

# Computational Simulations at Sandia National Laboratories



PRESENTED BY

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Computational Solid Mechanics & Structural Dynamics



Sandia National Laboratories Overview

Engineering Sciences Center

Computational Simulation Group

Computational Solid Mechanics & Structural Dynamics

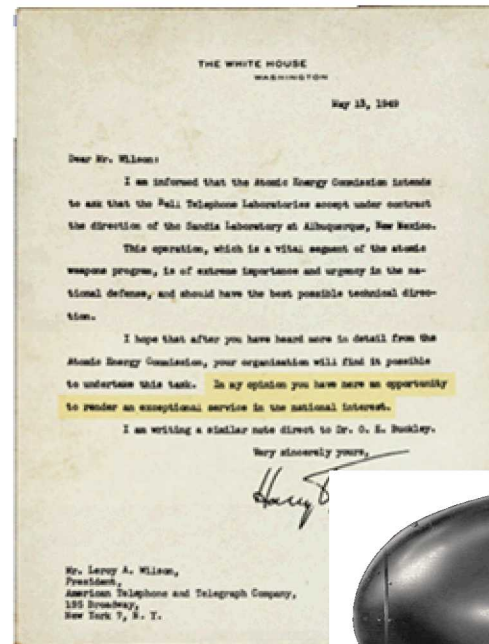
Research Topics:

- Inverse problems
- Blast-Induced Traumatic Brain Injuries
- Very large problems in structural dynamics

# SANDIA'S HISTORY IS TRACED TO THE MANHATTAN PROJECT

*...In my opinion you have here an opportunity to render an exceptional service in the national interest.*

- July 1945  
Los Alamos creates Z Division
- Nonnuclear component engineering
- November 1, 1949  
Sandia Laboratory established
- AT&T: 1949–1993
- Martin Marietta: 1993–1995
- Lockheed Martin: 1995–2017
- Honeywell: 2017–present





## SANDIA HAS FACILITIES ACROSS THE NATION

### Activity locations

- Kauai, Hawaii
- Waste Isolation Pilot Plant, Carlsbad, New Mexico
- Pantex Plant, Amarillo, Texas
- Tonopah, Nevada

### Main sites

- Albuquerque, New Mexico
- Livermore, California





Sandia develops  
advanced technologies  
to ensure global peace



# Sandia's Current Nuclear Weapons Activities



*An extensive suite of multi-disciplinary capabilities are required for Design, Qualification, Production, Surveillance, Experimentation / Computation*

Gas  
Trans  
Systems



Design Agency for

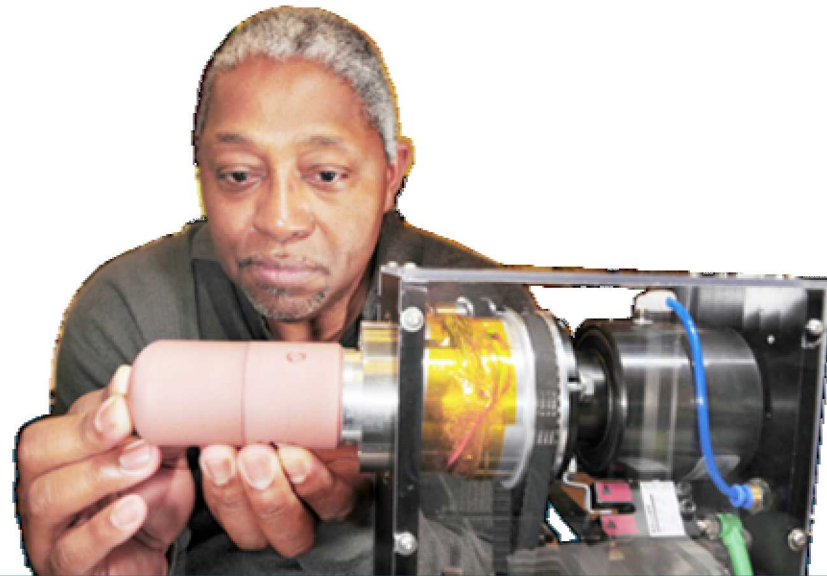


Arming, Fuzing, and Firing Systems

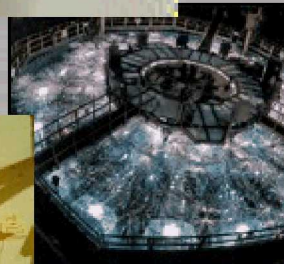
Safety Systems



MESA Microelectronics



Major Environmental Test Facilities and Diagnostics



Z Machine



Light Initiated High Explosive

Annular Core Research Reactor

# Energy



## Energy Research

ARPAe, BES Chem Sciences, ASCR, CINT, Geo Bio Science, BES Material Science

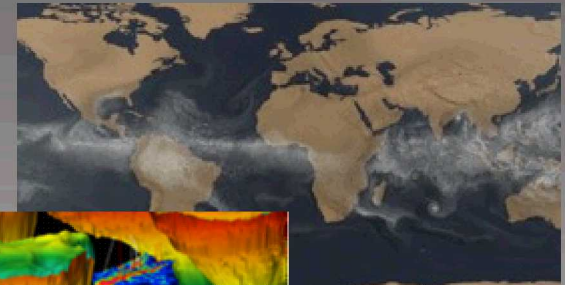
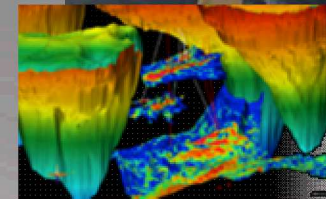
## Climate & Environment

Measurement & Modeling, Carbon Management, Water & Environment, and Biofuels

## Nuclear Energy & Fuel Cycle

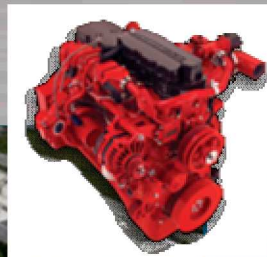
Commercial Nuclear Power & Fuel, Nuclear Energy Safety & Security, DOE Managed Nuclear Waste Disposal

