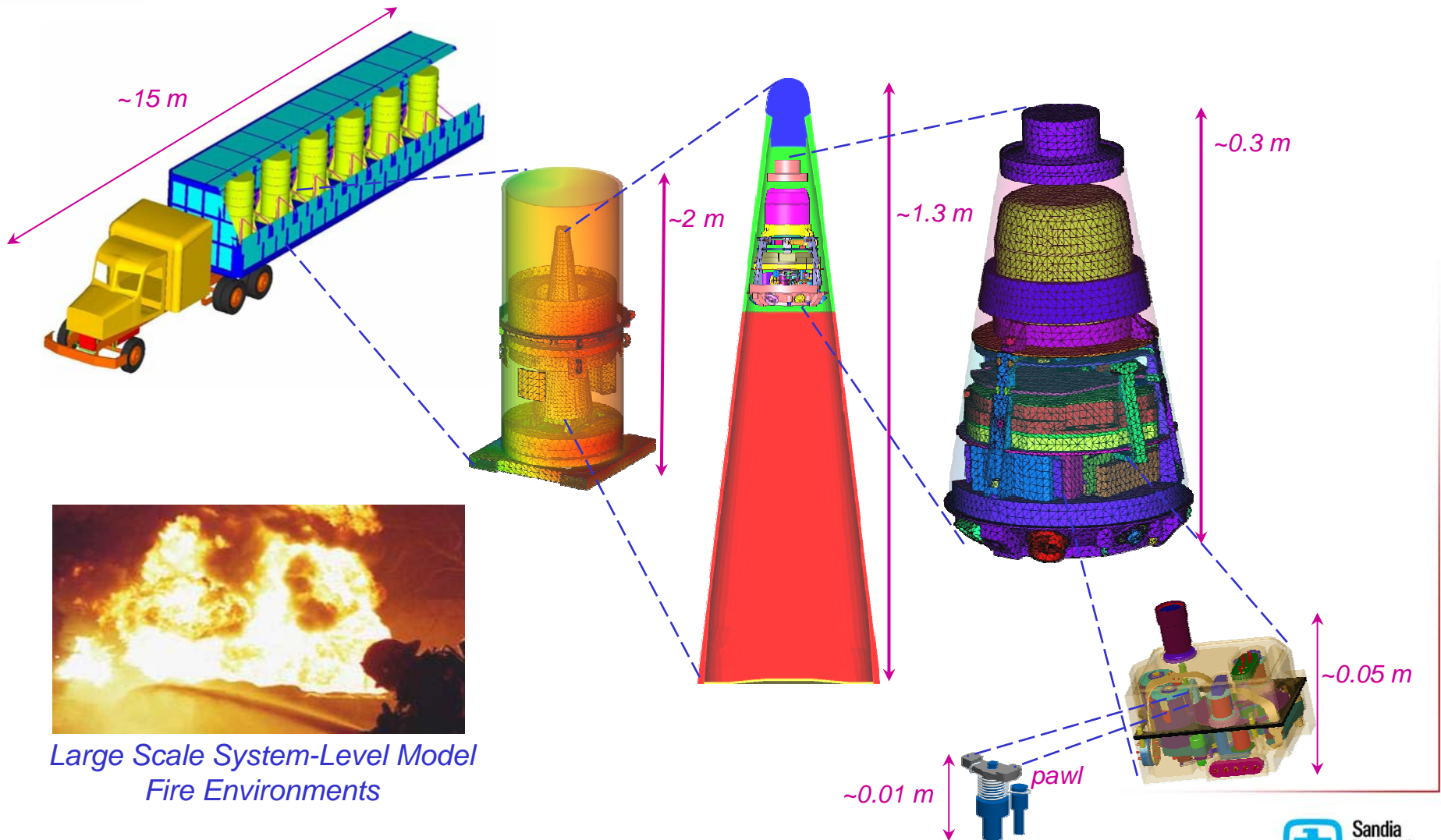


Resolution of weapon Issues uncovered in surveillance



System Design Improvements: W76-1 System in Abnormal