SAND2009-6962C

CTH and ALEGRA: Sandia Shock Physics Software

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Sandia National Laboratories

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL84000.

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Current State of Shock Physics Analysis Codes

- Shock physics analysis packages are mature
  - under development since ~1945
  - widely used for the simulation of complex high strain rate, large deformation, strong shock continuum mechanics
  - widely used in the defense industries, NASA, DoD, and DOE laboratories.
- Numerical techniques are relatively stable
- Codes compare favorably to many experimental datasets
  - When we understand how material behaves, we can accurately predict the material deformation.
  - An understanding of material behavior is critical to being able to predict any material characteristic.

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Numerical Techniques

- Most hydrocodes solve the conservation equations of mass, momentum, and energy using explicit time stepping.
- Solution methods fall into two groups.
  - Lagrangian - mesh moves with material (Presto)
  - Eulerian - mesh fixed in space (CTH)
- ALE (Arbitrary Lagrangian-Eulerian) methods combine characteristics of both Lagrangian and Eulerian, generally more similar to Lagrangian (ALEGRA)
- SPH (Smooth Particle Hydrodynamics) methods are Lagrangian based without mesh restrictions
- Both Eulerian and Lagrangian methods have pluses and minuses and have significant quirks depending on the specific code.

The constant debate: Eulerian vs. Lagrangian

Eulerian Methods – "An approximate solution to an exact problem"

Lagrangian Methods – "An exact solution to an approximate problem"

…as paraphrased from Gordon Johnson, Alliant Tech Systems, the developer of the EPIC series of codes.

Verification and Validation (V & V)

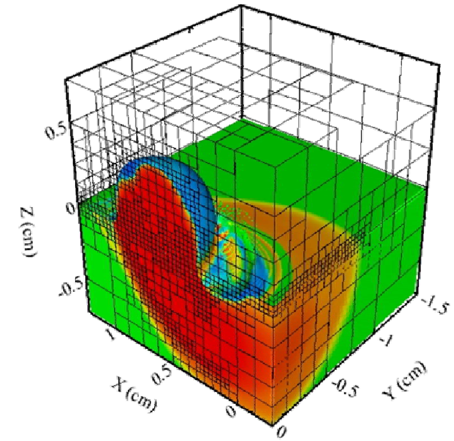
- **Code comparisons with analytical or experimental data critical to developing confidence in solution accuracy**
- **Shock physics codes are solving nonlinear phenomenology**
  - **discontinuous behavior (shocks, phase transitions, fracture)**
- **Wide ranging parameter space**
  - **many orders of magnitude in strain rate**
  - **solid, liquid, vapor, plasma, reaction chemistry**
- **Incumbent on the analyst to perform V&V in their regime of interest.**
  - **Don’t rely on assertions by others!**

Sandia's Shock Physics Simulation Codes

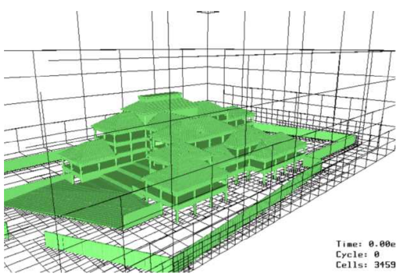
- CTH
  - Eulerian shock physics code
- ALEGRA
  - Arbitrary Lagrangian Eulerian shock physics code
- Presto (part of Sierra)
  - Lagrangian transient solid dynamics with some shock capabilities
  - ongoing effort to expand shock capabilities
- Fortissimo (part of Sierra)
  - Presto coupled with CTH

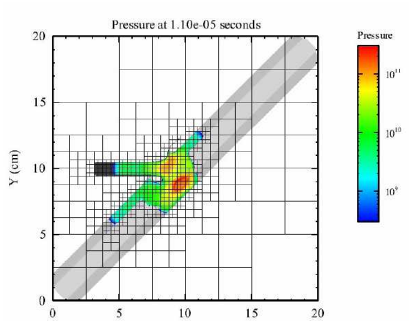
CTH Overview

CTH is a massively-parallel Eulerian shock-physics code.



- Eulerian shock wave physics computer code solving conservation equations of mass, momentum, & energy for up to 20 materials including gases, fluids, solids, & reactive materials
  - **Analytic & Tabular Equation-of-State representations**
  - **Advanced Strength & Fracture models**
  - **Adaptive Mesh Refinement**
- Applications (partial list):
  - **National Missile Defense (NMD), Nuclear Emergency Response (NEST), Weapon effects & vulnerability**
  - **Armor, Anti-Armor, Munitions Design, Blast Effects**
- CTH licensed to hundreds of external DOE & DoD agencies and their subcontractors
  - **300-1000 users**