## Renewable Systems & Energy Infrastructure



## Transportation Energy & Systems

Vehicle Technologies, Biomass, Fuel Cells & Hydrogen Technology

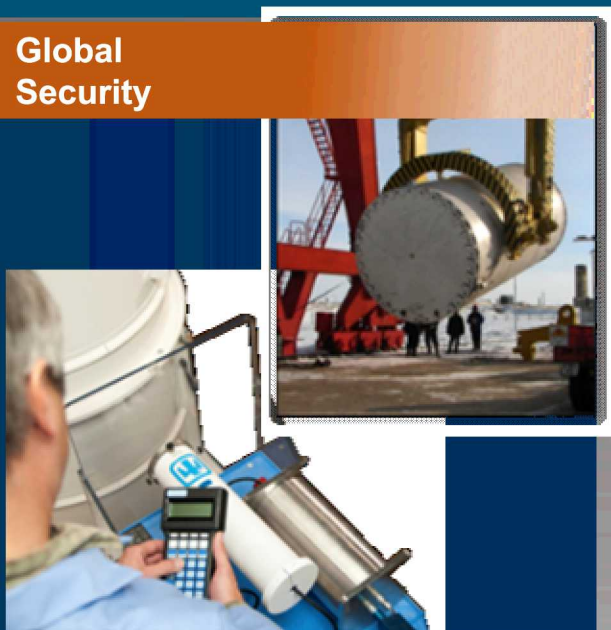




# Global and Homeland Security



## Global Security



## WMD Counterterrorism and Response



## Homeland Defense and Force Protection



## Homeland Security Programs

## Cyber and Infrastructure Security

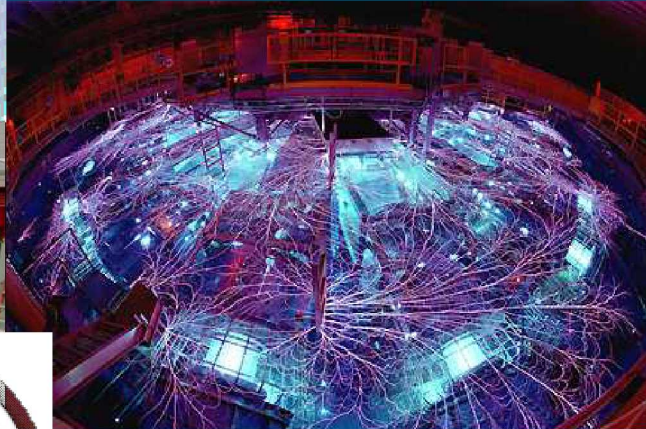




# Our Research Framework

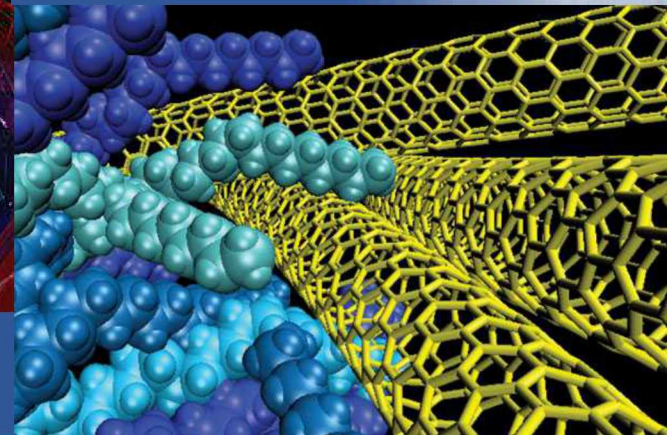
*Strong research foundations play a differentiating role in our mission delivery*

## Computing & Information Sciences

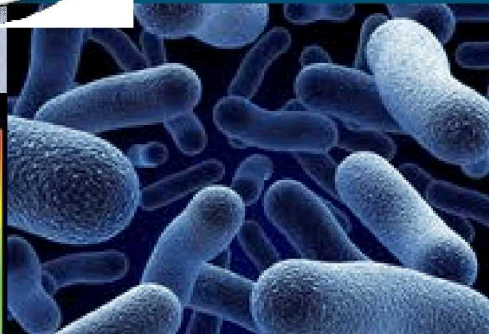
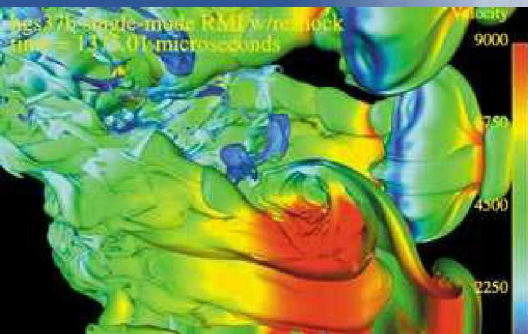


