

# Overview of Sierra Codes

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**Sandia National Laboratories**  
**Albuquerque NM**  
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Sandia is a multi program laboratory operated by Sandia Corporation, a Lockheed Martin Company,  
for the United States Department of Energy's National Nuclear Security Administration  
under contract DE-AC04-94AL85000.

# The national code strategy establishes Sandia as the engineering simulation capability provider

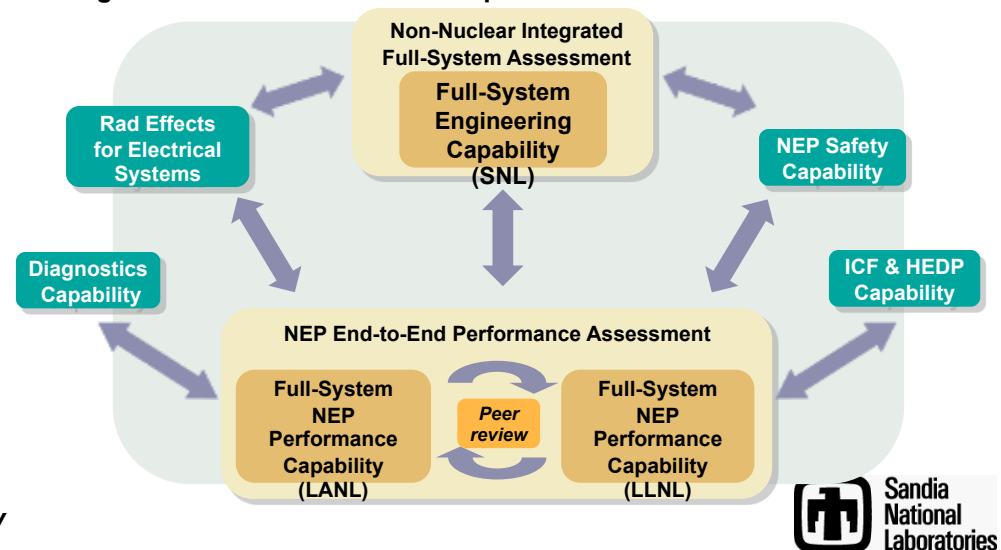
Focus Areas	Current State	Strategies	Future State
Integrated Simulation Capabilities (Application Codes)	<ul style="list-style-type: none"> <li>14 modern + numerous legacy codes across 6 broad application areas</li> <li>Core physics simulation competencies established</li> </ul>	Establish the National Simulation Portfolio for Stockpile Certification	<ul style="list-style-type: none"> <li>7 modern national capabilities</li> <li>End legacy development</li> <li>Core competencies sustained</li> </ul>
Computational Science	<ul style="list-style-type: none"> <li>Tera scale computational science established (MPI programming model)</li> <li>Basic capabilities for uncertainty quantification</li> </ul>	Advance computational algorithms to enable predictive simulation and QMU	<ul style="list-style-type: none"> <li>Algorithms &amp; programming models supporting predictive simulation at petaFLOP and exaFLOP scales</li> <li>Advanced capabilities for uncertainty quantification and QMU studies</li> </ul>
Scope of Applications	<ul style="list-style-type: none"> <li>ASC simulation capabilities focused on certification for tail numbers</li> </ul>	Broaden the impact of ASC simulation capabilities in national security	<ul style="list-style-type: none"> <li>Capabilities for broader national security applications, including NNSA nuclear security and non-proliferation missions</li> </ul>

## Strategic Components

- Establish the National Simulation Portfolio for Weapons Science and Engineering, and Stockpile Certification**
  - Define the core simulation capabilities needed
  - End development funding for legacy codes
  - Establish the capability to couple between codes of national portfolio
- Advance Computational Algorithms to Enable Predictive Simulation and QMU**
  - Advance scalability of computational algorithms
  - Collaborate on evolution of programming models
  - Deliver advanced capabilities for QMU and UQ
- Broaden the Impact of ASC Simulation Capabilities in National Security**
  - Develop a business "prospectus" for major capabilities
  - Develop and support interagency partnerships
  - Develop enhanced capabilities for expanded national security missions

## Objectives

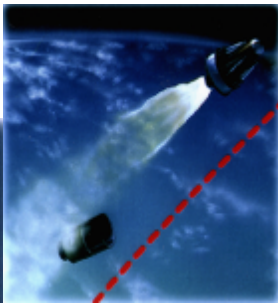
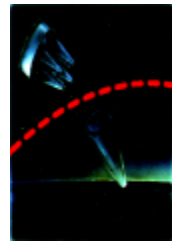
- Advance world-leading predictive science**, providing the capability to sustain stockpile stewardship without returning to underground nuclear testing as weapons age and we move further from the test base.
- Enable Quantification of Margins and Uncertainties (QMU)-based certification**, transforming the broader certification process to allow more effective and selective use of aboveground experiment, certification tests, flight tests, and other tests.
- Catalyze a responsive infrastructure** through pervasive simulation across all aspects of the stockpile lifecycle, such as design, certification, manufacturing, Significant Finding Investigation resolution, transportation, security, safe dismantlement, outputs and environments, etc.
- Enable a broadened national security mission**, in which simulation tools extend beyond stockpile stewardship and enable the next-generation mission of the Complex



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

## Delivery

Separation shock/  
Aerodynamic Heating



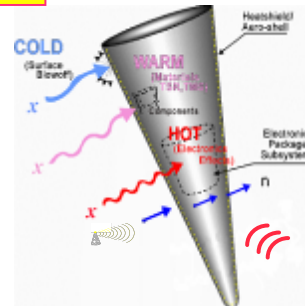
Staging shock



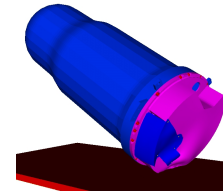
Random vibration

## Survivability

Radiation Effects



## Assured Safety and Security



Mechanical Insult



Thermal Insult



Electromagnetic Insult

Security Components

## Assured Performance & Manufacturing

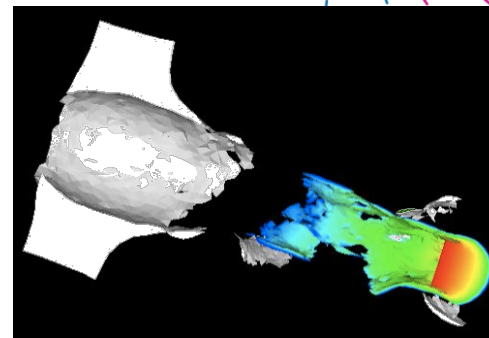
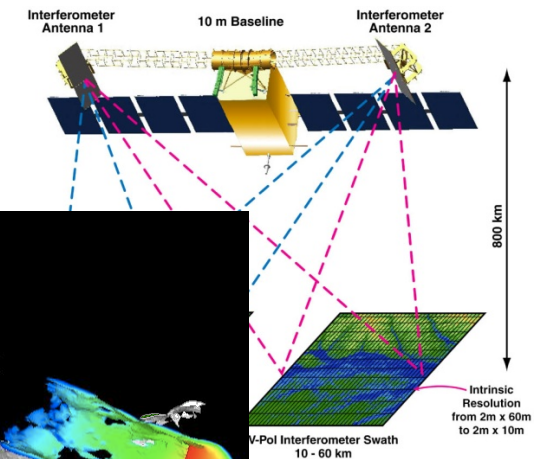
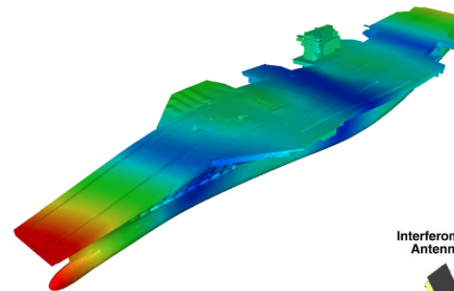
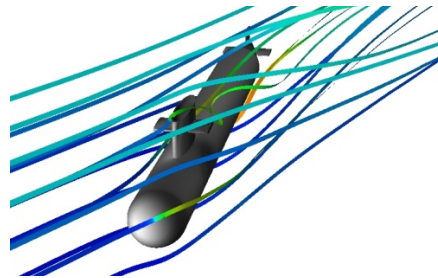
Safe &  
Secure  
Transport



