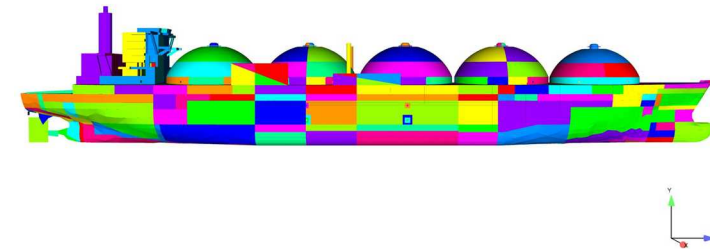
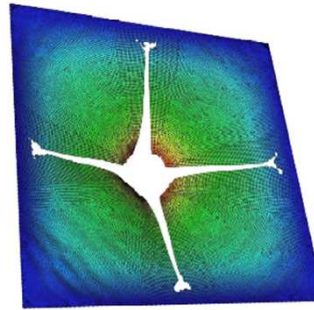
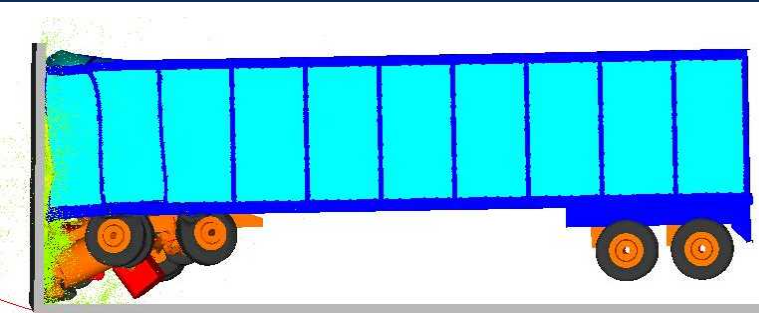


*Exceptional service in the national interest*



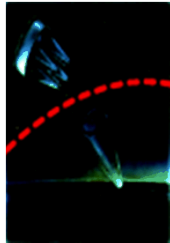
## Mechanics Simulation Capabilities at Sandia National Laboratories