## Radiation Effects & High Energy Density Science

## Materials Sciences

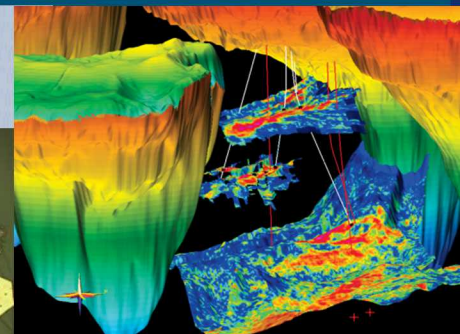


## Engineering Sciences



## Bioscience

## Nanodevices & Microsystems



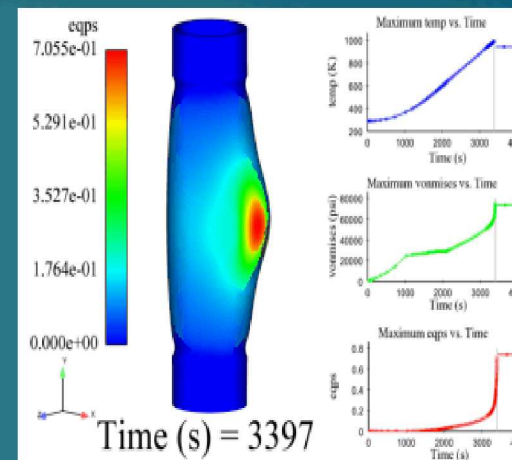
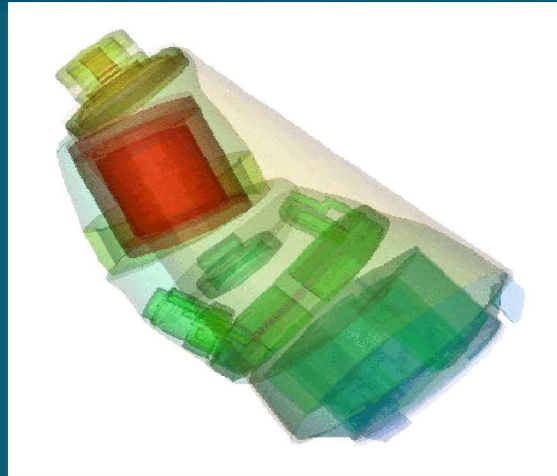
## Geoscience



# Engineering Sciences as The Capability Steward

*Integrated theory, computational simulation, and experimental discovery/validation across length and time scales is critical to develop the technical basis for complex engineered systems.*