Thermal Environments

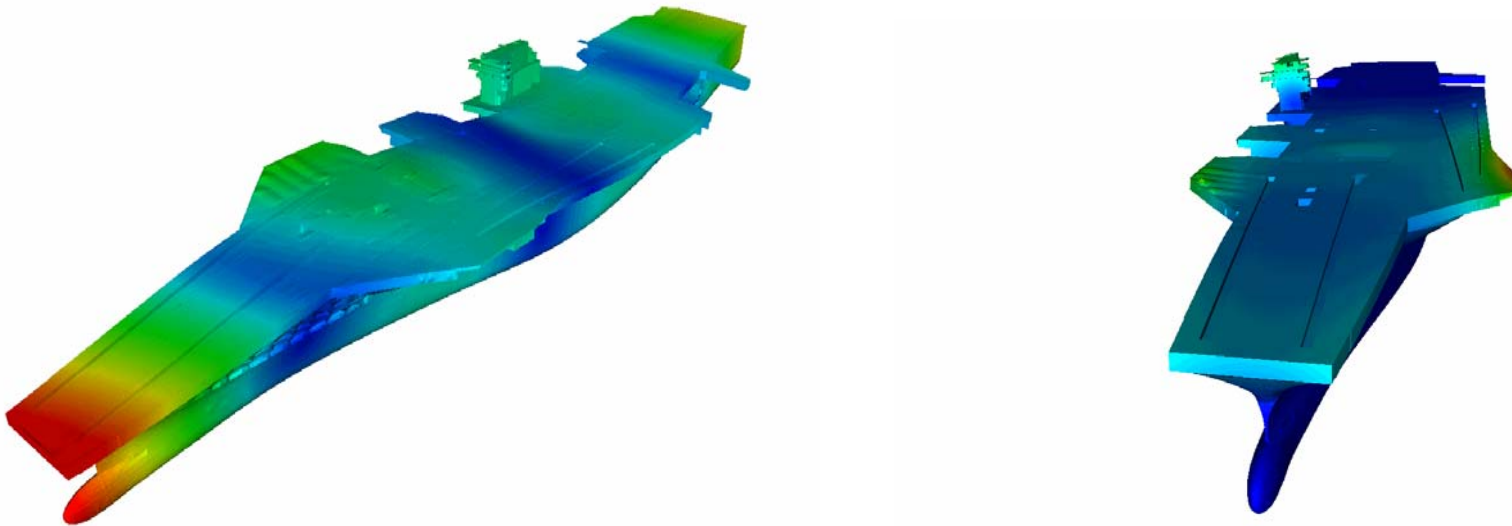
From Transporter Walls to Stronglink Pawls Over 3 Orders of Magnitude in Part Size