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

# Non-NW customers contribute significant resources

- **Other Sandia mission areas and projects, for example**
  - Energy
  - LNG
  - Satellite programs
- **Industry**
  - Goodyear,
  - Proctor & Gamble,
- **DoD**
  - CREATE
  - ARDEC, TARDEC, Picatinny, ARL, etc.
- **NASA (and JPL)**
- **AWE**



# SIERRA has a wide range of coupled mechanics simulation capabilities

- **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



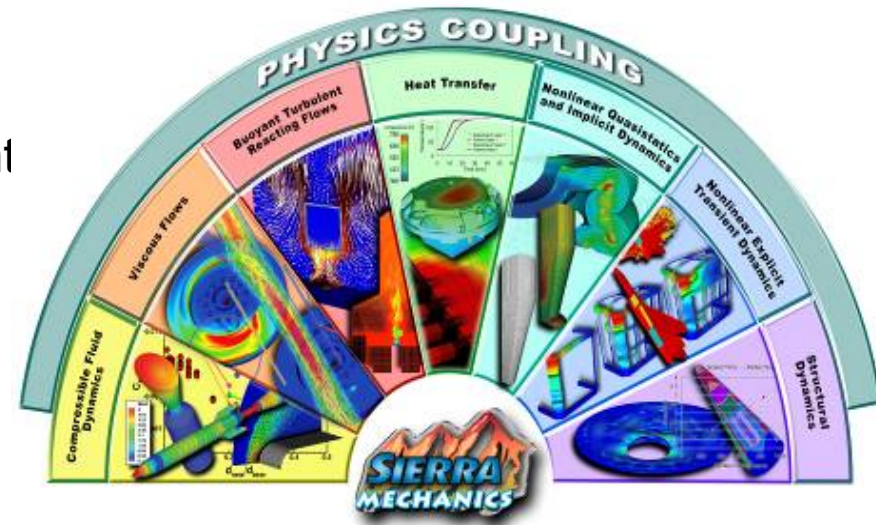
- **Solid mechanics/structural dynamics**

- 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 is the engineering mechanics simulation code supporting the NW mission, as well as other customers

- **Distinguishing strengths**

- “Application aware” development
- Scalable
- SQA and V&V
- Multiple scales
- Coupling



- **Explicit tie to SNL workflow, including**

- Geometry and meshing
- Visualization
- Design and optimization

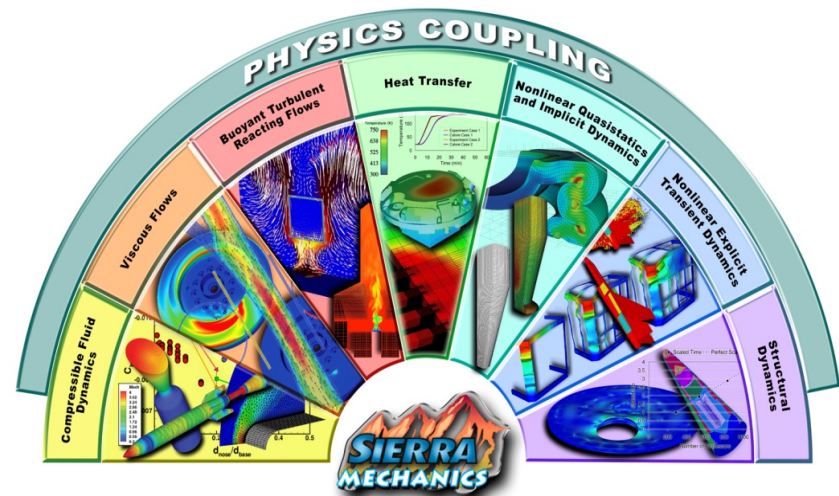
- **“Partner” applications include**

- CTH and ALEGRA for shock physics simulations
- RAMSES suite for radiation effects, electrical and electronics simulations