Speaker: Michael R. Tupek, PhD  
Sandia National Laboratories

# The Nuclear Weapons Program is the principal driver for Sandia's Computational Simulation efforts

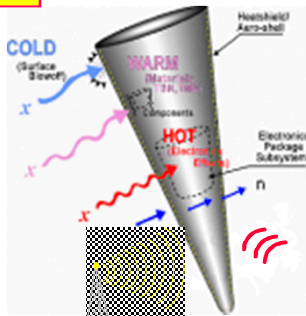
## **Delivery**

Separation  
shock/  
Aerodynamic  
Heating



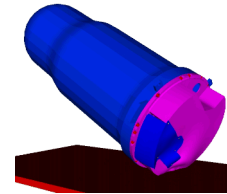
## **Survivability**

Radiation  
Effects



## **Assured Performance & Manufacturing**

## **Assured Safety and Security**



Mechanical Impact



Thermal Load



Electromagnetic  
Pulse

Security  
Components

Safe &  
Secure  
Transport

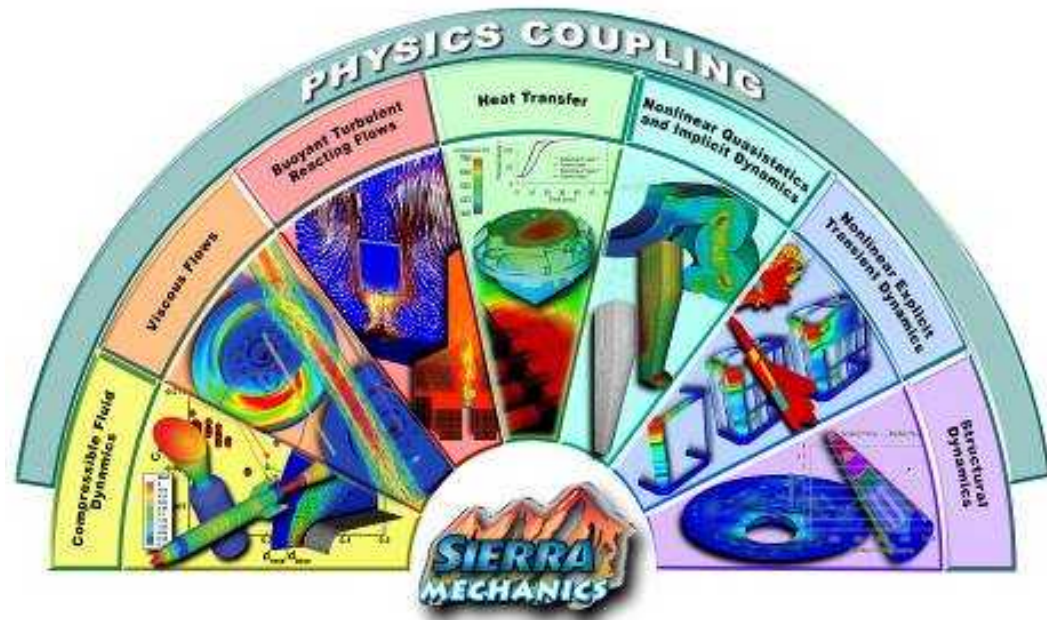


**SNL Engineering Codes are positioned to support the engineering needs of the complex**

# SIERRA coupled physic software

## ■ Thermal/fluids/aerodynamics

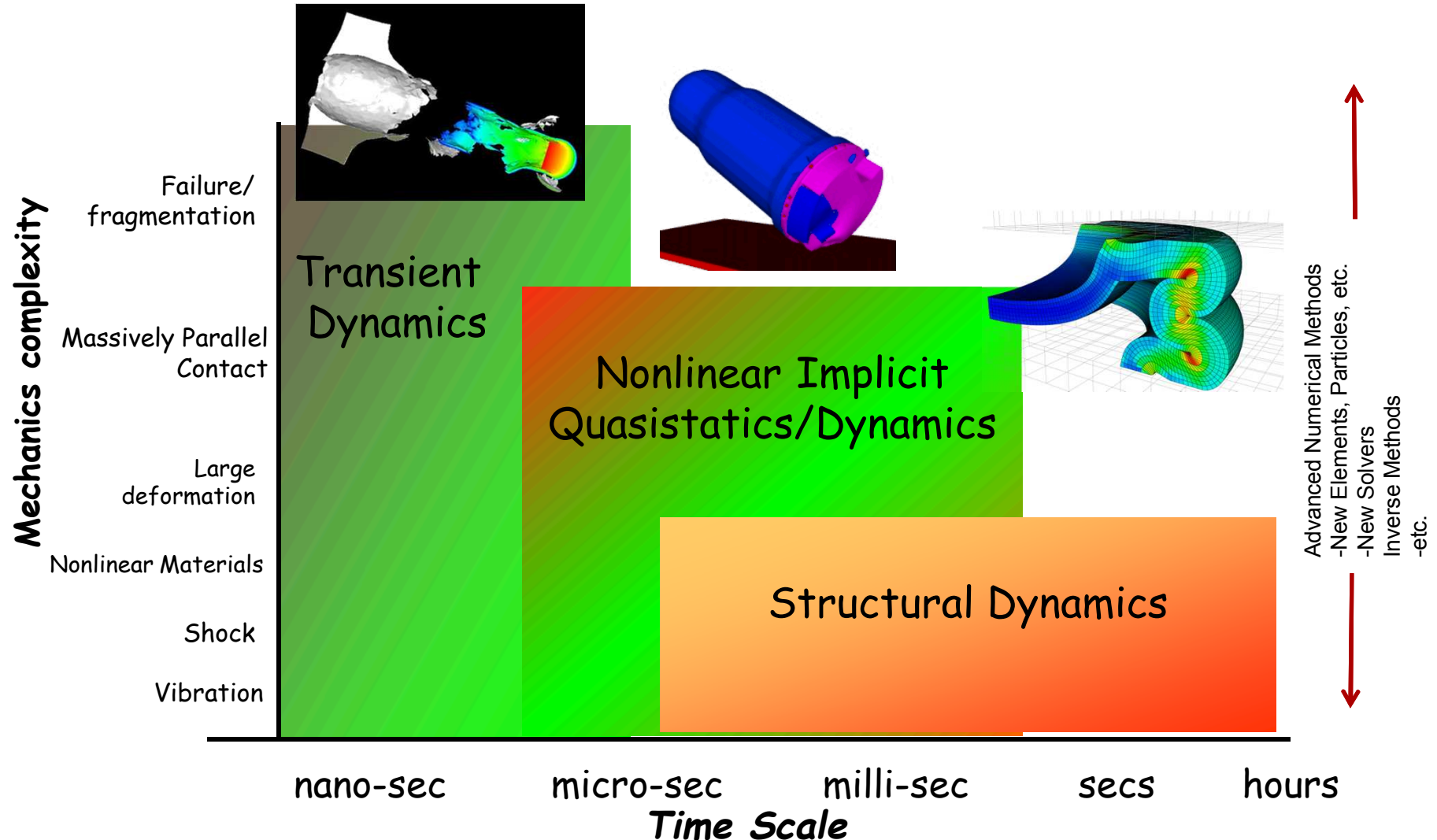
- Compressible fluid mechanics with subsonic through hypersonic flows
- Non-newtonian reacting flow with free surfaces and complex material response
- Low mach number turbulent reacting flow participating media radiation
- Heat transfer with limited convection, chemistry, and enclosure radiation



## ■ Solid mechanics/structural dynamics

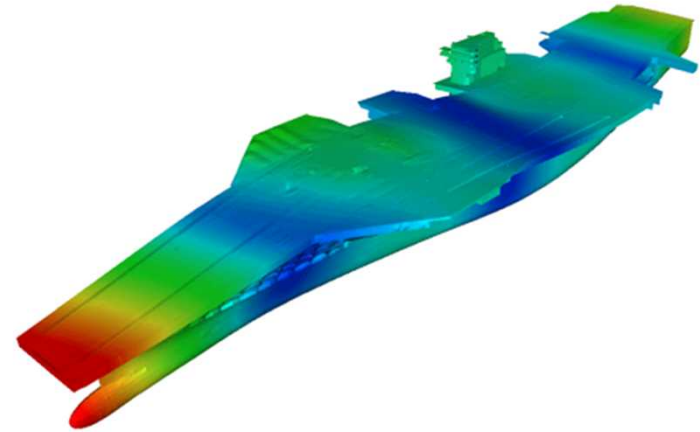
- Nonlinear solid mechanics, quasistatics, implicit dynamics, failure and tearing
- Nonlinear solid dynamics with explicit time integration, nodal-based tets, remeshing, particle methods, cohesive surface elements, contact, and material failure
- Linear structural dynamics and modal analysis of complex structures

# Sierra includes solid mechanics and structural dynamics capabilities

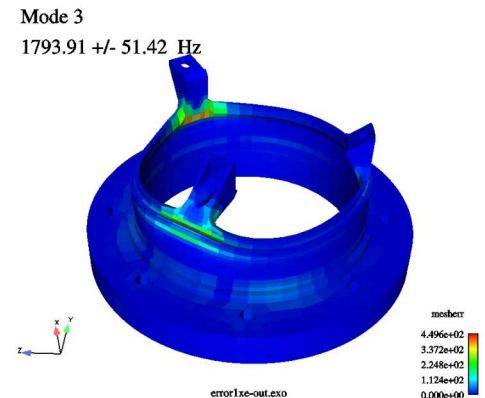


# Sierra/SD: Structural Dynamics

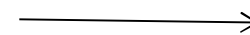
- Predicts the response of a system under dynamic conditions.
  - Time and Frequency Response
  - Stresses (particularly in the operating regime)
  - Fatigue
  - Energy dissipation in joints
  - Rotating Systems
- Efficient for very large problems
  - Many millions of coupled equations
  - Serial, direct matrix solutions scale to order  $N^3$
  - Parallel, iterative solvers are typically more complex, but scale as  $O(N)$ 
    - FETI
    - GDSW Solvers (Sandia)
- Structural-Acoustics
  - Infinite Elements
- Inverse Problem Capability
  - Source Inversion for Structural-Acoustics
  - Material Property
  - Shape