Large Scale System-Level Model
Fire Environments

Modal Analysis of an Aircraft Carrier

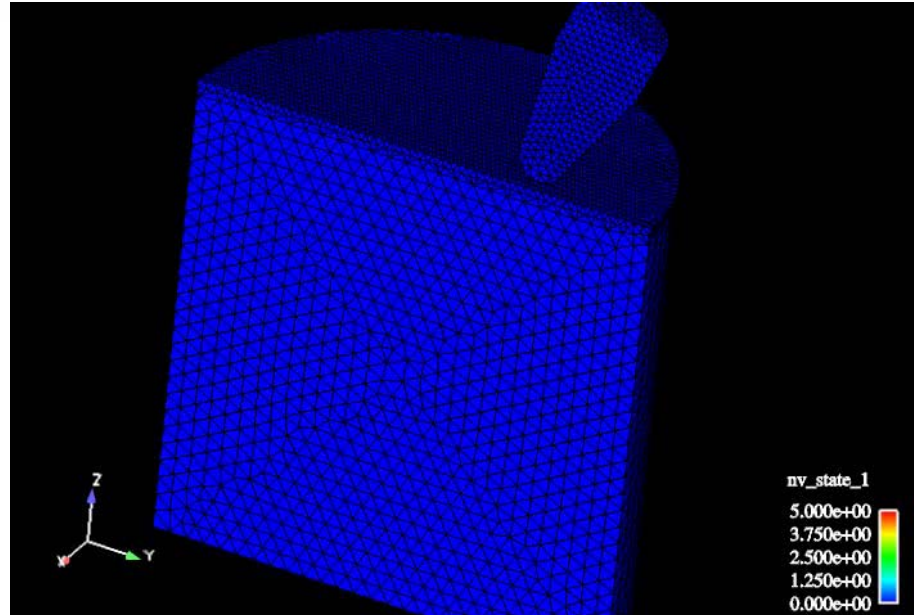
- Extremely complex model (1000's of material regions, offset shells and beams)
- 2.0M DOFs, solved on 64 processors



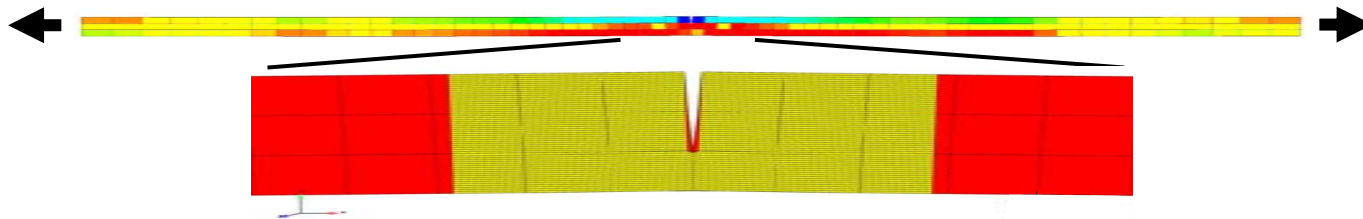
Von Mises Stresss Overlaid on Mode Shapes

Explicit Dynamics - Presto

- Fully Three-Dimensional
- Massively Parallel
 - Thousands of processors
- Finite Elements and Particles
 - SPH particles
 - Other particle methods planned (e.g., GPA, HPM, RKPM)
- Material models: 40+, including energy-dependent materials
- Contact: Massively parallel, momentum balance, accurate friction response
- Boundary conditions:
 - Kinematic and Force
 - Specialized: cavity expansion, silent BC
- Failure modeling:
 - Material failure/element death
 - Cohesive zones (elements, contact surfaces)
 - Phenomenological models (spot weld, line weld)

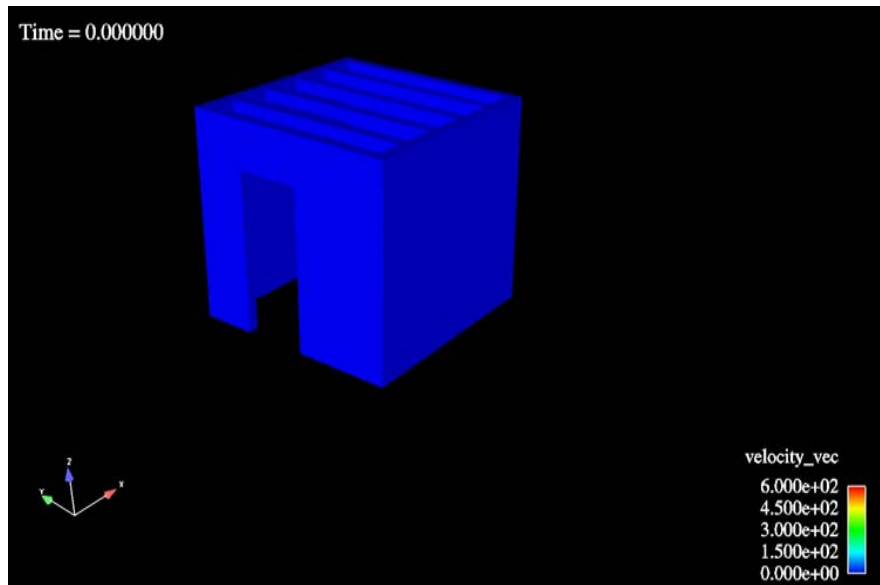


Penetration simulation using node-based tet element with re-meshing
(Similar accuracy as hex elements)