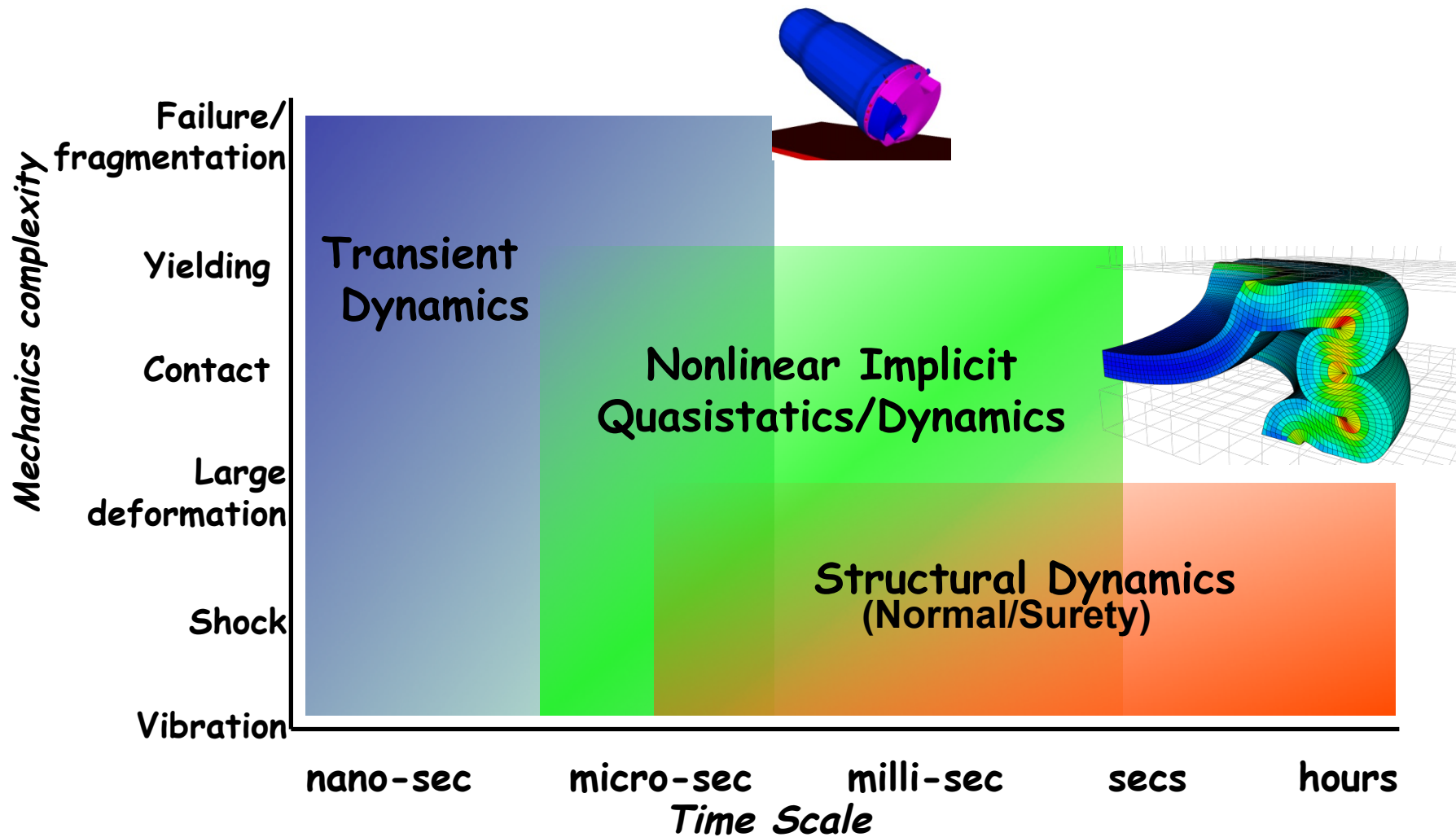


# There are three facets to the current code capability & consolidation efforts

- **Thermal/Fluids Consolidation**
  - Compressible Flow
  - Thermal Response
  - Multiphase
  - Turbulent Reacting Flow
- **Solid Mechanics Consolidation**
  - Explicit Transient Mechanics
  - Implicit Transient Mechanics
  - Quasistatics
  - Structural Dynamics
- **SIERRA Framework → SIERRA Toolkit**

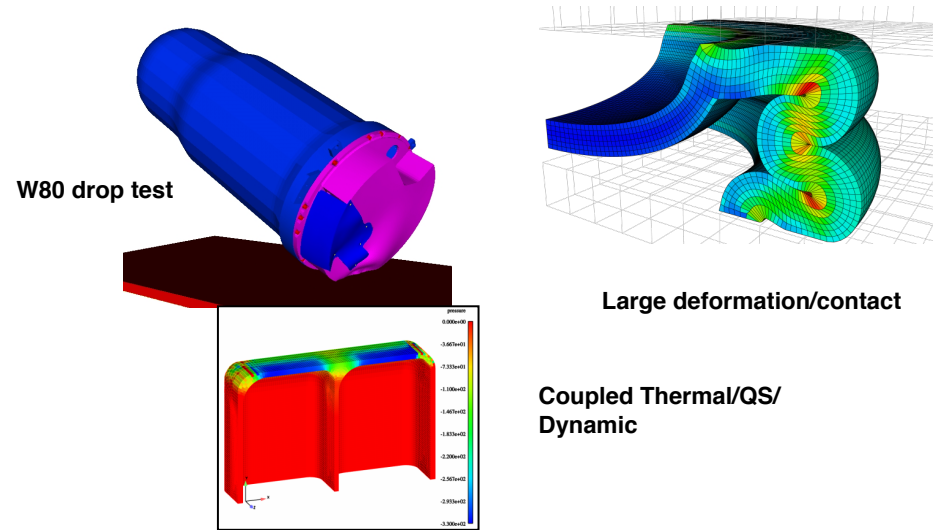


# Sierra includes solid mechanics and structural dynamics capabilities



# Explicit transient dynamics and implicit quasi-statics and dynamics capabilities

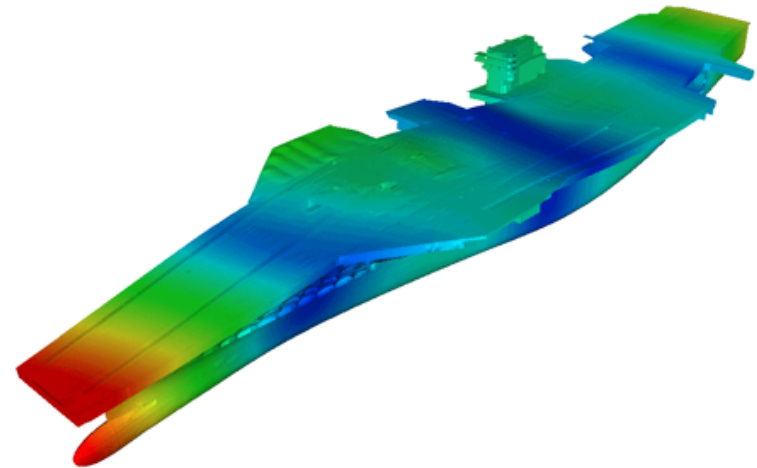
- **Fully Three-Dimensional**
- **Finite Elements and Particles**
  - Hex and Nodal Based Tets
  - Shell and Beams
  - SPH and Mass particles
- **Material models: 50+, including energy-dependent materials**
- **Explicit contact: Massively parallel, momentum balance, accurate friction response**
- **Multi-length Scale**
- **Boundary conditions:**
  - Kinematic and Force
  - Specialized: cavity expansion, silent BC
  - CONWEP integration (Analytic Blast Pressure Loads)
- **Explicit Failure modeling:**
  - Material failure/element death
  - Cohesive zones (elements, contact surfaces)
  - Phenomenological models (spot weld, line weld)
  - Automatic remeshing using Nodal Based Tets
  - X-FEM (pervasive failure modeling)
- **Quasi-static failure modeling**



- **Provides scalable parallel solvers for highly nonlinear problems**
  - Contact
  - Nonlinear material response
  - Large deformation
- **Utilizes services provided by the Sierra Framework/Toolkit to enable**
  - Coupled physics
  - Multi-length scale modeling techniques
  - Preloading

# Structural Dynamics

- **Predicts the response of a system under dynamic conditions.**
  - Stresses (particularly in the operating regime)
  - Fatigue
  - Energy dissipation in joints
- **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
    - CLIP, CLOP Solvers (Sandia)
- **Structural Acoustics**
- **Inverse Problem Capability underdevelopment**



**Recent Past:**  
**NASTRAN**  
**MC2912**  
**30,000 dof**



**Today:**  
**Sierra MP**  
**>10M dof**

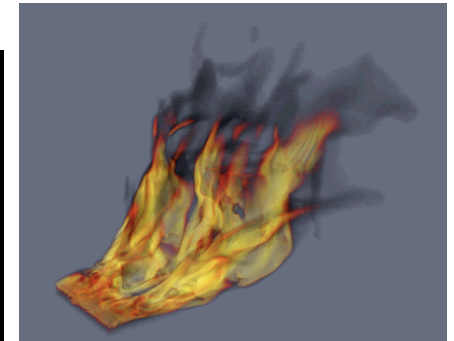
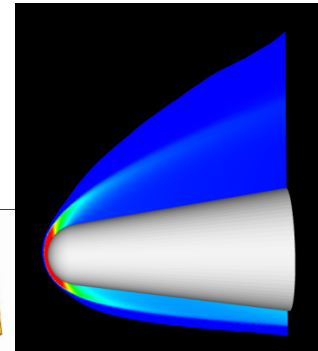
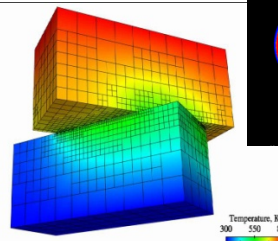
# Computational Thermal & Fluid Mechanics