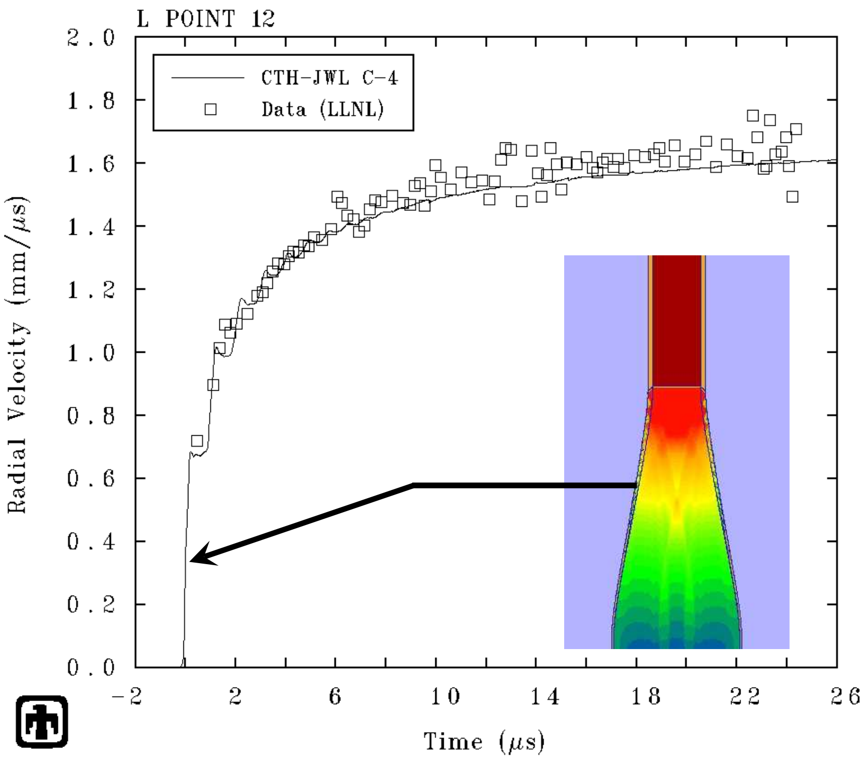


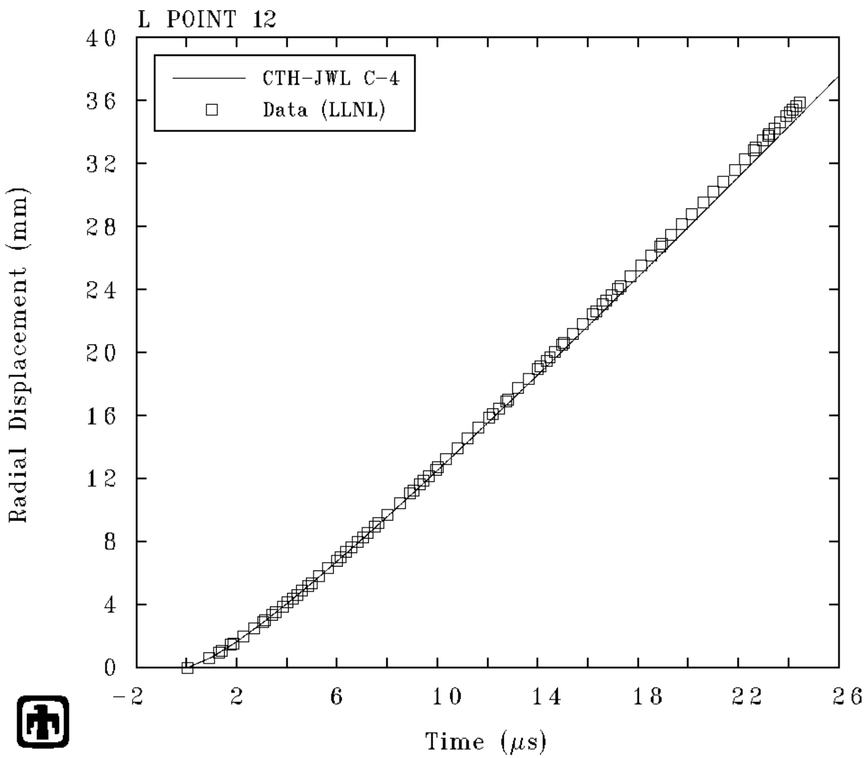
Examples to Illustrate CTH Capabilities

- Cylinder test to evaluate explosive model accuracy (Kipp)
- Research into non-ideal explosive behavior (Baer)
- Mesoscale studies of hotspot mechanisms in explosives (Brundage)
- Cylinder fragmentation (Kipp)
- Modern composite material models (Schumacher)

C-4 Explosive / Copper Cylinder Test

- Copper tube filled with explosive, initiated at one end
- Compare calculation with velocity and displacement data for expanding copper surface