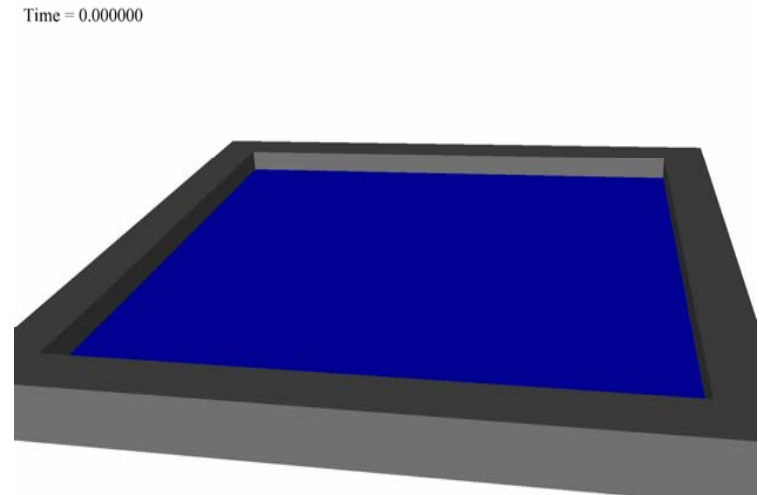
Multi-length scale and explicit control modes capabilities

One-Way Coupled CTH/Presto



CTH Loading: 5 kg TNT at the center of a room, for 2.5 ms

Blast Response



Sierra Thermal/Fluids Capabilities

- **Calore – Heat Transfer, Enclosure Radiation, & Chemistry**

- Dynamic Enclosures
- Element birth/death
- Contact

- **Fuego – Low Speed, Variable Density, Chemically Reacting flows (Fire)**

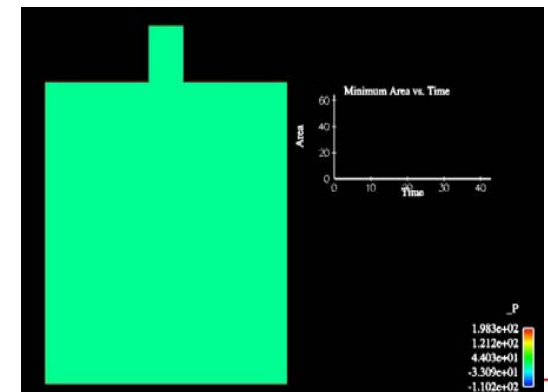
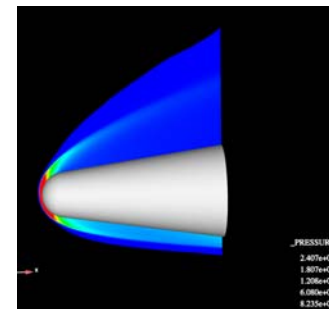
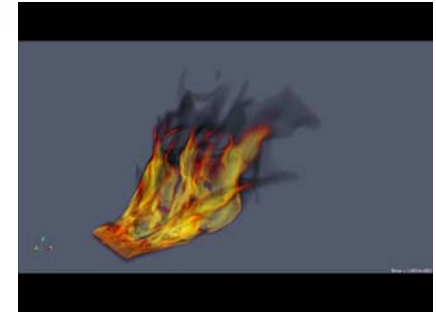
- Eddy dissipation and mixture fraction reaction models
- RANS and LES based turbulence models
- Unstructured Mesh
- Pressurization models