- **Thermal – Heat Transfer, Enclosure Radiation and Chemistry**

- Dynamic enclosures
- Element birth death
- Contact

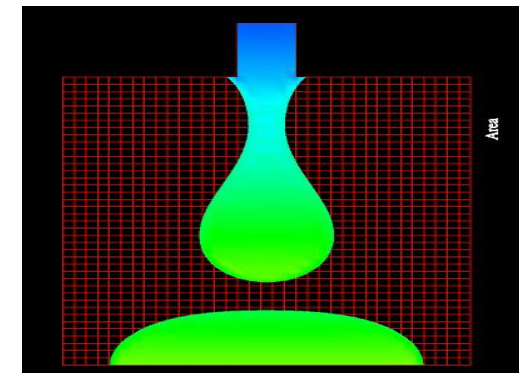
- **Aero – Compressible Fluid Mechanic**

- Subsonic through hypersonic
- Laminar and turbulent
- Unstructured mesh



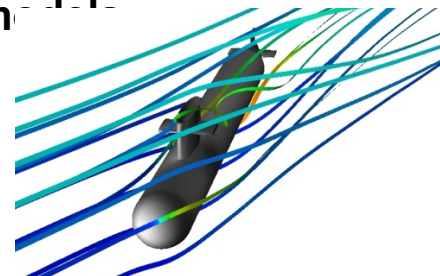
- **Multiphase – Non-Newtonian, Multi-physics, and Free Surface Flows**

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



- **Fire/Combustion – Low Speed, Variable Density, Chemically Reacting Flows**

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



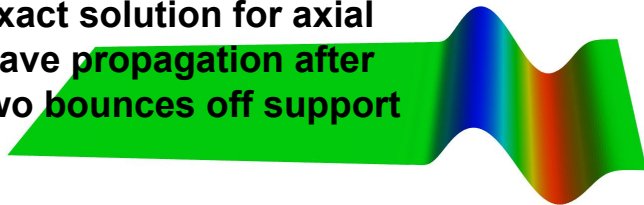
# Sierra will continue to invest in new capabilities

- Nonlinear stress response (w/ multi-level solvers)
  - Interface problems (contact)
  - Large deformations (automatic remeshing, particle methods)
  - Failure Modeling
    - Element death
    - Element to Particle
    - Dynamic Cohesive Zone
    - X-FEM
  - Multi-Scale Modeling:
    - RVE (representative volume element)
    - Embedded Finite Element models
    - Time
  - Performance
    - Solvers
    - Contact Algorithms
    - Element calculations
  - Nonlinear Structural Acoustics
  - Energy Dissipation
  - Time and Frequency Domain vibrations
- Unified FEM algorithms for high speed compressible flows, fire applications, and porous flow with deformable media applications
    - Improved accuracy via analytic enrichment for steep gradients
  - Improved thermal contact and enclosure radiation
  - Improved finite rate chemistry and fluid/thermal ablation coupling for re-entry
  - Improved Fluid (Aero)-Structure interaction
  - Couplings to: Thermal, Solid, Fluid, Shock Hydro
    - Including large deformation Fire-Thermal-Structural coupling
  - Intrinsic V&V
    - Testing and verification
    - Uncertainty quantification
  - Support
    - User support
    - Documentation and training
    - Usability and workflow
  - Continued development of the toolkit
    - MPP capabilities and advanced architectures
  - Inverse problems and design

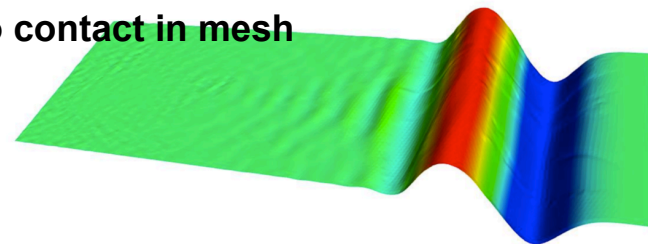
# Capabilities 1: High Velocity Contact

- **Automated contact is a core technology in Sierra**
  - Recent improvements use face-face contact algorithm to handle hypervelocity contact
    - Remedies well-known defects of node-face contact
    - Improves accuracy and performance in remeshing

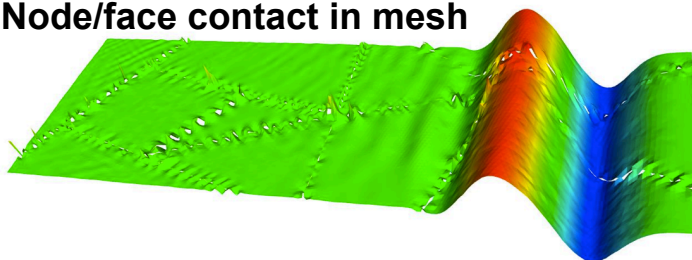
Exact solution for axial wave propagation after two bounces off support



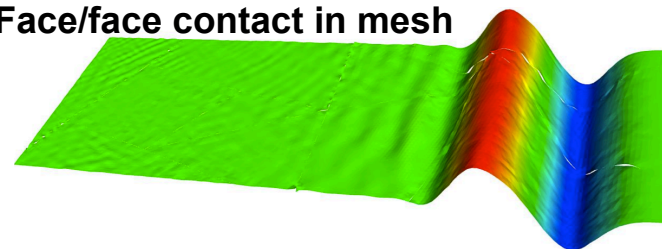
No contact in mesh



Node/face contact in mesh

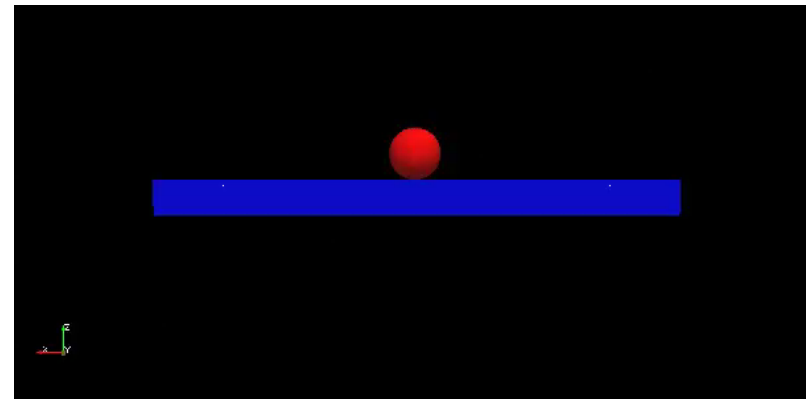
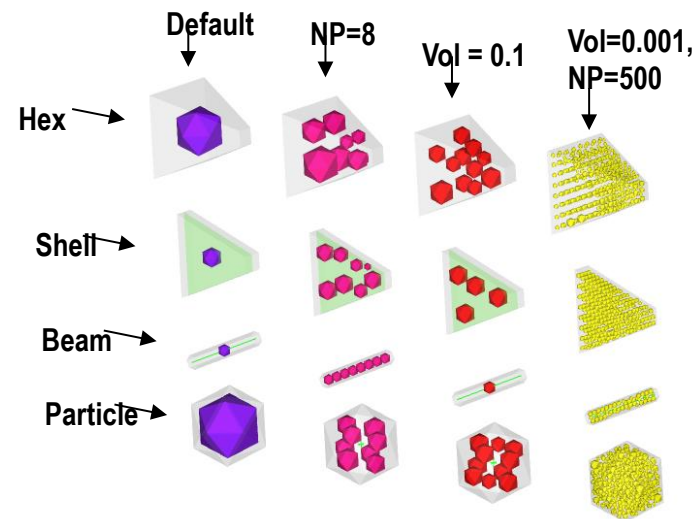