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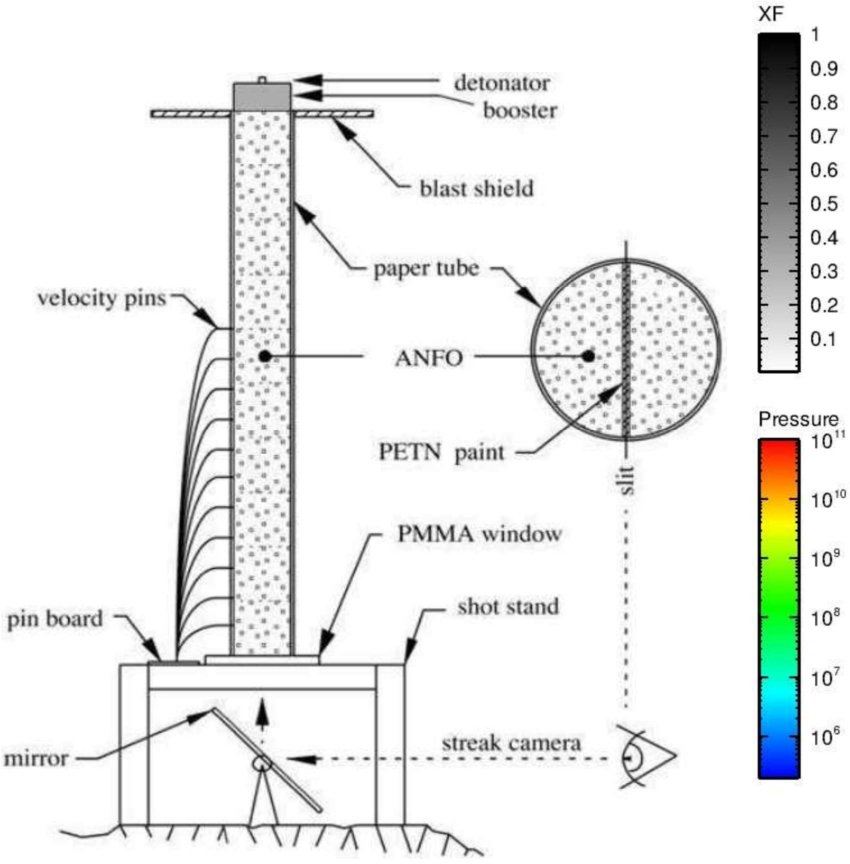
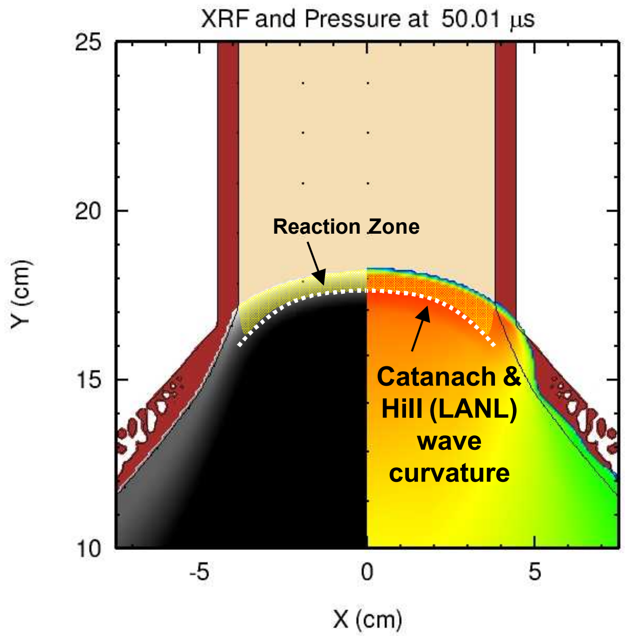
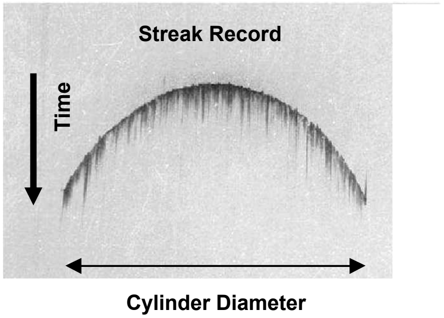
Research on Non-Ideal Explosives