## Error Estimation



Recent Past:  
NASTRAN  
MC2912  
30,000 dof



Today:  
Sierra MP  
>1B dof



# PDE Constrained Optimization:

## Acoustic Source Inversion:

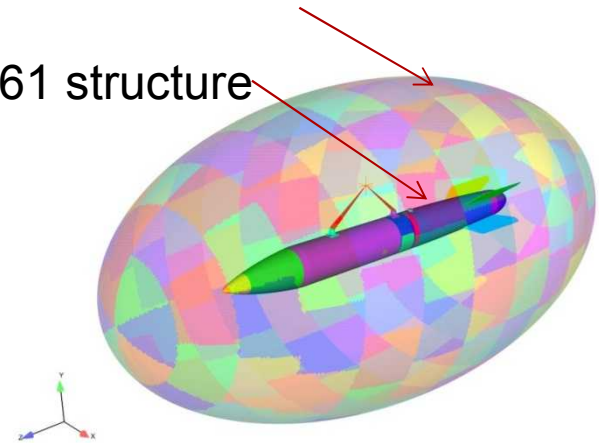
Solve inverse problem to obtain acoustic patch inputs that produce the given 17 experimental microphone measurements.

## Material property inversion:

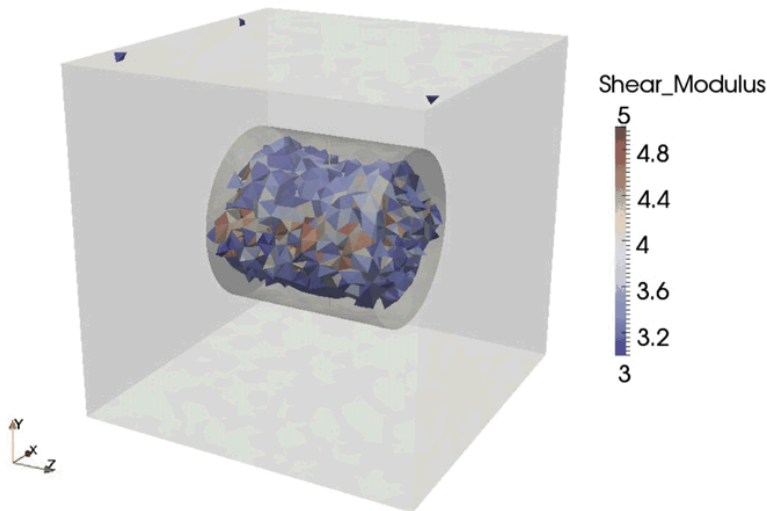
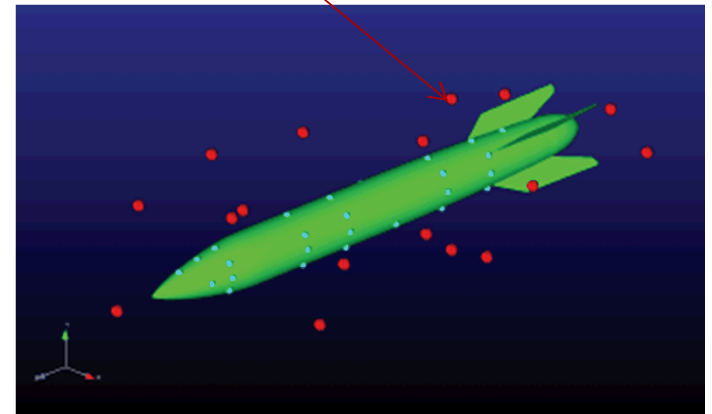
Solve inverse problem to determine spatially varying material properties given structural response.

Surface with 174 acoustic patches

B61 structure

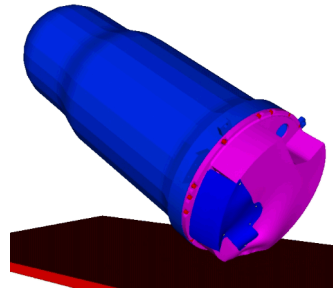


17 Microphone locations

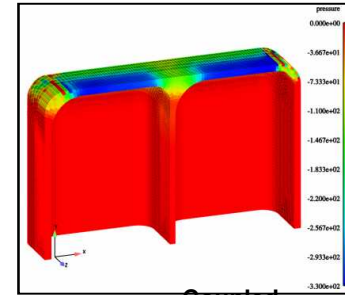


# Sierra/SM: Explicit and Implicit quasi-statics and Dynamics Solid Mechanics

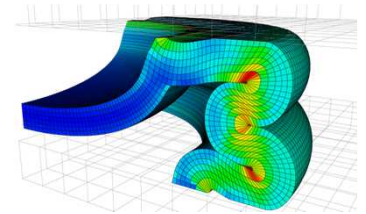
- Fully Three-Dimensional
- Finite Elements and Particles
  - Hex and Nodal Based Tets
  - Shell and Beams
  - SPH, RKPM, Peridynamics
- 50 + Material models
- Explicit and Implicit contact: Massively parallel, accurate friction response
- Explicit Failure modeling:
  - Material failure/element death
  - Cohesive zones (elements, contact surfaces)
  - Phenomenological models (spot weld, line weld)
  - Automatic remeshing
  - X-FEM (pervasive failure modeling)
- Quasi-static failure modeling