Face/face contact in mesh

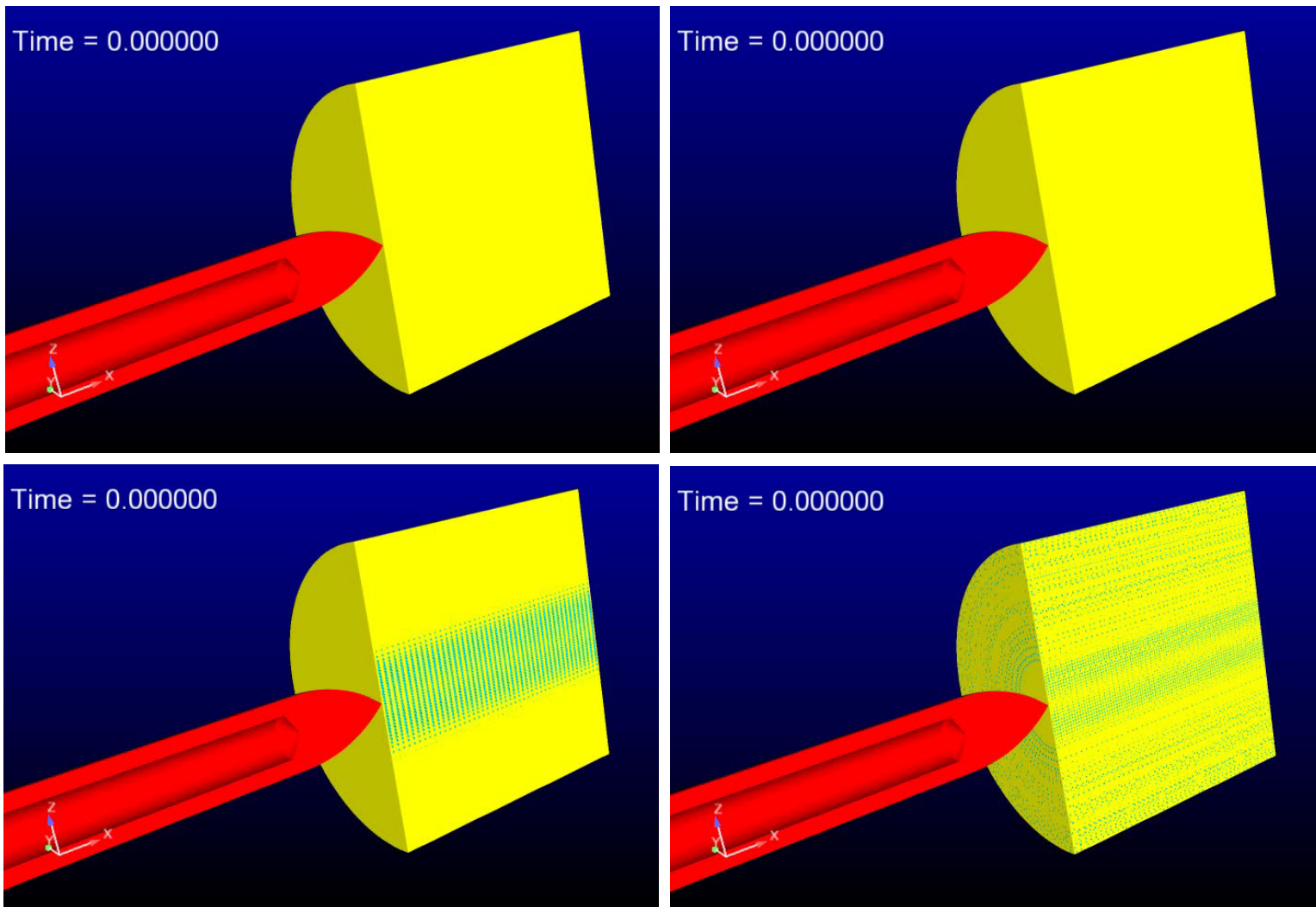


## Capabilities 2: Element/Particle Conversion

- **Ability to convert element to arbitrary number of particles**
  - Used with all element types
- **Ability to embed particles into initial solid mesh instead of creating via element death**
- **SPH mechanics applied after particle conversion**
  - For example, convert to SPH upon element death
- **Key tasks remaining:**
  - Combine EOS & remeshing
  - Develop analysis guidelines



## Capabilities 2: Element/Particle Conversion



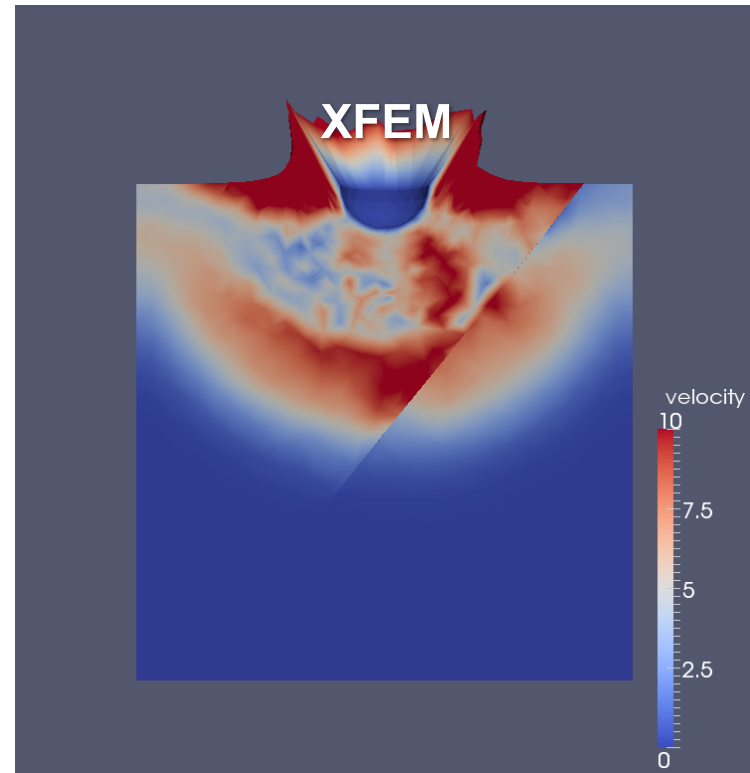
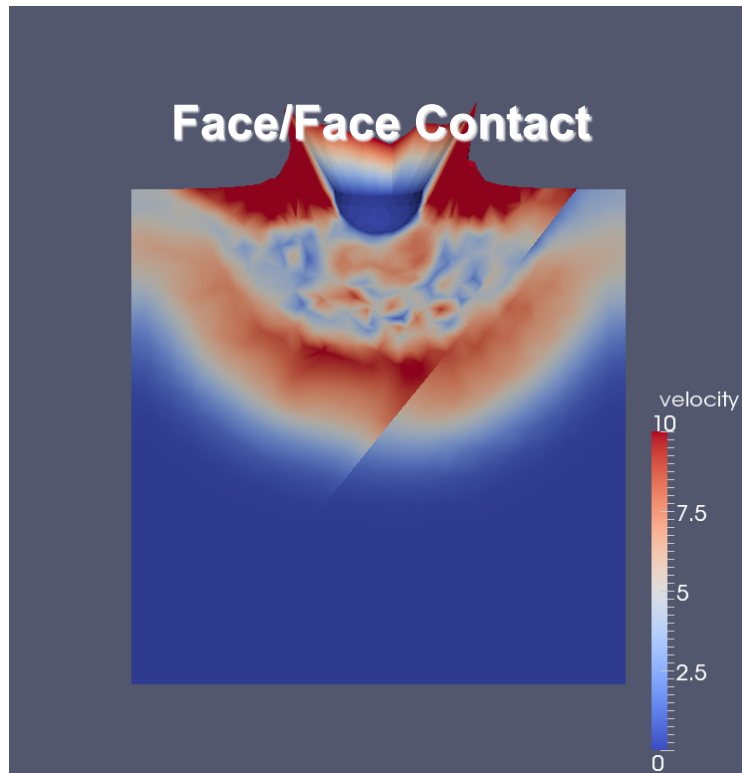