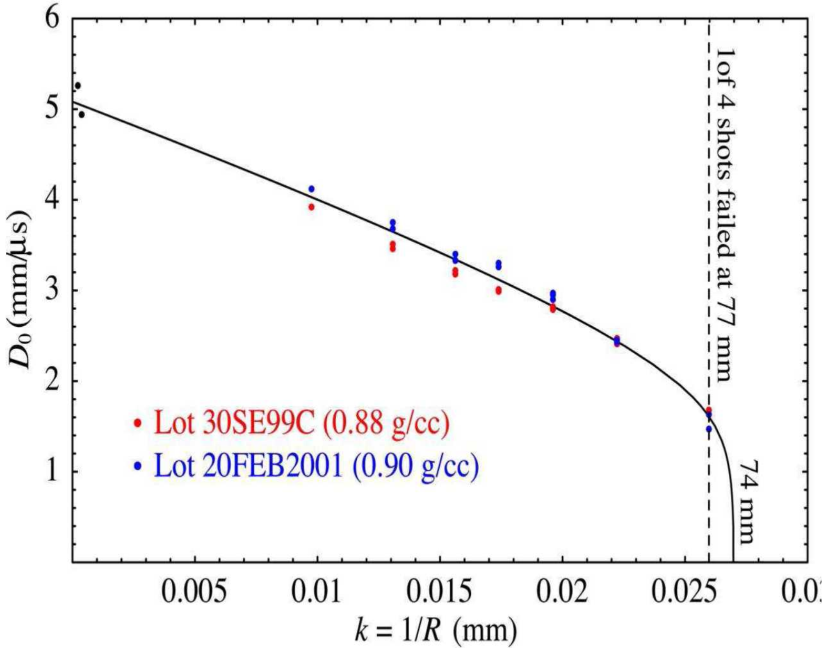


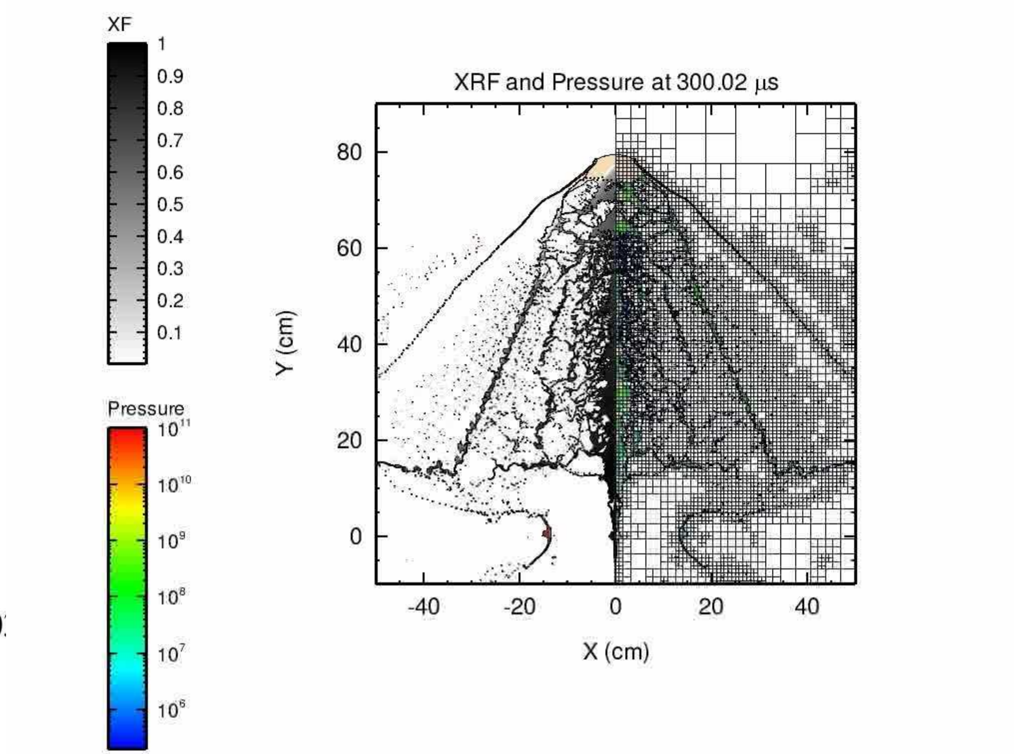




- Partition of energy release to support shock vs. reaction in the expansion region
- Multistep chemistry behavior can be represented using a simplified global model

Research on Non-Ideal Explosives (cont.)





- Detonation failure behavior is replicated
- Model framework in place – improved EOS and chemistry inputs
- Application to other non-ideal materials

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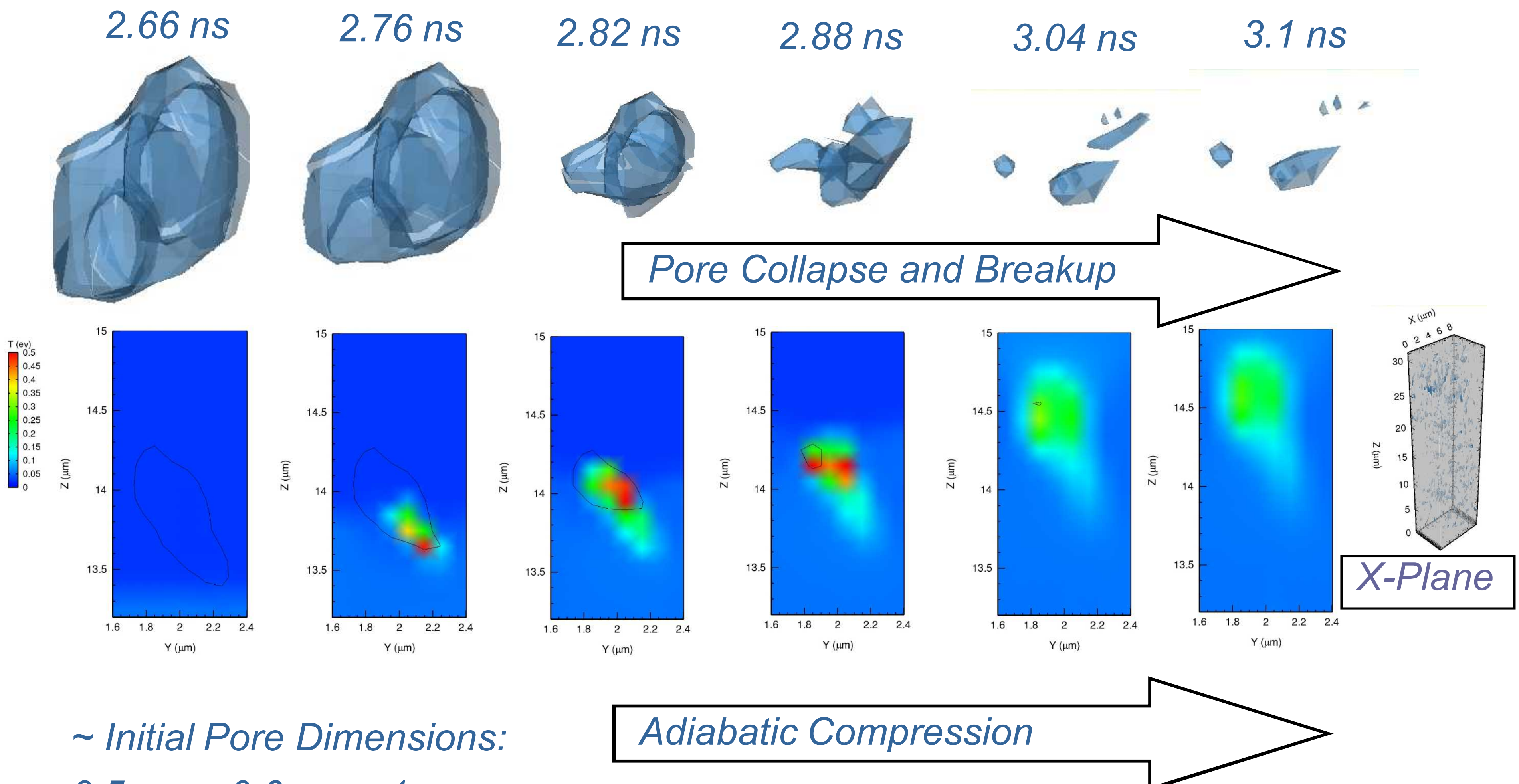
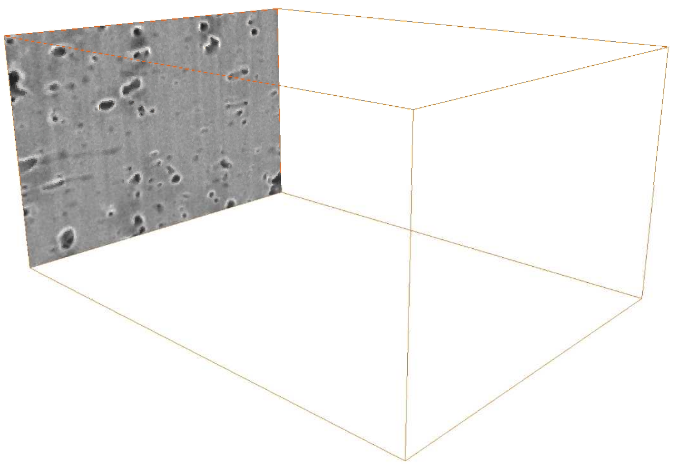
Mesoscale Studies of Hotspot Mechanisms in Explosives (e.g. HNS)