- **Premo – Compressible Fluid Mechanics**

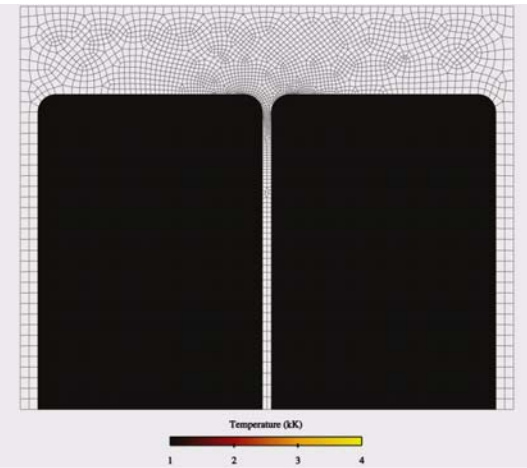
- Subsonic through hypersonic
- Laminar and turbulent
- Unstructured mesh

- **Aria – Non-Newtonian, Chemically Reacting, & Free Surface Flows**

- Complex material response
- Level sets for surface tracking
- Flexible coupling schemes



Coupled Physics Examples



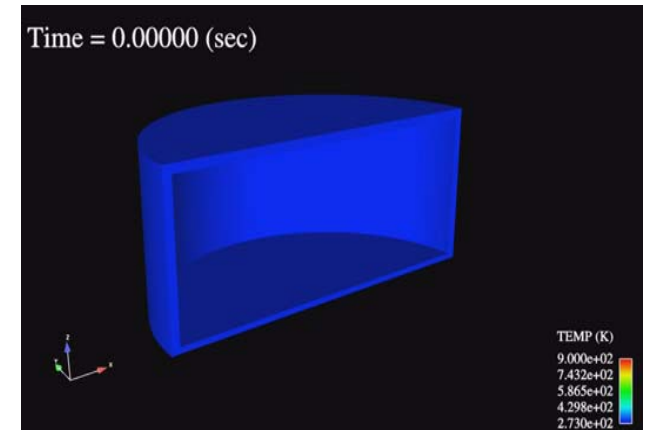
Residual stress prediction for a laser welding process.

Coupled heat transfer, fluid mechanics, quasi-static solid mechanics.



Temperature and internal pressure prediction for an object in a hydrocarbon fire.

Coupled chemically reacting flow, heat transfer, quasi-static solid mechanics.

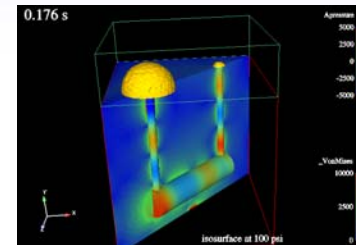


Internal pressure prediction for a decomposing foam in a thermal environment.

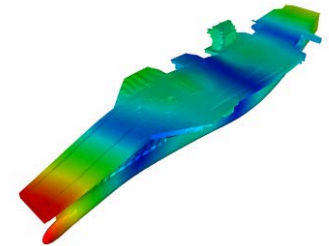
Coupled heat transfer, foam chemistry, quasi-static solid mechanics.

Sandia engineering codes enable predictive simulation for broad national impact

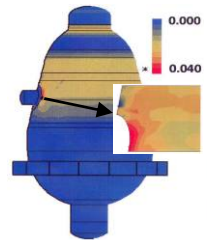
- Strategic Partnership with the Navy to transform
 - Live Fire Test & Evaluation
 - Product Acquisition
- Extend other DOE interactions
- Leadership in nuclear energy initiatives in safety/security
- Help realize success in American Competitiveness Initiative (Goodyear, Procter & Gamble, Lockheed Martin, etc)