W80 drop test



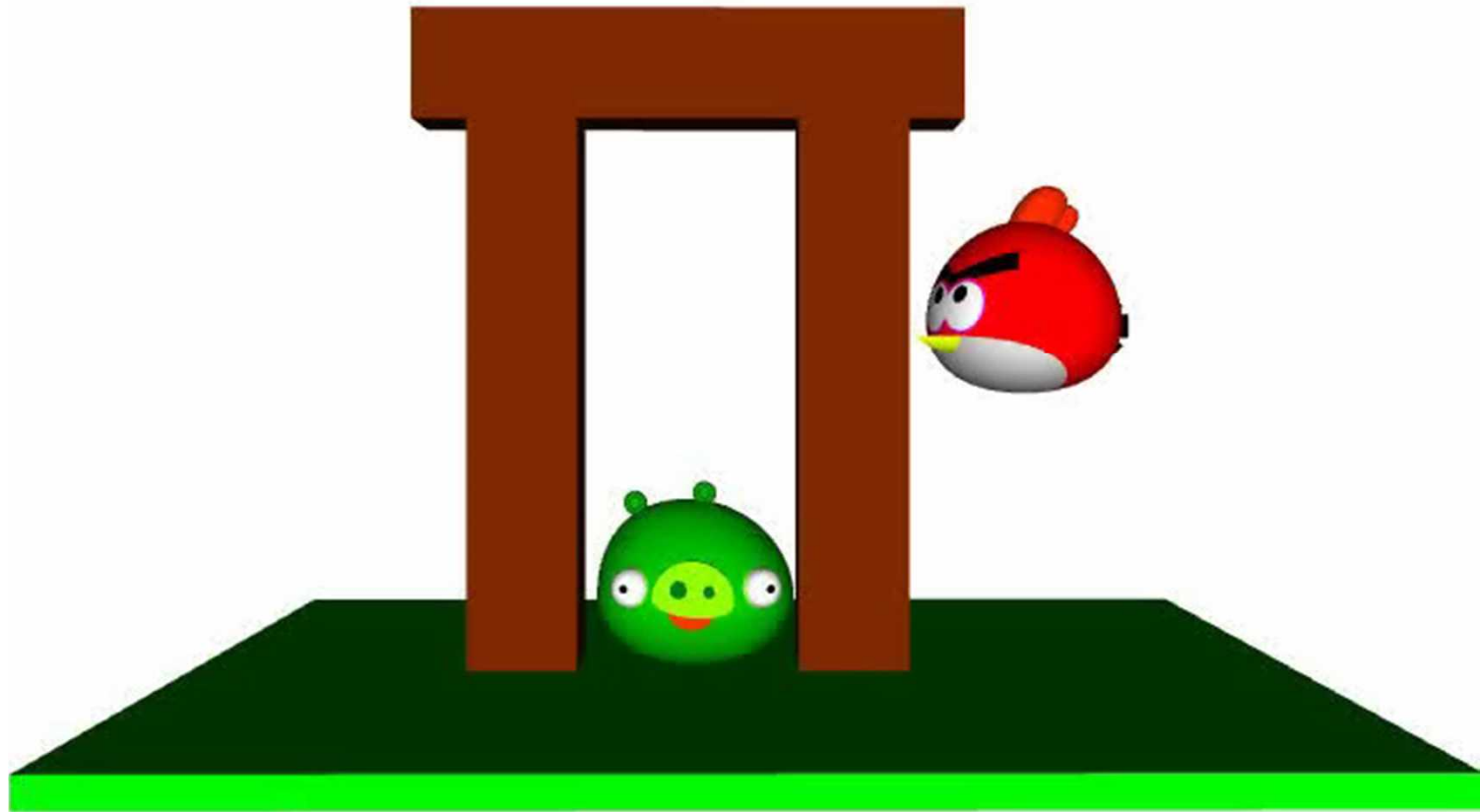
Coupled  
Thermal/QS/Dynamic



Large deformation/contact

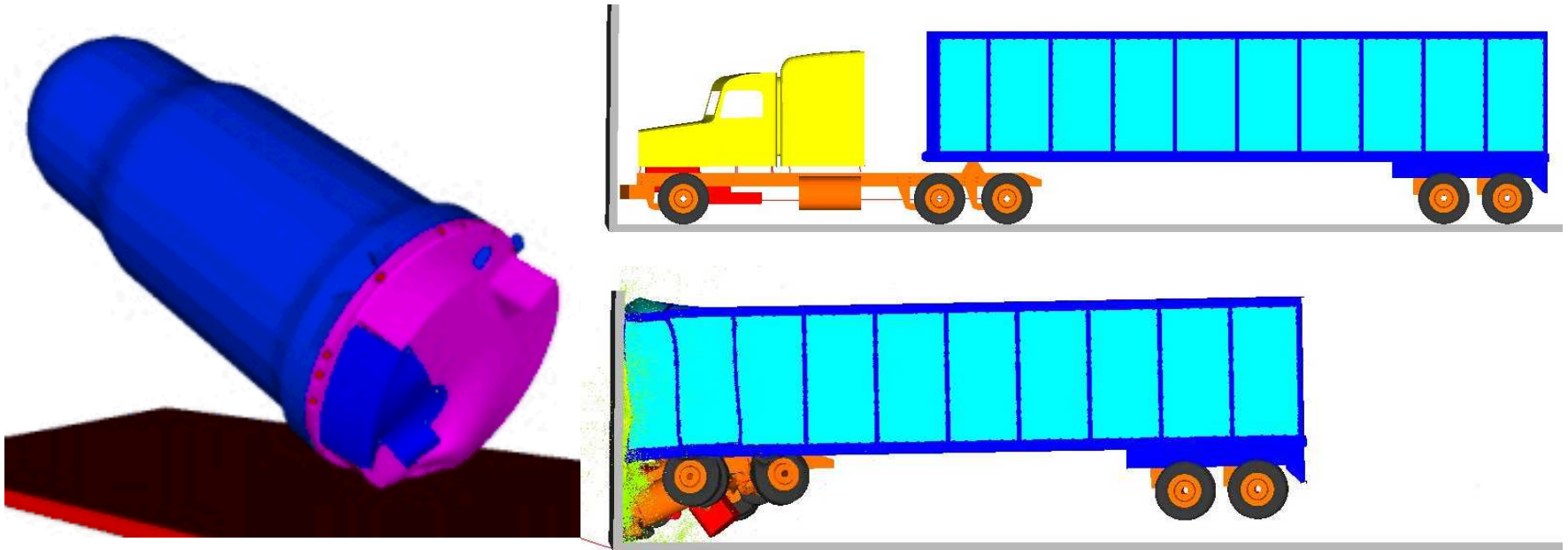
- Scalable parallel solvers for nonlinear problems
  - Contact
  - Nonlinear material response
  - Large deformation
- Coupling to internal and external modules
  - Sierra/TF
  - CTH (Blast)
- Multi-scale approaches