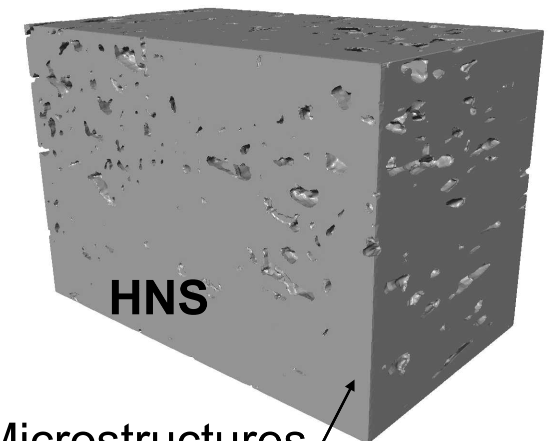
~ Initial Pore Dimensions:

0.5 μm x 0.6 μm x 1 μm

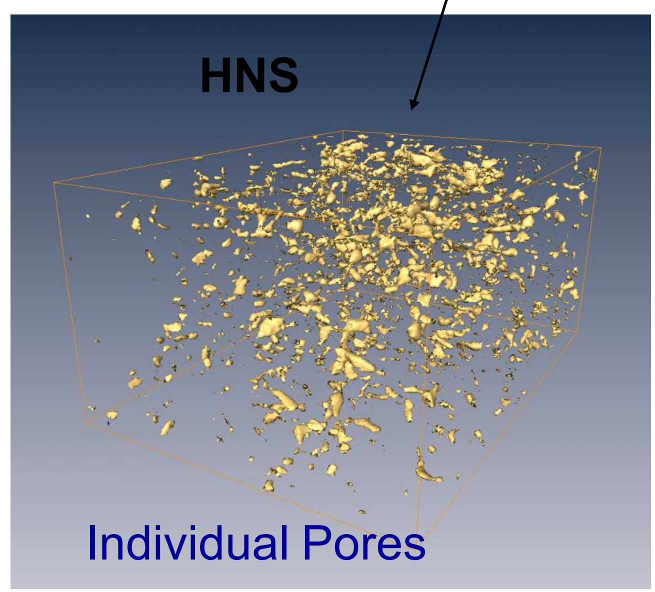
FIB/SEM nanotomography: 3D microstructures