## Capabilities 3: Extended FEM (XFEM)

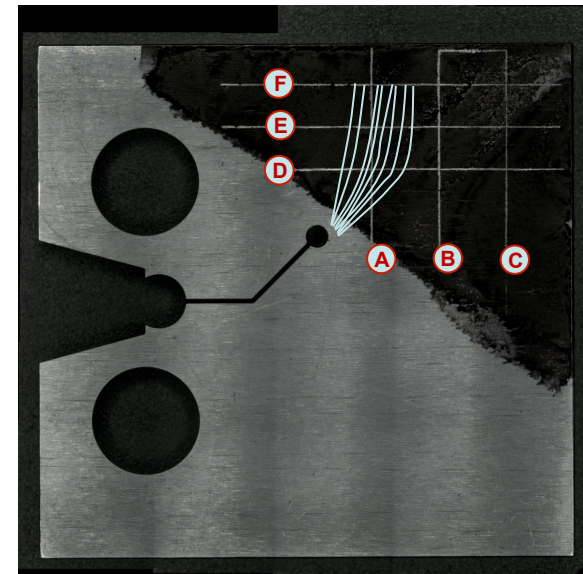
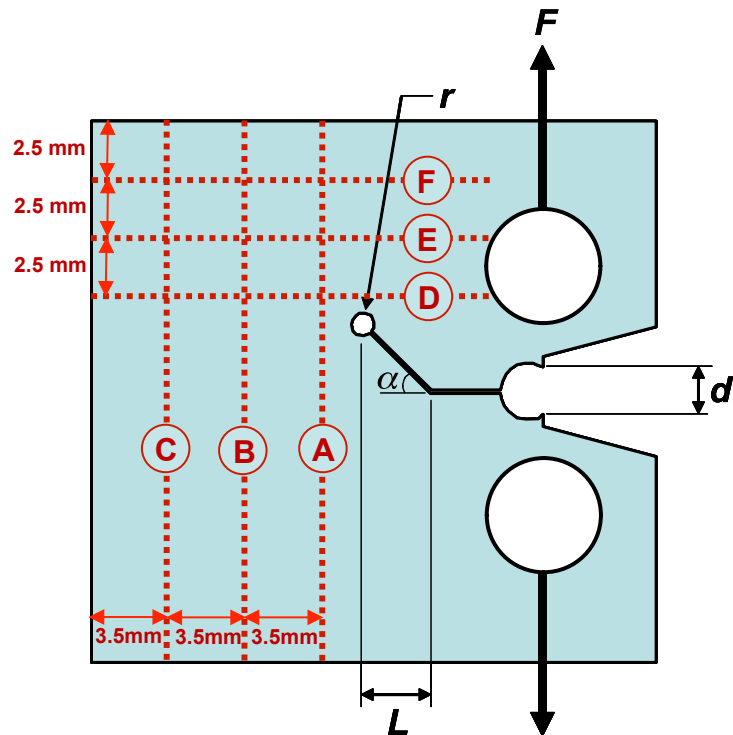
- **XFEM supports discrete localization within elems**
  - Remedies one of the few weaknesses of FEM
  - Supports physics-based crack propagation
  - Permits creation of cohesive zones on interfaces
  - Allows contact between faces of interfaces
- **Remaining work:**
  - Crack initiation capabilities
  - Improvements in crack propagation strategies
  - Implicit solves (currently explicit dynamics only)
  - Improve scalability on MPP architectures

## Capabilities 3: XFEM Results

- XFEM used to model frictional contact on arbitrary joint within blast-loaded geologic material



# Activities: Ductile Fracture X-Prize

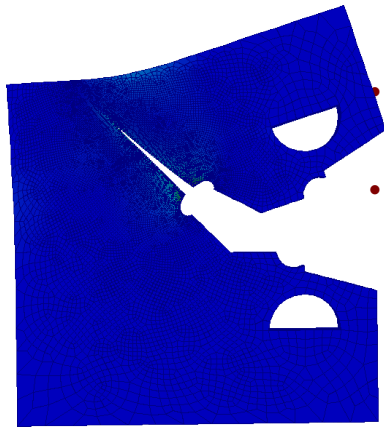


Experimental crack paths

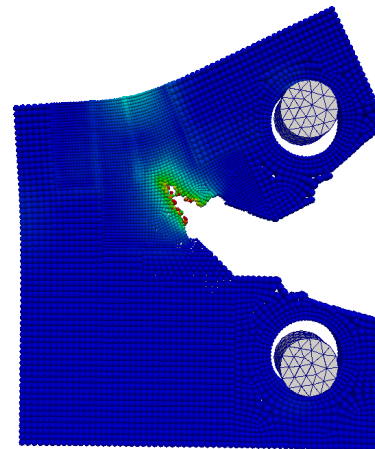
- Quasistatic loading, displacement control
- Predict crack trajectory,  $F$  &  $d$  at times when lines are crossed

# Activities: Sierra-Based X-Prize Entries

## Localization Elements



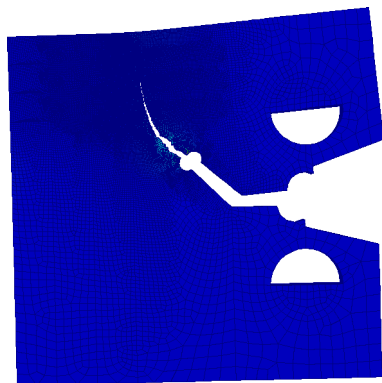
- Interface elements placed in mesh *a priori*
- 3 potential crack paths competed against each other to determine most likely path