# Sierra/SM Explicit Contact Mechanics addresses real world problems





# Sierra/SM Contact Mechanics addresses system level contact

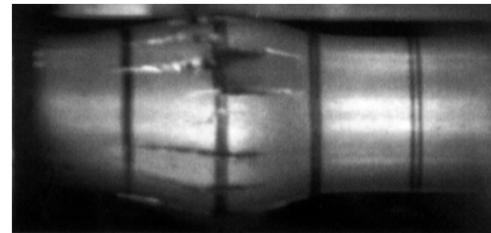
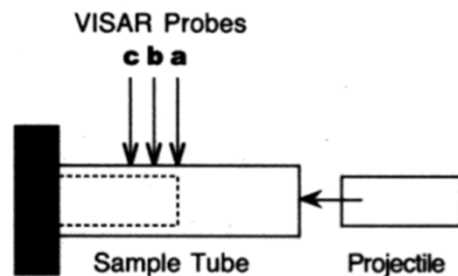


# Meshless Capabilities

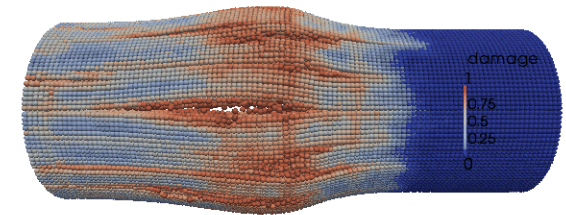
- Peridynamics is a non-local continuum method with great promise for handling fracture and damage

## Expanding Tube Experiment

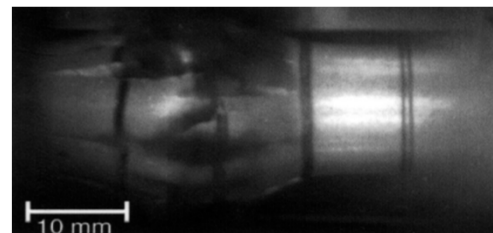
- Lexan discs impact w/in tube
  - Discs modeled with FE
  - Johnson-Cook with EOS
- AerMet high strength steel tube
  - Tubes model is peridynamics
  - Elastic-plastic with hardening
  - Bond failure on critical stretch



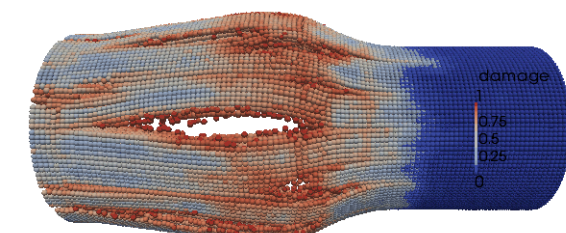
Experimental image  
[Vogler et. Al]



Simulation  
15.4 microseconds



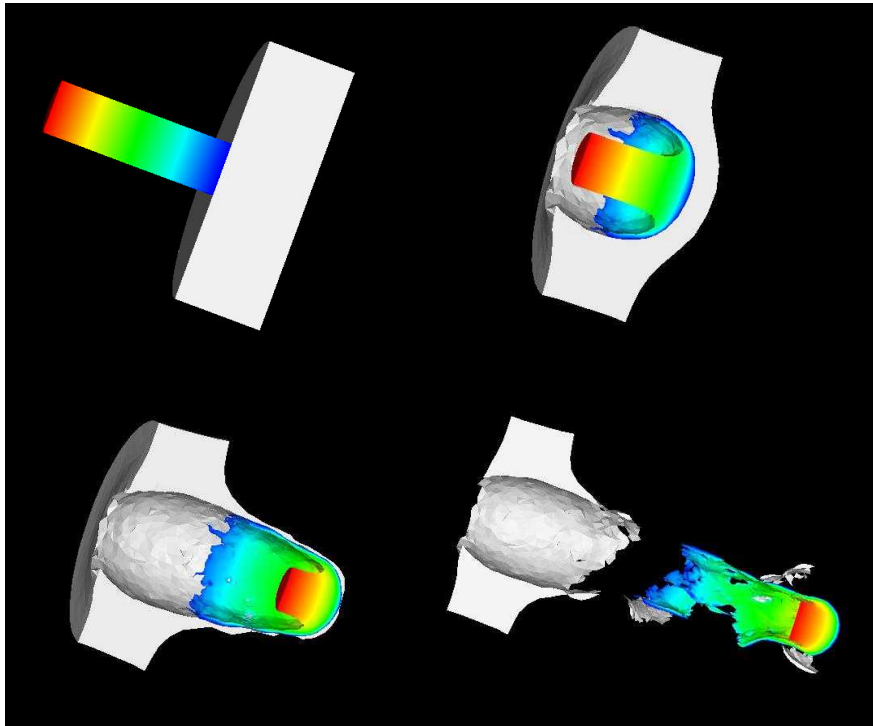
Experimental image  
[Vogler et. Al]



Simulation  
23.4 microseconds

# Nodal-Based Tetrahedra (NBT)

- This element blurs the boundary between element and particle methods, and has advantages of both
  - **Since all data resides at nodes, amenable to remeshing**