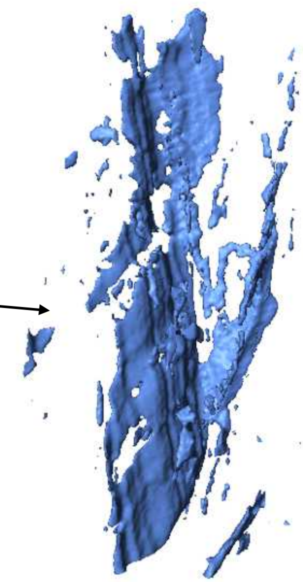


Stack up of 2D SEM Images



3D Microstructures





PETN

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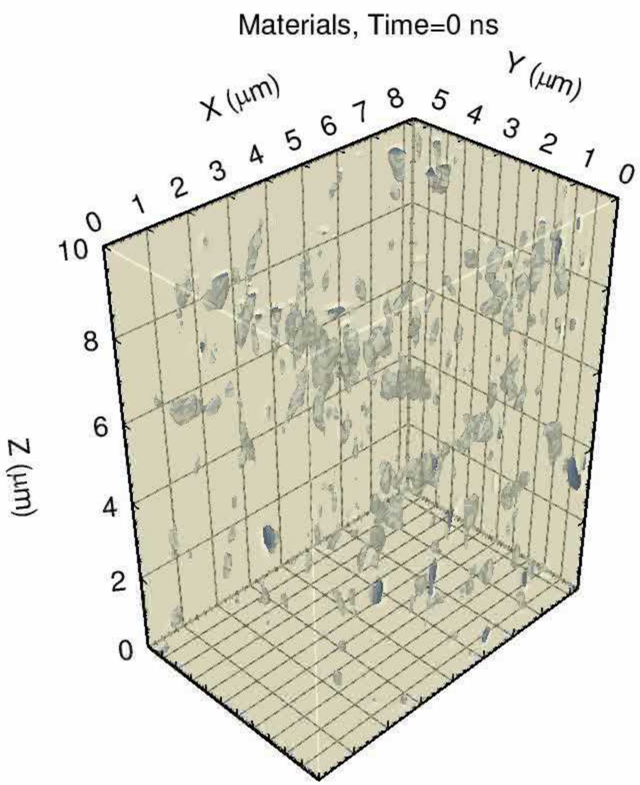
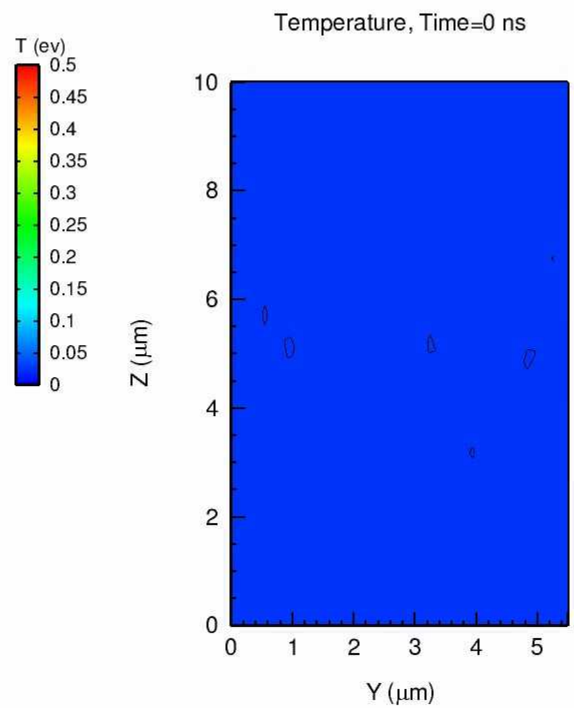
Mesoscale Studies of Hotspot Mechanisms in Explosives (cont.)





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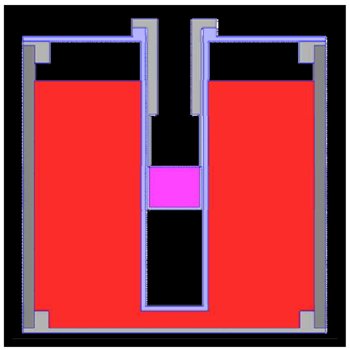
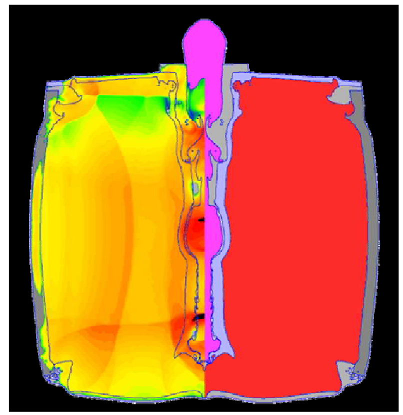
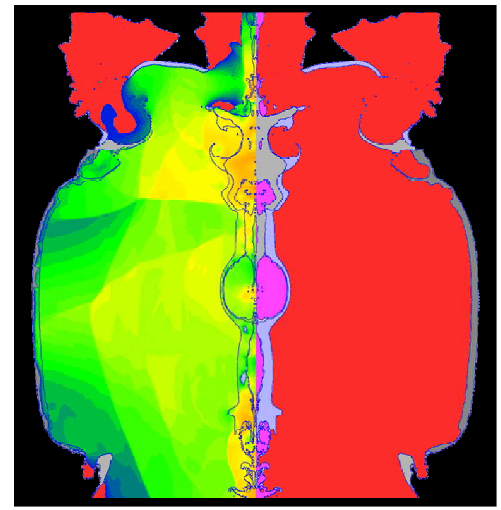
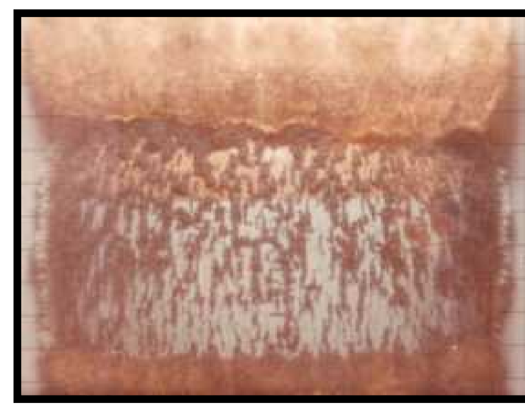
Explosive Cylinder Tests (NSWC - Dahlgren)