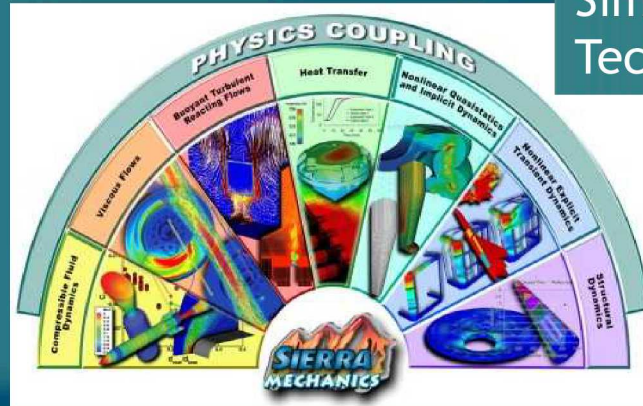
Engineering  
Analysis



Engineering  
Science Physical  
Phenomena

Computational  
Simulation  
Technology

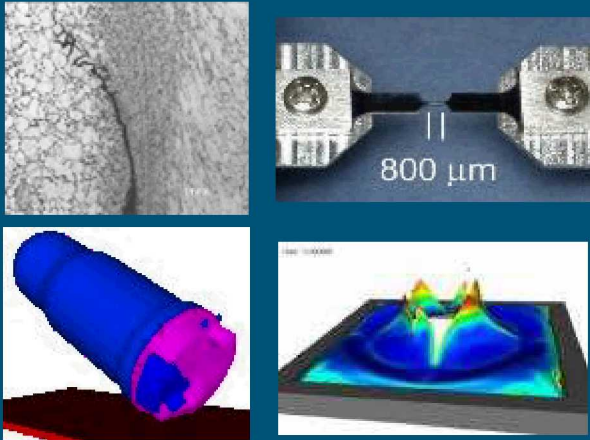
Environmental  
Simulation  
& Test



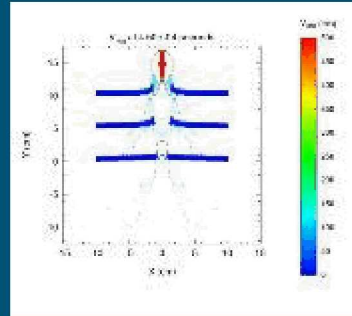


# Engineering Sciences Core Technical Areas

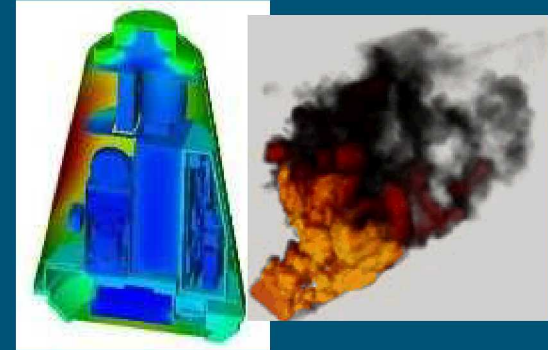
## Solid Mechanics



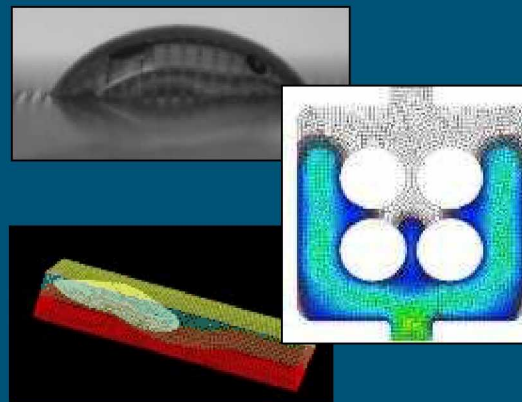
## Shock Physics and Energetics



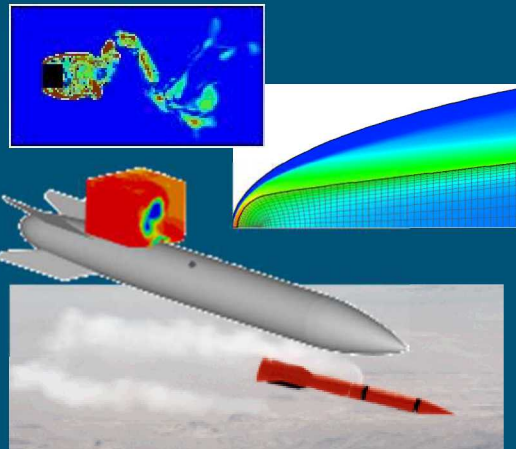
## Thermal & Fire Sciences



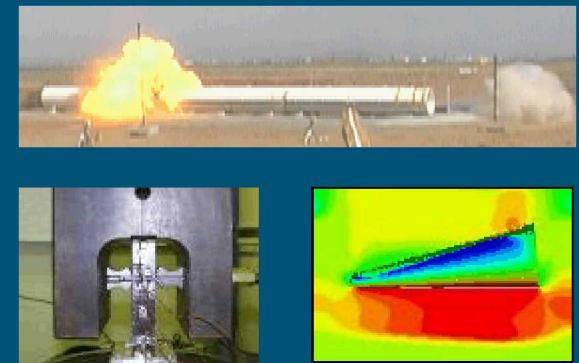
## Fluid Mechanics



## Aerosciences



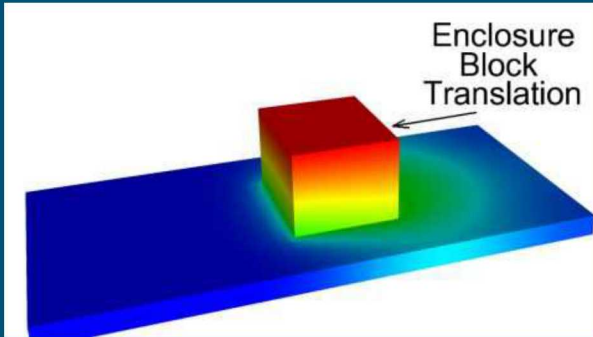
## Structural Dynamics



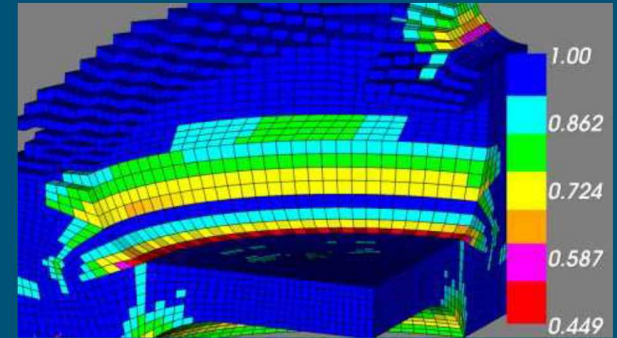
# Engineering Sciences Video







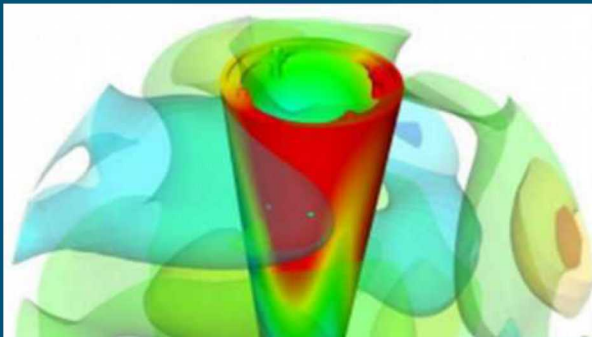
Computational Thermal And Fluid Mechanics



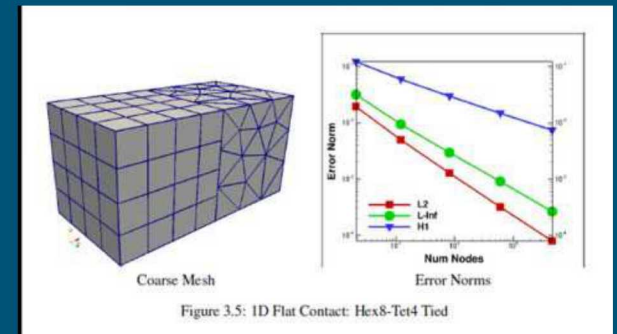
Simulation Modeling Sciences



Computational Simulation Infrastructure



Computational Solid Mechanics And Structural Dynamics



V&V, UQ, Credibility Processes

**Solid Mechanics** – Quasi-static, implicit & explicit transient dynamic**Shared capabilities**

- large deformations, large-strain nonlinear material behavior
- implicit-explicit solution switching, multi-sequence analyses
- continuum & structural finite elements, particle methods
- parallel scalable frictional contact
- geometric and temporal multi-scale methods
- coupled thermal-mechanical modeling, with failure

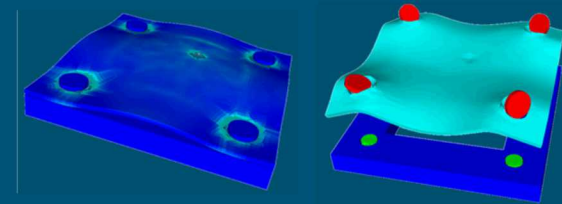
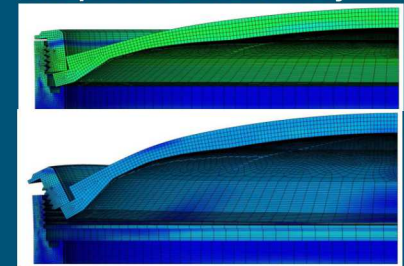
**Implicit Solid Mechanics**

- preloads, encapsulation & cure, incompressible material behavior

**Explicit Solid Mechanics**

- energy-dependent material models
- fracture & failure modeling (cohesive zones, XFEM, remeshing)
- empirical blast pressure loads (CONWEP)
- coupled to CTH shock-hydro (Zapotec), Alegra EM

Implicit→explicit switching

pressure & temperature loading  
snap-thru & disassembly

2D XFEM Fracture Simulation





## Structural Dynamics – Implicit Dynamics & Modal Response

Parallel Scalable Domain Decomposition Solver with many constraints

### Shared mechanics capabilities

- small deformations, small-strain linear material behavior
- solid & structural elements, constraint elements
- non-linear pre-load transfer from Sierra/SM