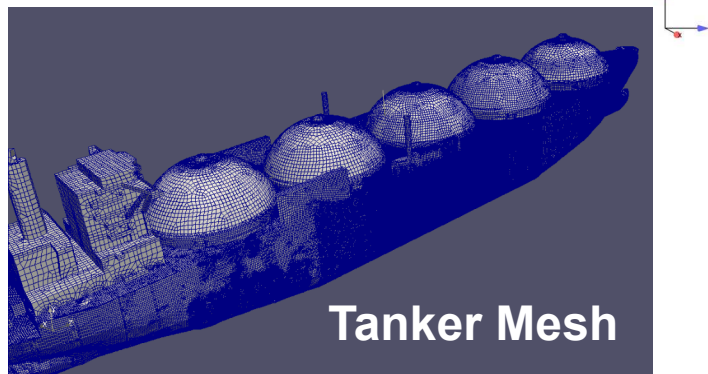
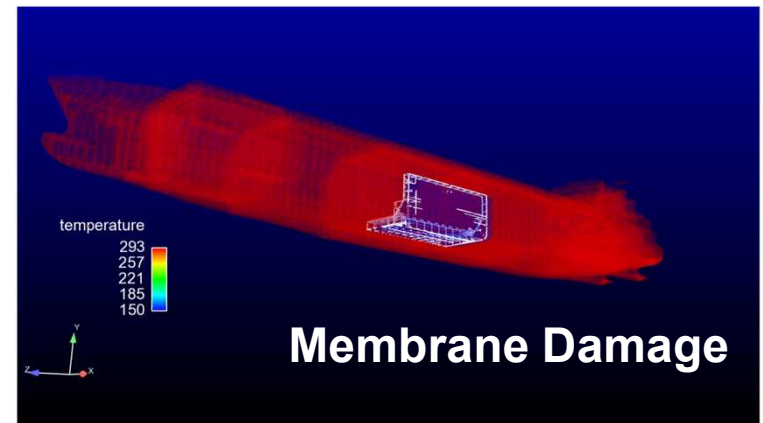
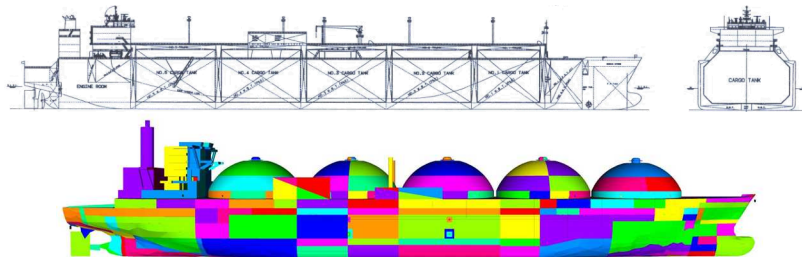
**Nodal-based tet  
transient analysis of  
impact of tungsten  
bar on steel plate**

**Impact velocity is  
2500 m/s, and explicit  
dynamics (Presto)  
code is used with  
pervasive remeshing**

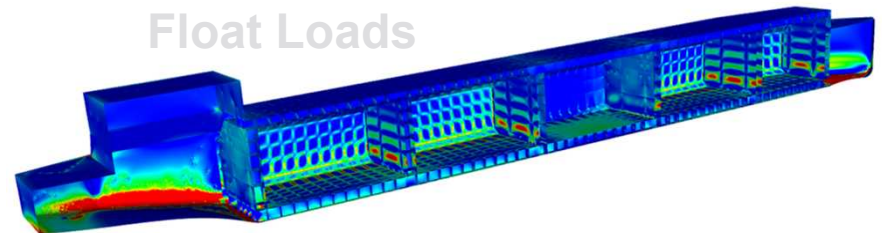
# Complex Systems Models

- Example large-scale coupled system model
  - LNG tanker analysis for disaster simulation response