Aermet 100 Steel









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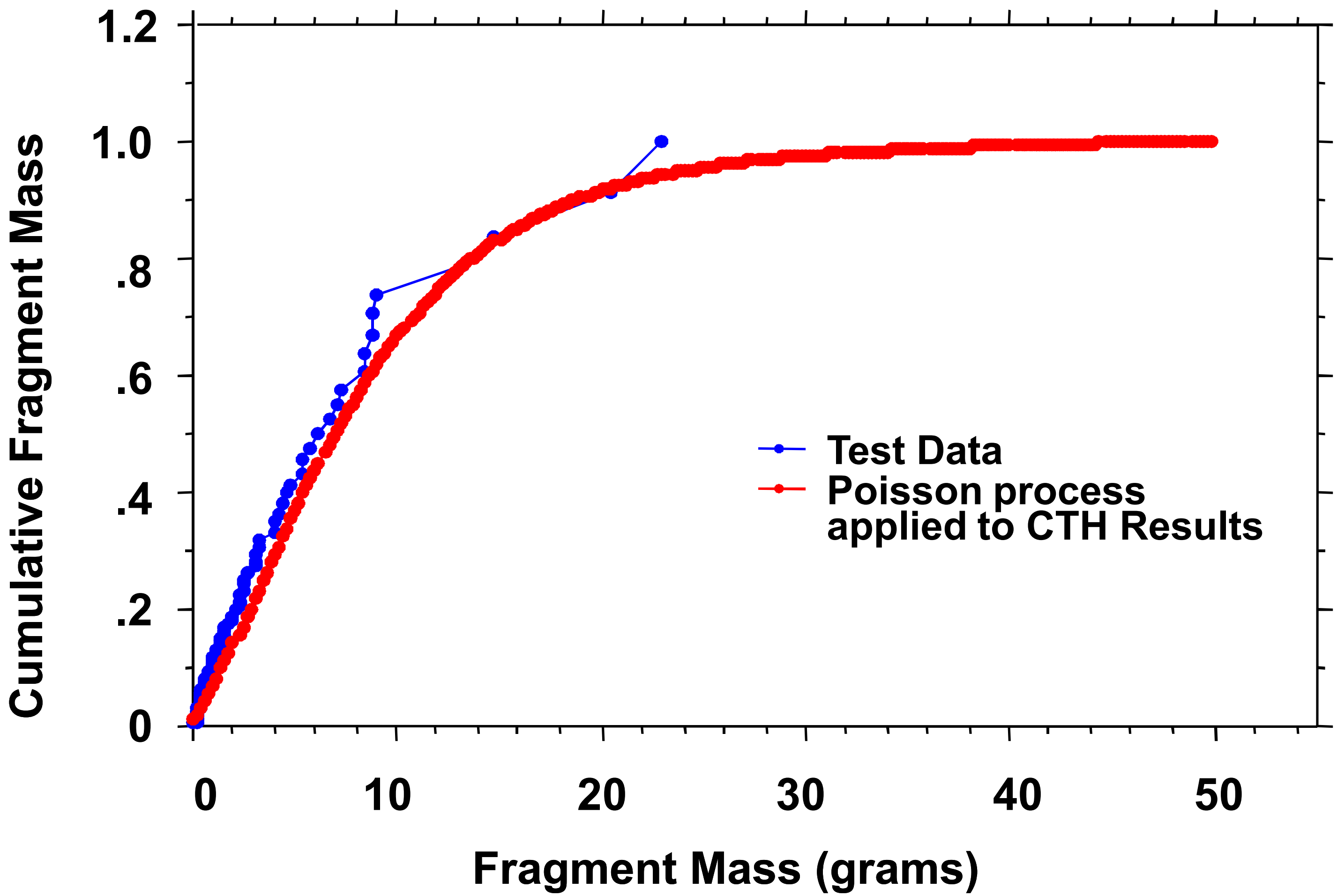
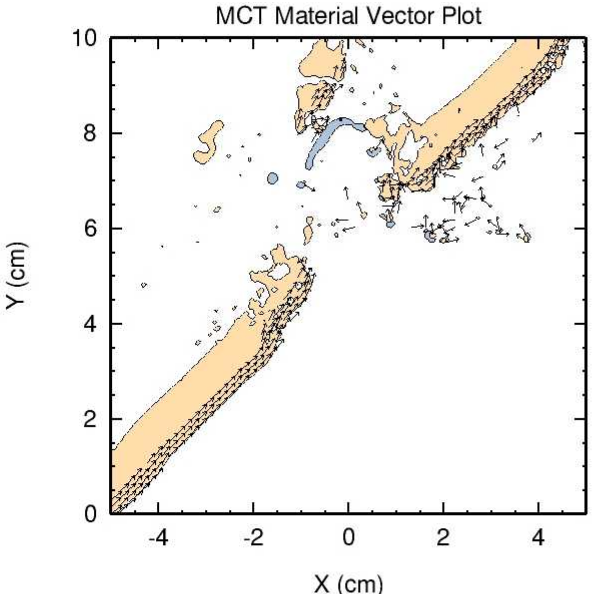
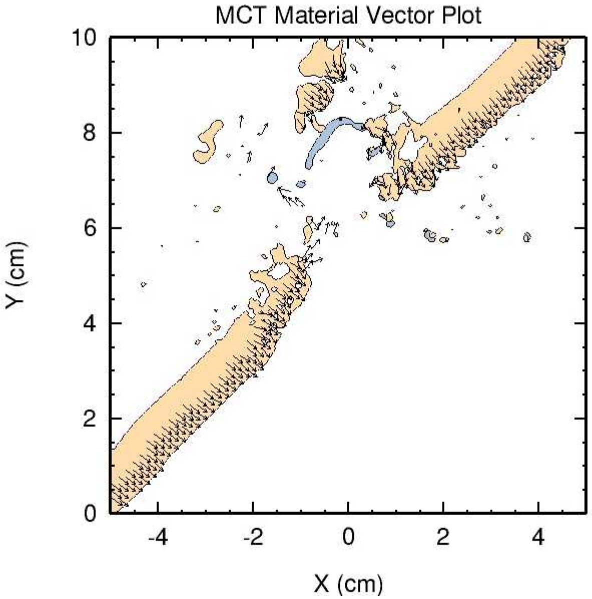
CTH / Data Fragment Distribution