### Time domain, statics & transients

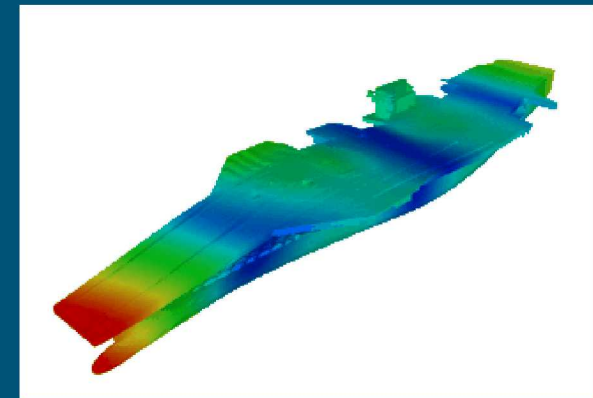
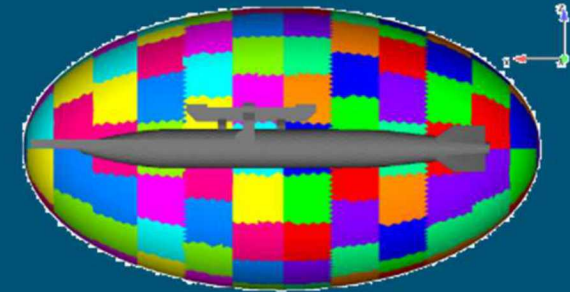
- joint models with dissipation
- material property inversion
- stochastic material (elastic) properties

### Frequency domain (Frequency Response Functions)

- Helmholtz solver for Direct FRF
- Modal FRF

### Acoustics – linear

- absorbing boundaries
- acoustic pressure source inversion
- monolithic coupling with structural response



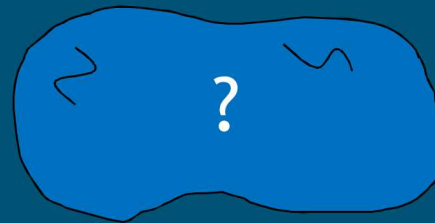
## Inverse Problems: Observing the Unobservable

Inverse problems arise when we have partial information and indirect observations of a system and need to infer (hidden) quantities of interest of the system.

Can we *non-destructively* interrogate a black-box system to “see what is inside”?

Typical quantities of interest:

- Material properties
- Loads
- Boundary conditions
- Residual stresses
- Size/shape/location of inclusions (e.g. composite materials)



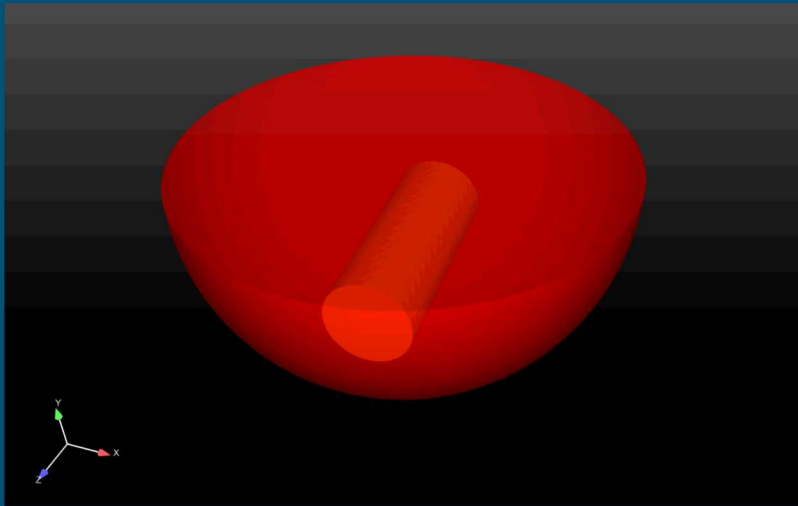
Applications include:

- Imaging: Medical ultrasound, seismic exploration (oil, gas)
- Calibration of material models and properties
- Force reconstruction
- Optimal experimental design, sensor locations
- Shape reconstruction