Membrane LNG Carrier



Float Loads



# CompSimUI

*Integrated Workflow Product*

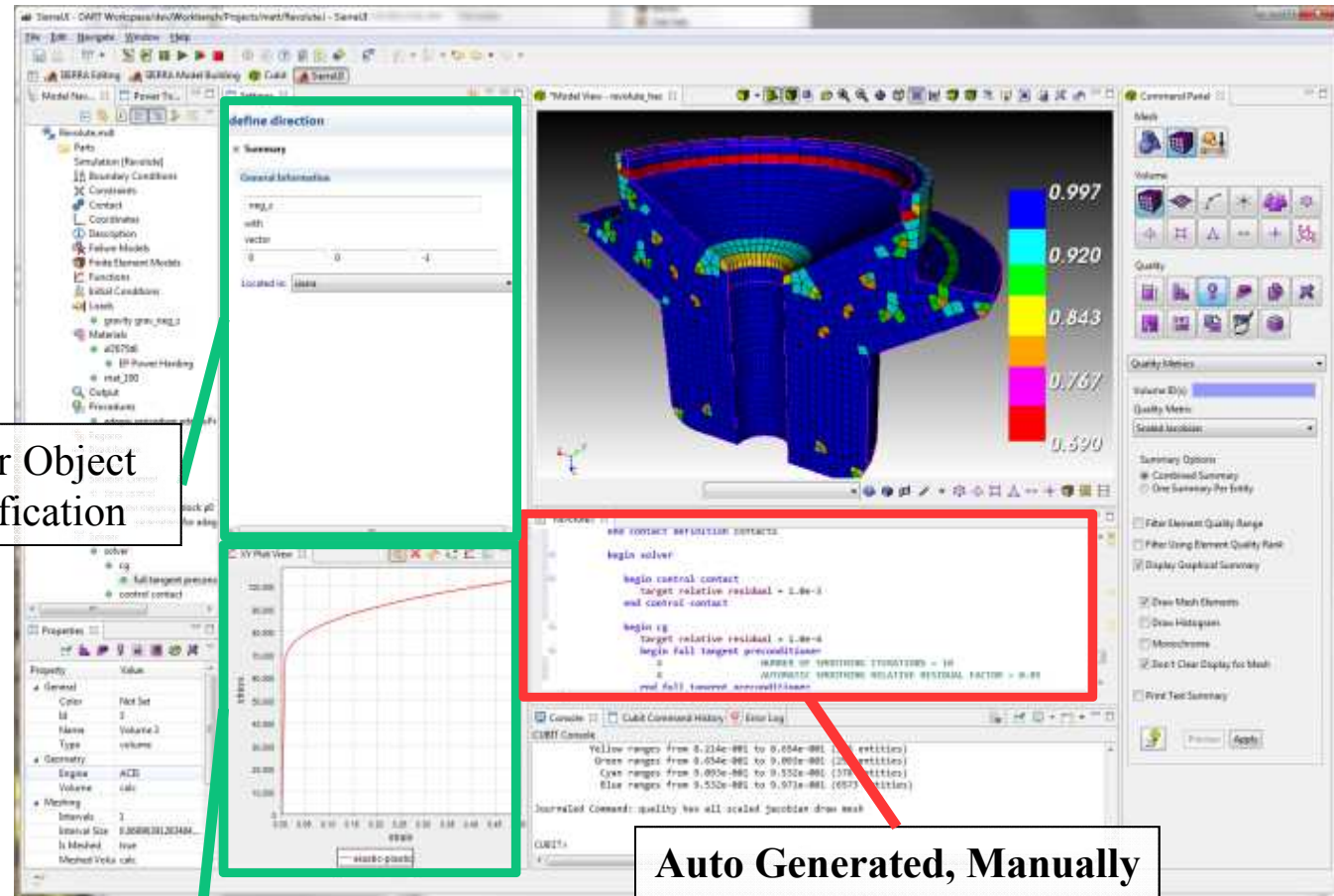
Synchronized  
Model

Customizable  
Solver Input

Solver Object  
Specification

Workflow Controls

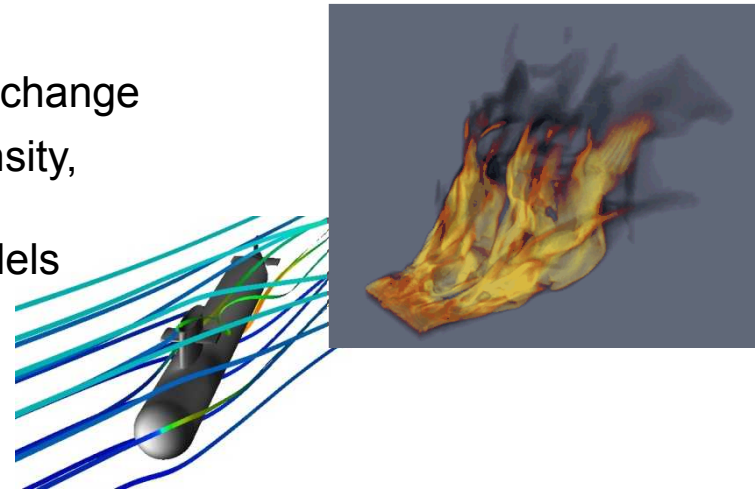
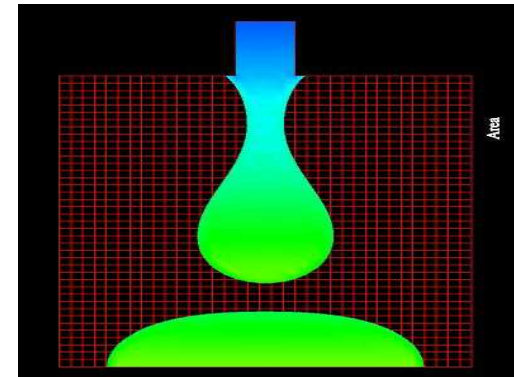
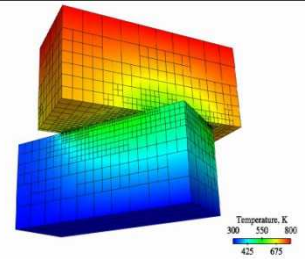
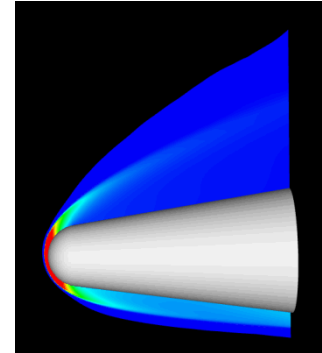
Function Editor