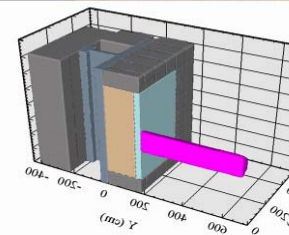
Acoustic Signatures



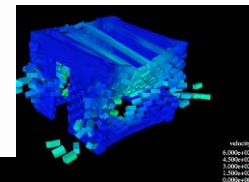
Live Fire Test & Evaluation



Reactor Safety



Vulnerability Analysis



DOD CHSSI & High Performance Computing Initiative

Sandia predictive simulation capabilities are directly adaptable to Other Federal Agency and industrial applications with appropriately funded development

Our customers are many & varied
with NNSA being our largest funding source



CORNING



P&G

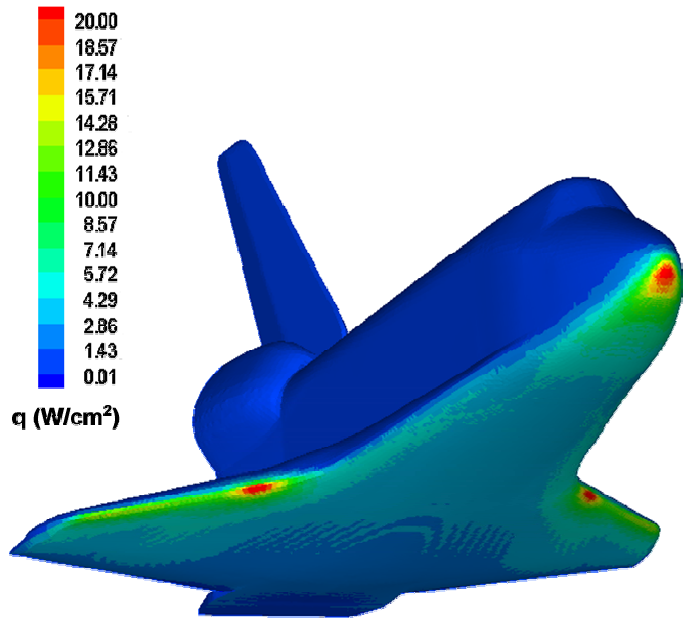
LOCKHEED MARTIN



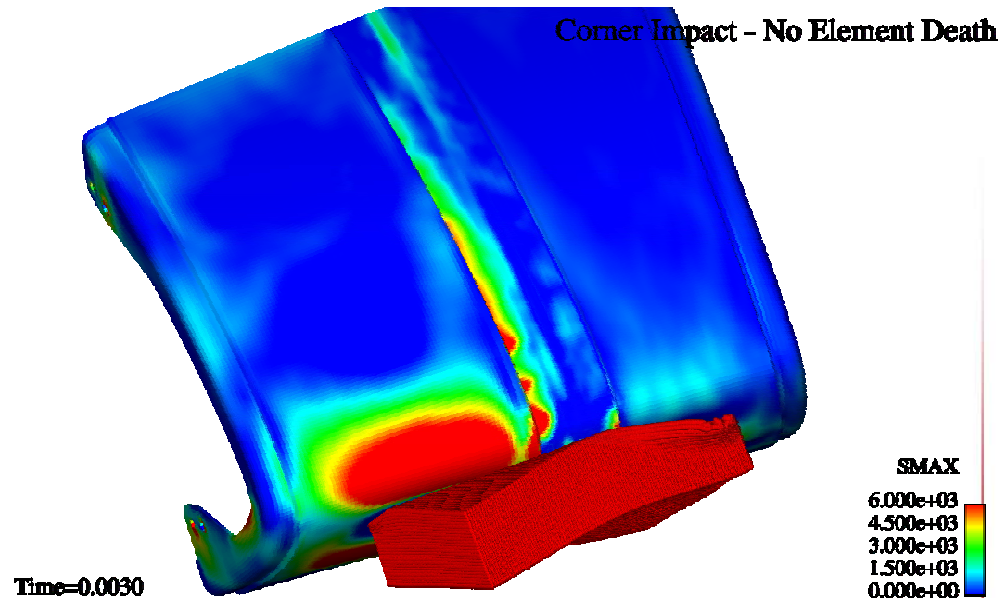
3M

~75% of Engineering Sciences Funding is
through NNSA

Sandia simulations drive resolution NASA Columbia orbiter accident investigation



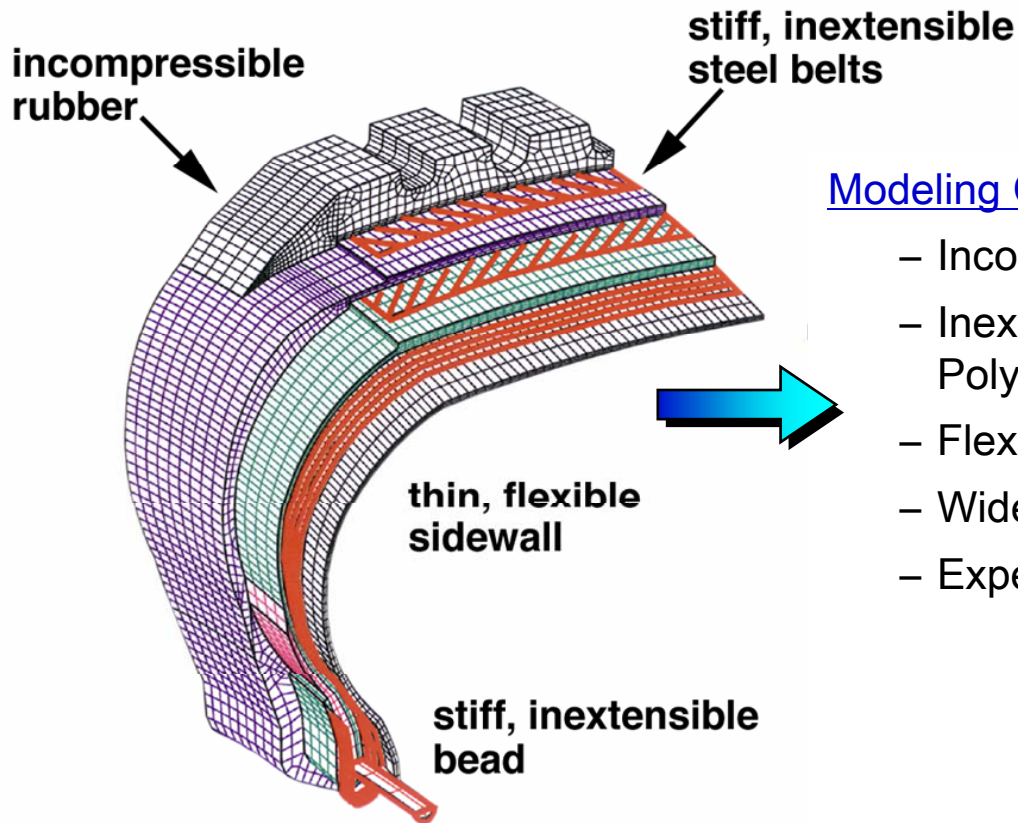
Heating during reentry



Foam impacting leading edge

“The Pneumatic Tire Represents One of the Most Formidable Challenges in Computational Mechanics Today”