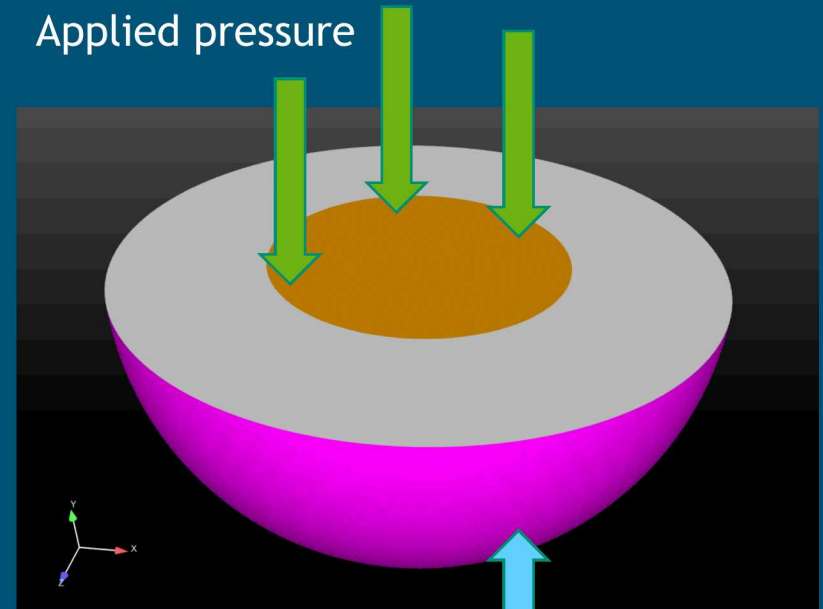


Goal: locate buried inclusion and surrounding material properties

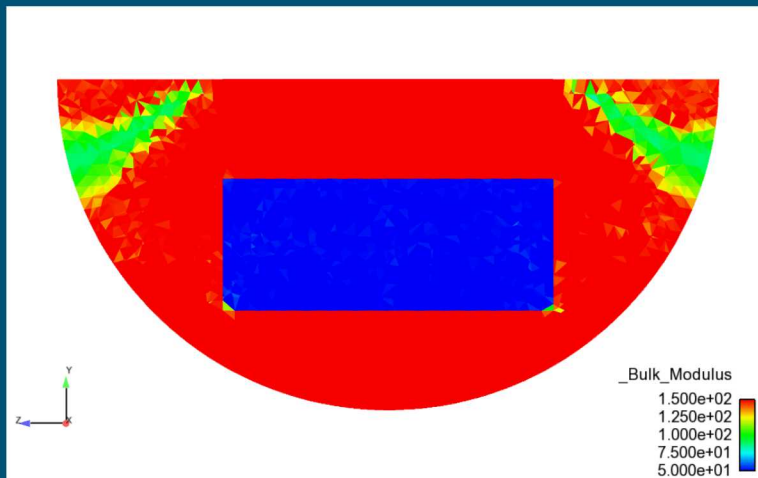
Buried inclusion model



Applied pressure



Fixed boundary

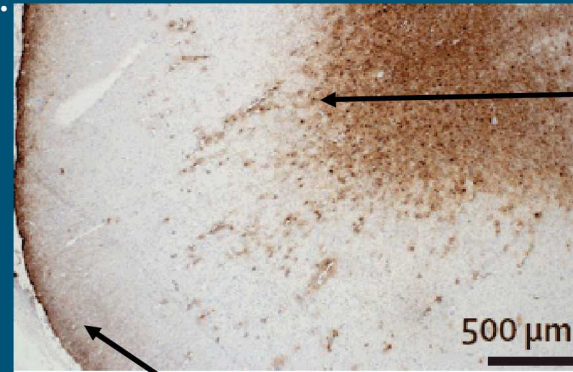
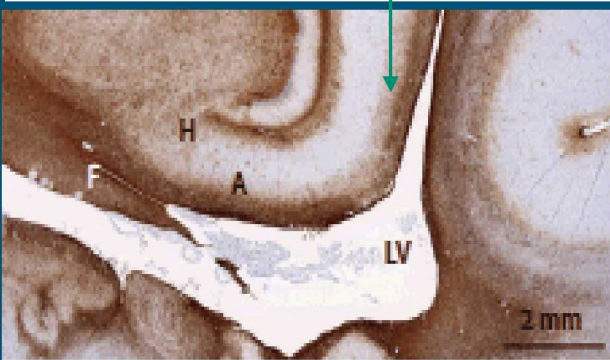
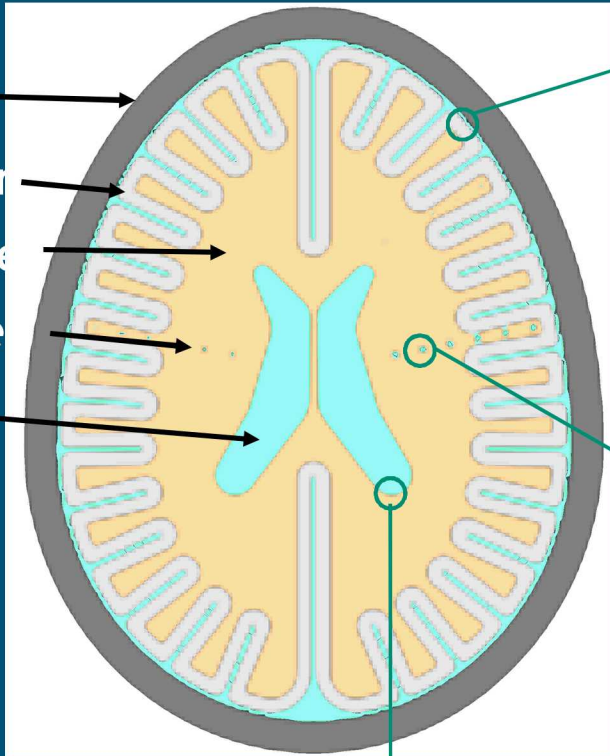


Inclusion identified in 30 iterations of inverse optimization!

# Blast-Induced Traumatic Brain Injuries (bTBI)

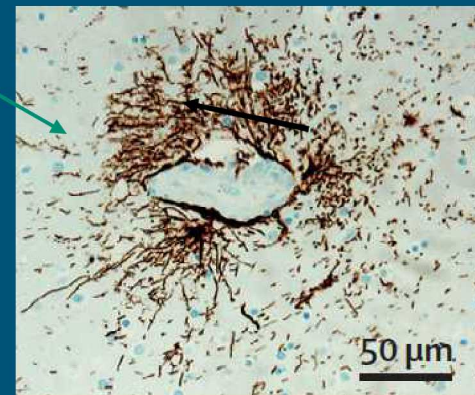
Unique neuropathological injury in bTBI :  
*interfacial injury*