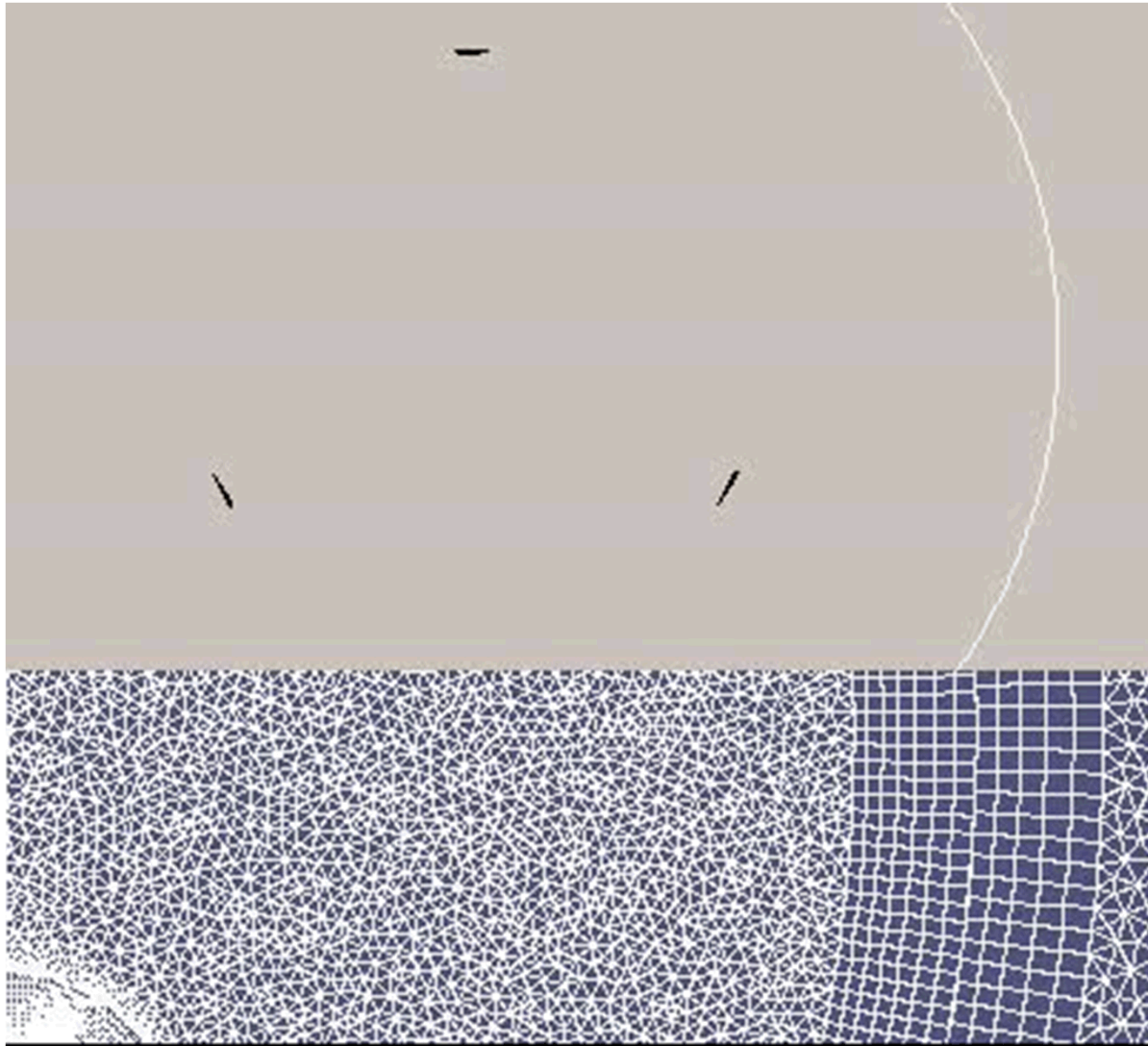


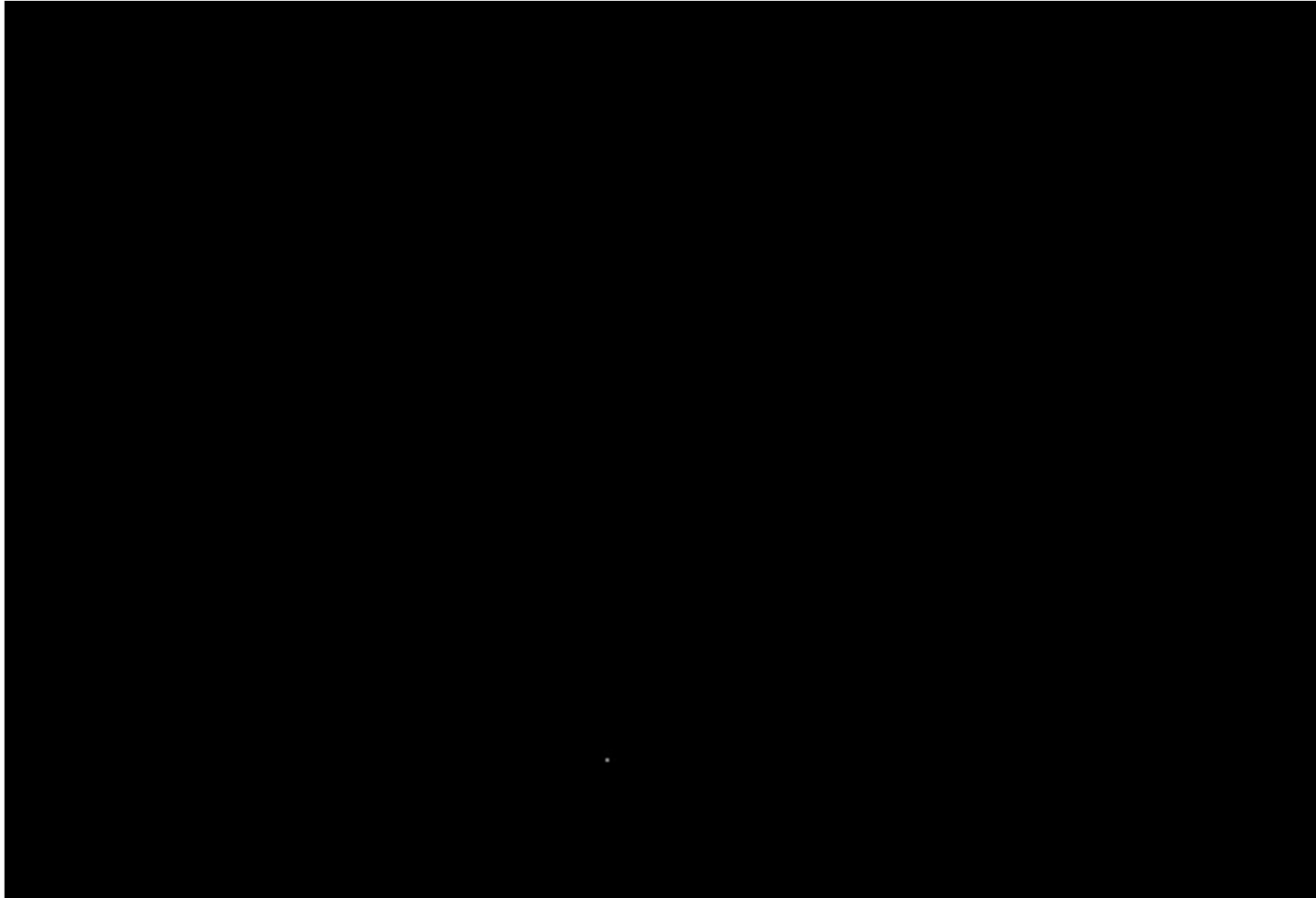
# Computational Thermal & Fluid Mechanics

- Heat transfer, enclosure radiation and chemistry
  - Dynamic enclosures
  - Element birth/death
  - Contact
- Compressible fluid mechanics
  - Subsonic through hypersonic
  - Laminar and turbulent
  - Unstructured mesh
- Non-Newtonian, free surface, and porous media flows
  - Complex material response
  - Level sets for surface tracking
  - Flexible coupling schemes
  - Porous media, with chemical reactions and phase change
- Low Mach number, high Reynolds number, variable density, chemically reacting flows
  - Eddy dissipation and mixture fraction reaction models
  - RANS and LES based turbulence models
  - Unstructured Mesh
  - Pressurization models









# Next Generation Scientific Computing

Sandia codes are undergoing refactor for next generation computer architectures

- Code capabilities include:
  - Mechanics, Electro-magnetics, Molecular dynamics, Radiation transport
  - Parallel solvers, Optimization

The architectures of the future are unknown!

- GPU clusters?
- Many-core architectures?
- ARM, other low power devices?

Modern architecture design is no longer determined by scientific computing

- Currently guided by Social Media! Facebook, Google, etc.
- Provides a unique challenge for developing and maintaining scientific codes