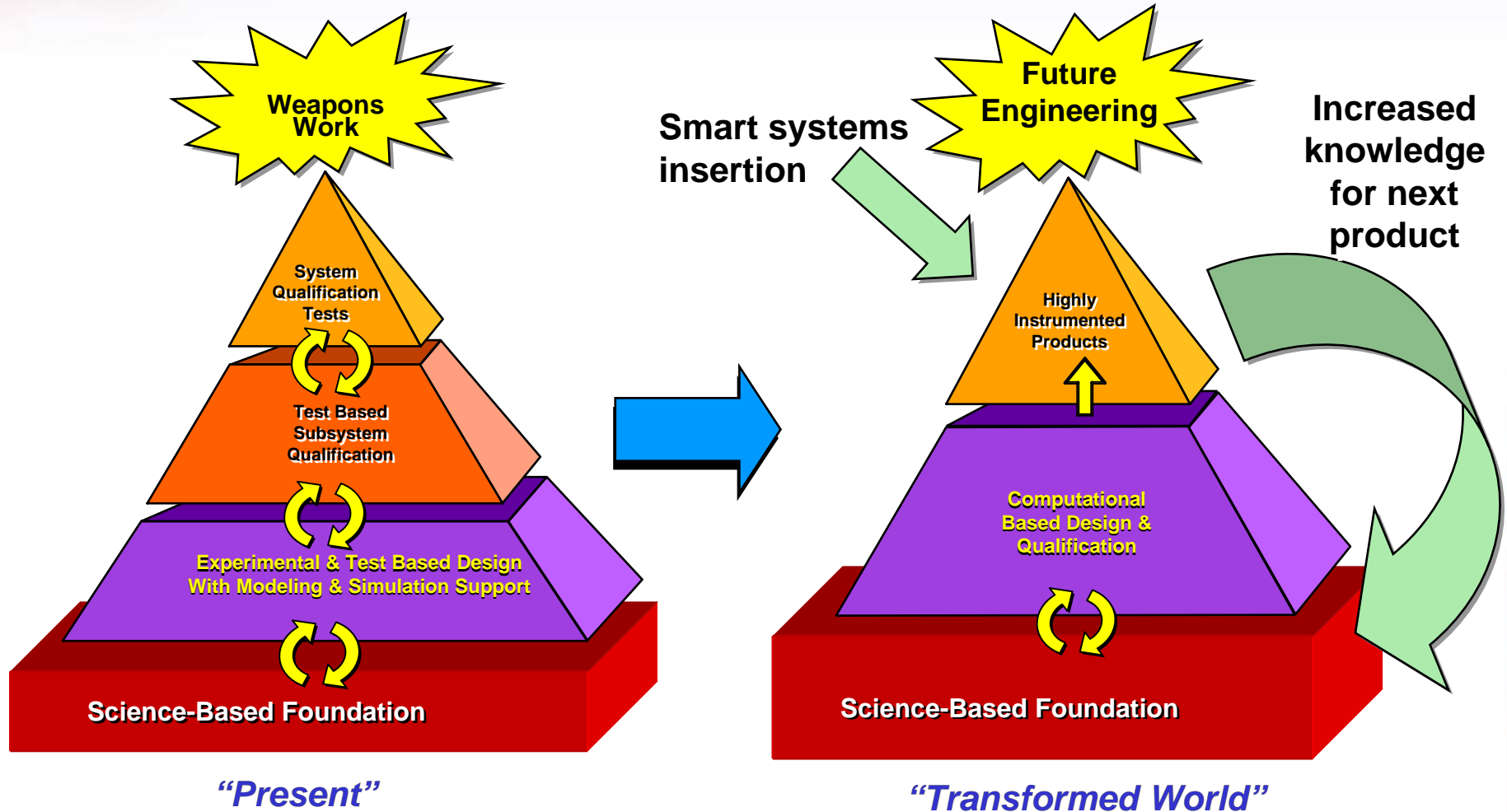
A. Noor, Journal of Computers and Structures



Modeling Challenges

- Incompressible Material (Rubber)
- Inextensible Fibers (Steel Belts & Polyester Ply)
- Flexible Structures (Sidewall)
- Wide Eigenvalue Spectrum
- Expensive Limited Accuracy Solutions

Computational simulation will enable changes in the way we do our business in the future



***Achieving the Science-based Engineering process:
Conceive, Understand, Build***