Skull  
Gray matter  
White matter  
Blood vessels  
CSF



Gray-white

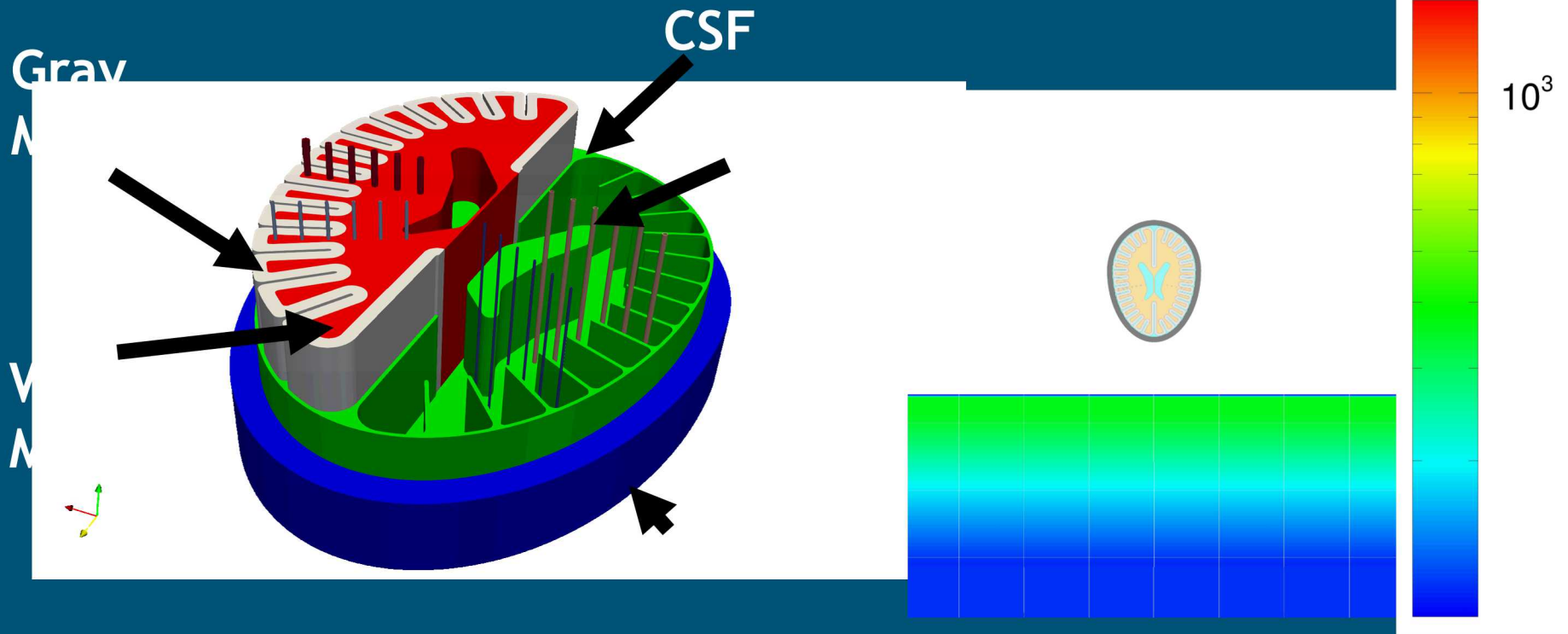
CSF - brain (sub-pial)



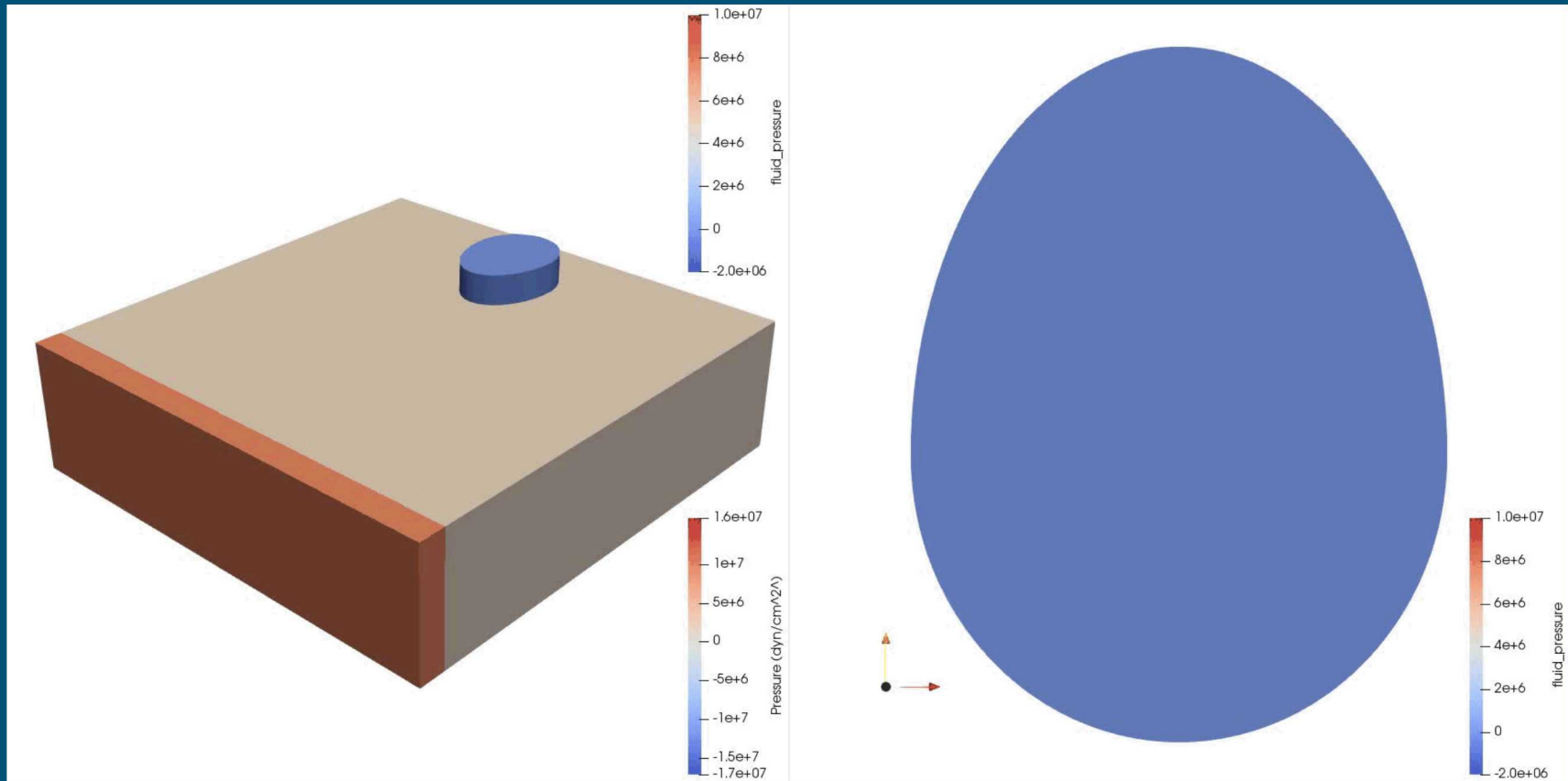
Peri-vascular

CSF-brain  
(Peri-ventricular)