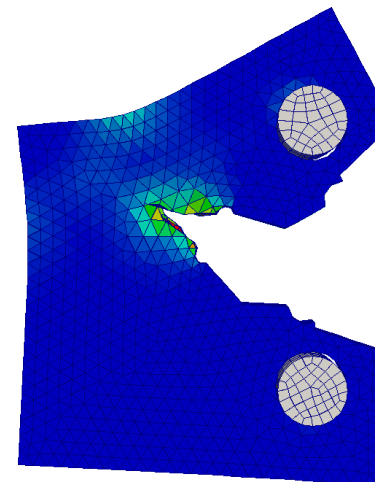
## Peridynamics

- Elastic-plastic continuum material used
- Bonds broken based on critical stretch
- Pins modeled with finite elements, interact with peridynamics via contact

## Element Death



- Elastic-plastic material with triaxial-based tearing parameter to determine failure
- Elements killed when failure criterion reached
- Used implicit solver with limited number of failed elements per iteration

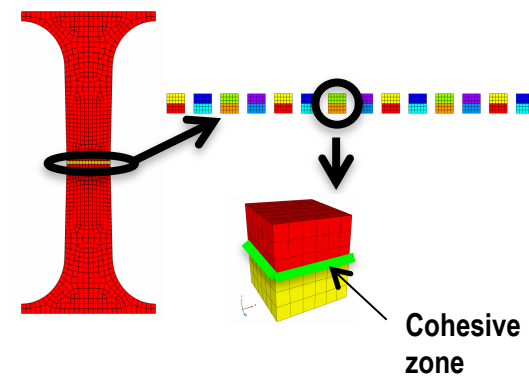
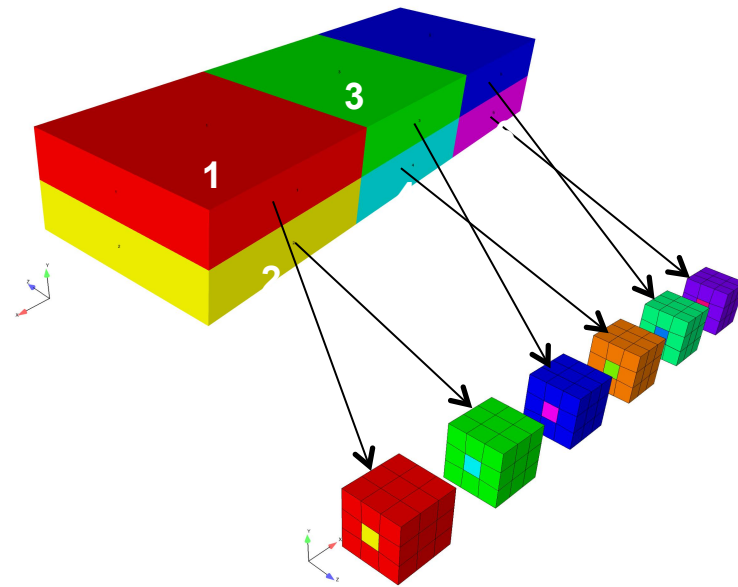


## XFEM

- XFEM in Sierra is still in development stage. This is one of first applications
- Elastic-plastic continuum material used, no cohesive zone law
- Coarse elements used for time step and because of crack tangling

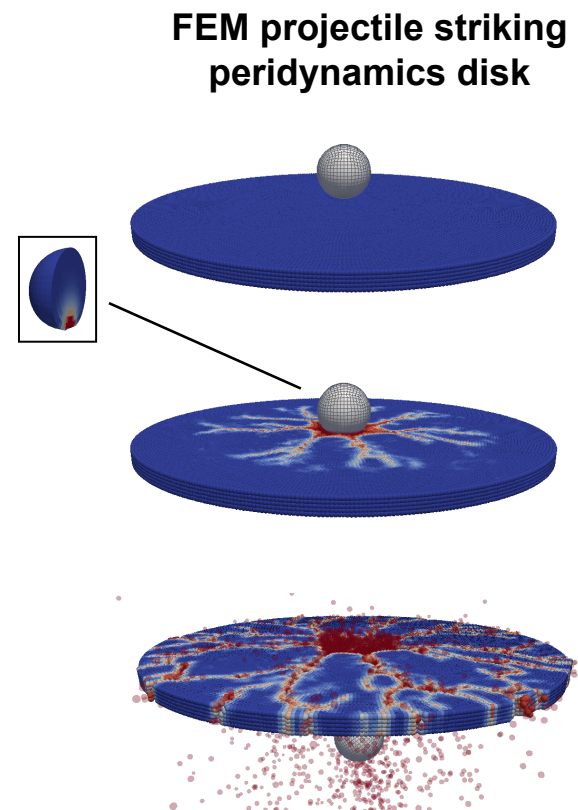
## Capabilities 4: RVE (Rep Vol Elems)

- **What are RVE's?**
  - Material microstructure
- **Work done to date:**
  - Testing and usability additions to RVE capability
  - Capacity for RVE meshes to be utilized without matching boundaries
  - Cohesive zones located within RVE mesh
- **Remaining work:**
  - Scalability improvements
  - Testing



## Capabilities 5: Peridynamics

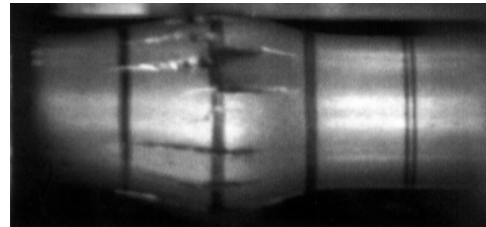
- **A nonlocal continuum mechanics**
  - Well-suited for modeling fracture
- **Initial implementation in Sierra**
  - Access to material models
  - Contact with finite elements
  - Bond slicing with mesh faces
- **Remaining work:**
  - Equation of state models
  - Implicit time integration
  - Direct coupling with finite elements
  - Verification & Validation
- **Funding source: ASC Algorithms**



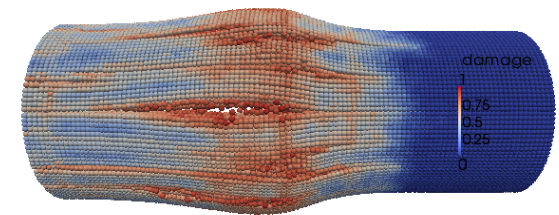
# Capabilities 5: Peridynamics Application

## Expanding Tube Experiment

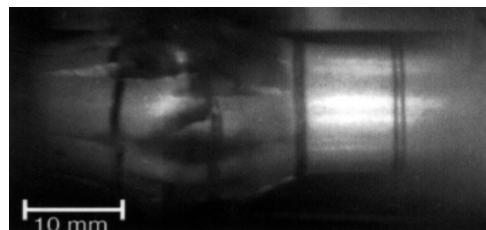
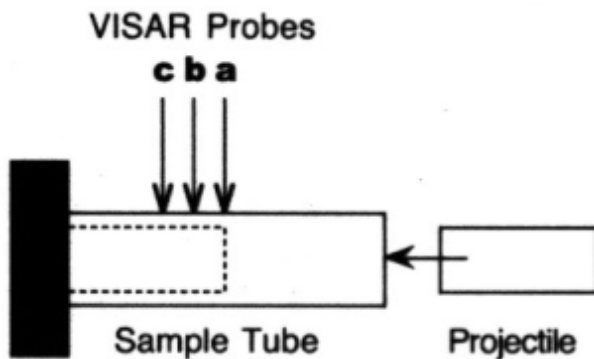
- **Lexan discs impact inside tube**
  - Discs modeled with finite elements
  - Johnson-Cook with EOS, failure
- **AerMet high strength steel tube**
  - Tubes modeled with peridynamics
  - Elastic-plastic with hardening
  - Bond failure on critical stretch



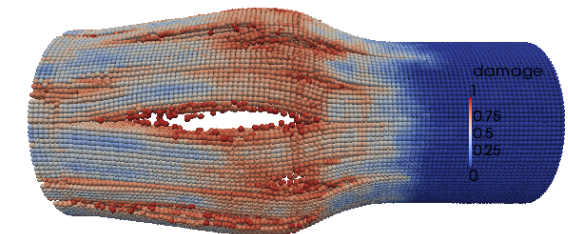
Experimental image  
[Vogler et. Al]



Simulation  
15.4 microseconds



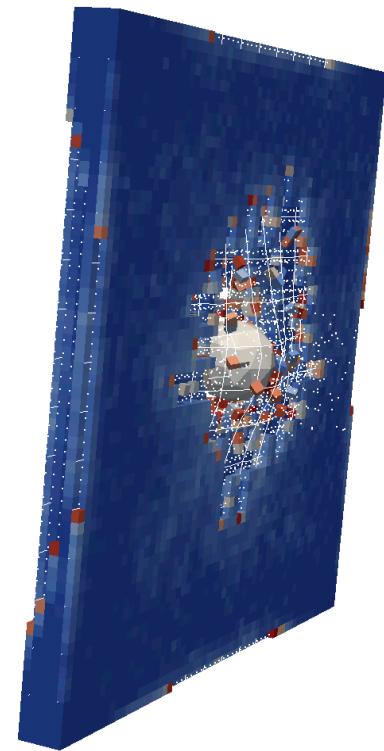
Experimental image  
[Vogler et. Al]



Simulation  
23.4 microseconds

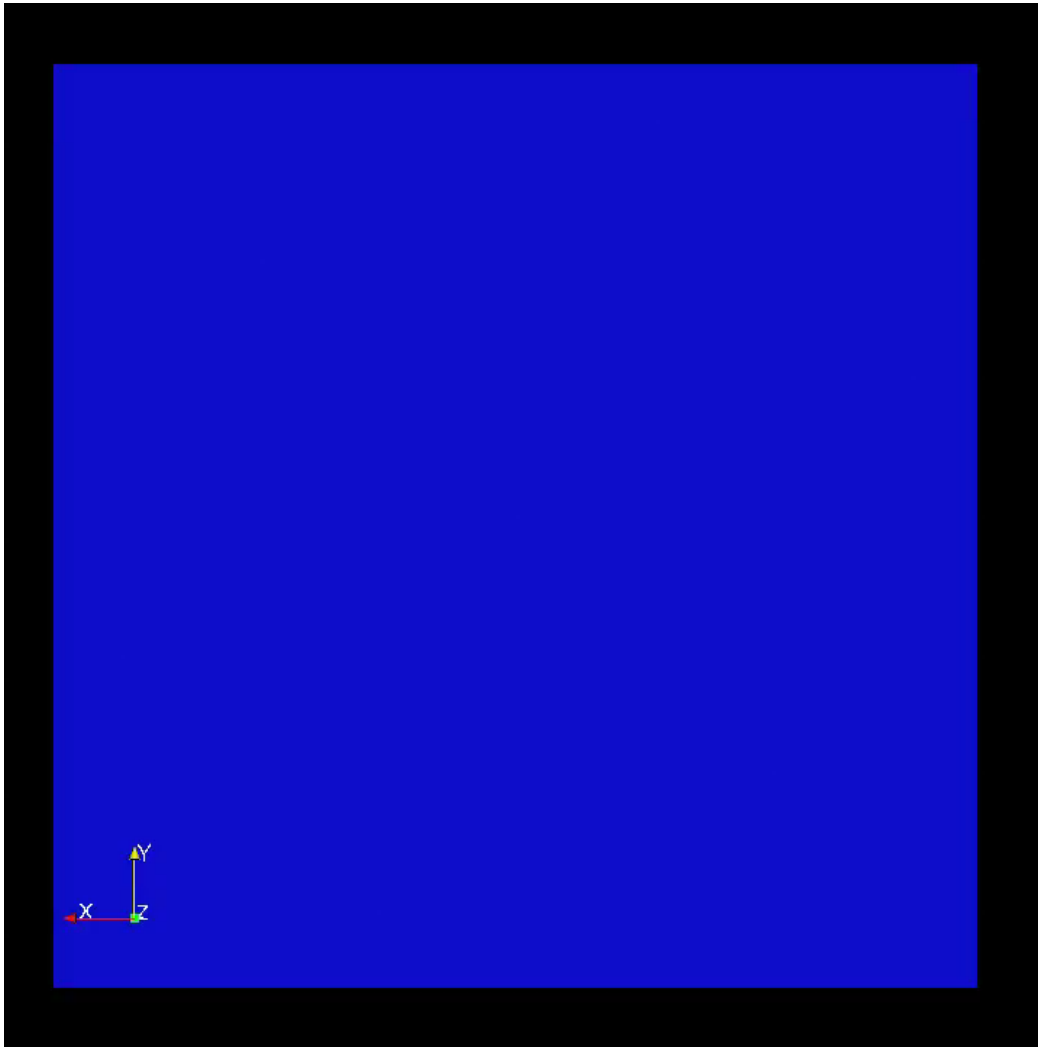
## Capabilities 6: Reinforced Concrete

- **Have developed robust modeling techniques for analysis of reinforced concrete structures of import to DoD**
- **Use K&C and other models (Epic, kayenta)**
- **Model reinforcing steel with embedded truss elements, which yields “exact” FE results**
- **Generate MPCs for composite response**
- **Work now in progress:**
  - Implicit solvers for progressive collapse
  - Test other candidate constitutive models
  - Analysis guidelines (theory and practice)



**RC plate/ball  
impact simulation**

## Capabilities 6: Reinforced Concrete



**Examine results  
from rear (spall)  
side of RC plate**

**Note localization of  
concrete damage  
into rotating blocks:  
this is how  
reinforced concrete  
fails under  
transverse load**

**Rebar elements not  
visible, but they help  
determine whether  
perforation occurs**



## Capabilities 7: Code Coupling

- **Proposed Exploratory R&D Effort**
  - Couple CTH and Sierra via Fortissimo code
  - One-way fluid-solid coupling technique
- **Results from coupled code effort**
  - Underpredicts pressures and displacements
  - Unconservative result for analysis and design
- **Path forward**
  - Perform iterative coupling strategy (e.g., Zapotec)
  - This is key initiative for Sierra team in FY11
  - Goal: provide general fluid-structure interaction capabilities for wide range of customer needs