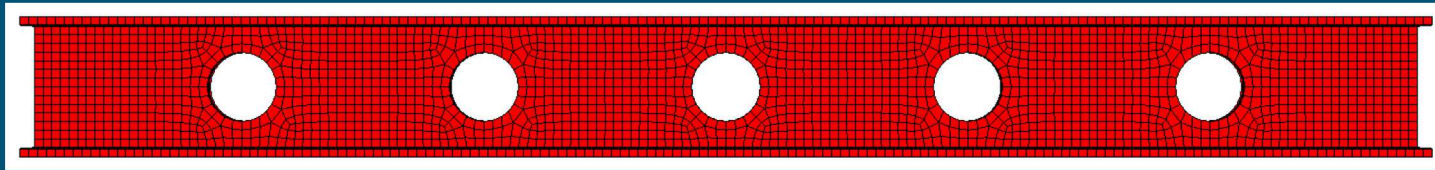


# Computational model: hybrid finite element model and shock physics code

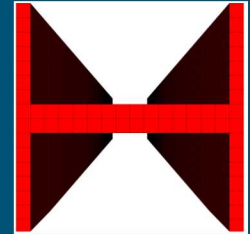




How large of a matrix system  $\mathbf{A}\cdot\mathbf{x}=\mathbf{b}$  can we solve?



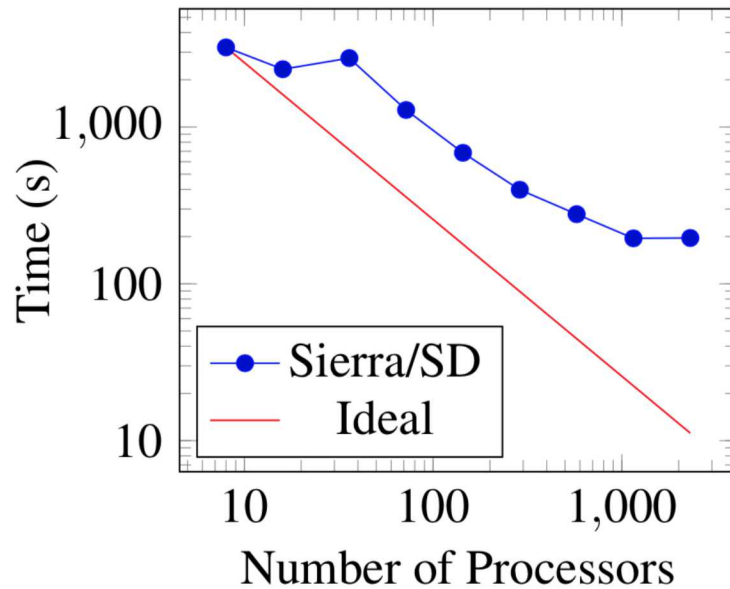
I-beam model



High Performance Computing/parallel processor computing

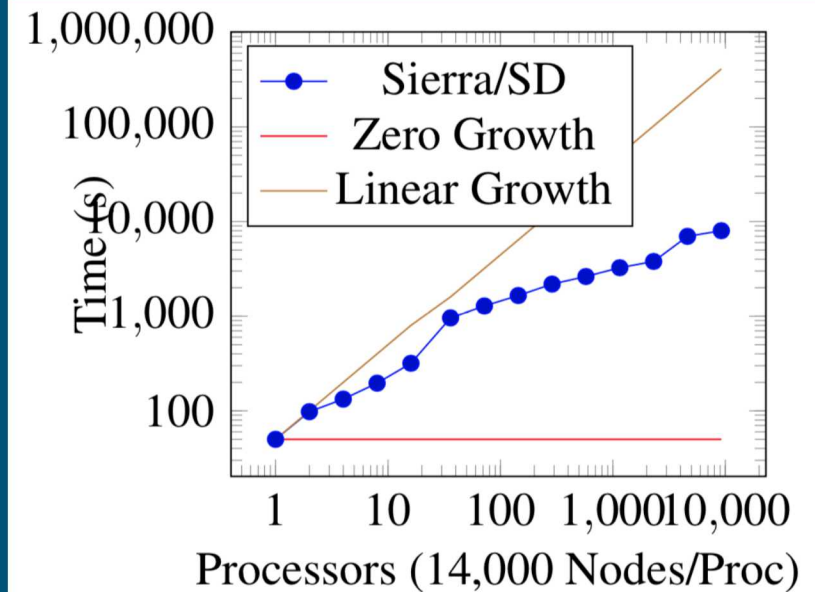
*Strong scaling:* how the solution time varies with the number of processors for a fixed total problem size

*Weak scaling:* how the solution time varies with the number of processors for a fixed problem size per processor



**Figure 8.** Scaling of Mesh 7 - 1,079,941 Nodes

Strong scaling



Weak scaling



# How do you know the number of processors needed?

	Mesh Number																	
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
NumProc	Salinas Complete						Not Run						Failed (Memory)					
1	Green	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
2	Green	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
4	Green	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
8	Green	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
16	Green	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
36	Green	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
72	Green	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
144	Yellow	Yellow	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
288	Yellow	Yellow	Green	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
576	Yellow	Yellow	Green	Green	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red	Red	Red	Red
1152	Yellow	Yellow	Yellow	Green	Green	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red	Red	Red
2304	Yellow	Yellow	Yellow	Yellow	Green	Green	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red	Red
4608	Yellow	Yellow	Yellow	Yellow	Yellow	Green	Green	Green	Green	Green	Green	Green	Red	Red	Red	Red	Red	Red
9216	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow
18432	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow

**Table 2.** Matrix of Successful Sierra/SD Runs

Consider: speed, memory usage, and *availability*!

## The End. Questions?

Interested in Sandia National Labs?

Summer internships: [sandia.jobs](http://sandia.jobs)

Career opportunities: [sandia.jobs](http://sandia.jobs)

There are many opportunities (not just at Sandia) to use your engineering and science skills to national service!