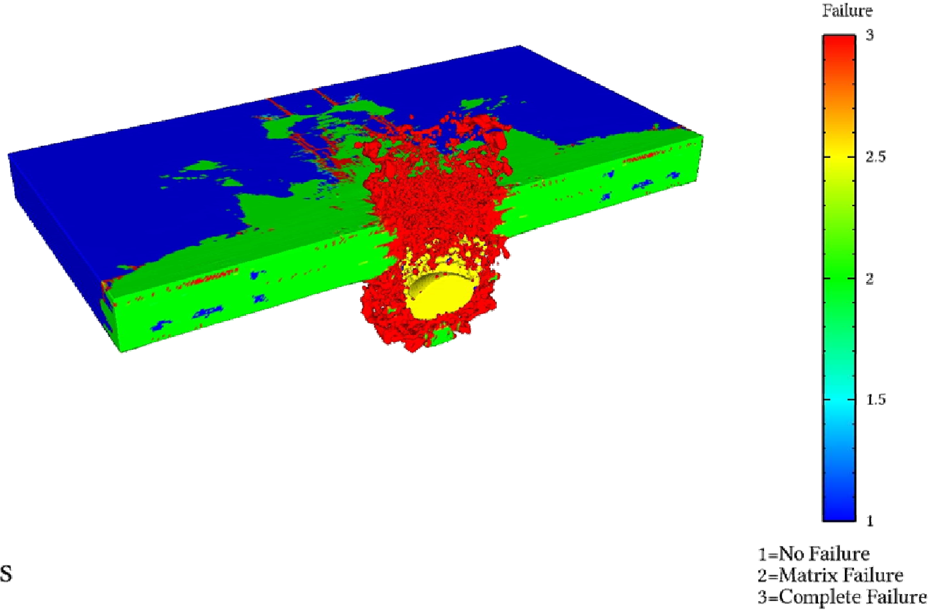


Modern Composite Material Models in an Eulerian Hydrocode





CTH Analysis of a Directional 8 lamina Composite
Impacted by a Copper Sphere at 1 km/s



Time = 24.51 μs

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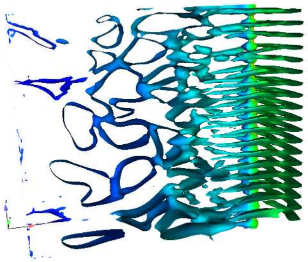
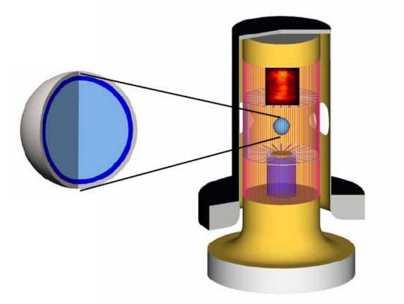
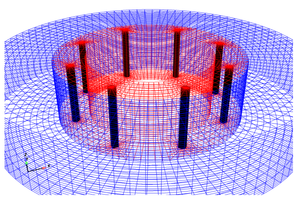
ALEGRA Overview





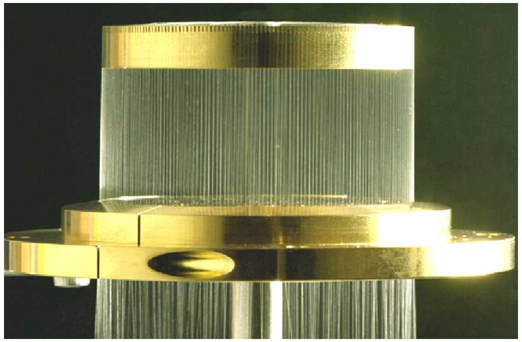


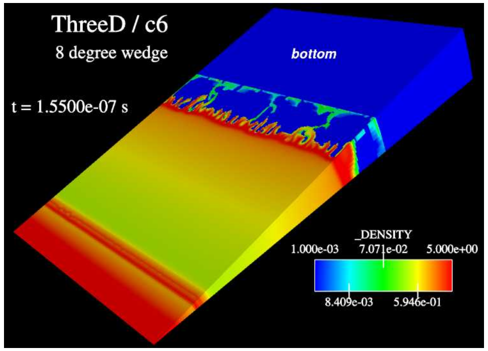
ALEGRA models shock and high energy environments for solids, fluids and plasmas using a multi-material arbitrary Lagrangian-Eulerian (ALE) multi-physics methodology designed for use on massively-parallel platforms.

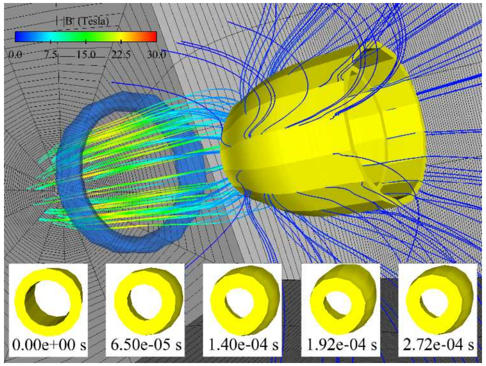
Current MHD Applications:

- **Z-pinch**
- **ICE/Magnetic Flyers**
- **Electromagnetic Launch**

Z-Pinch

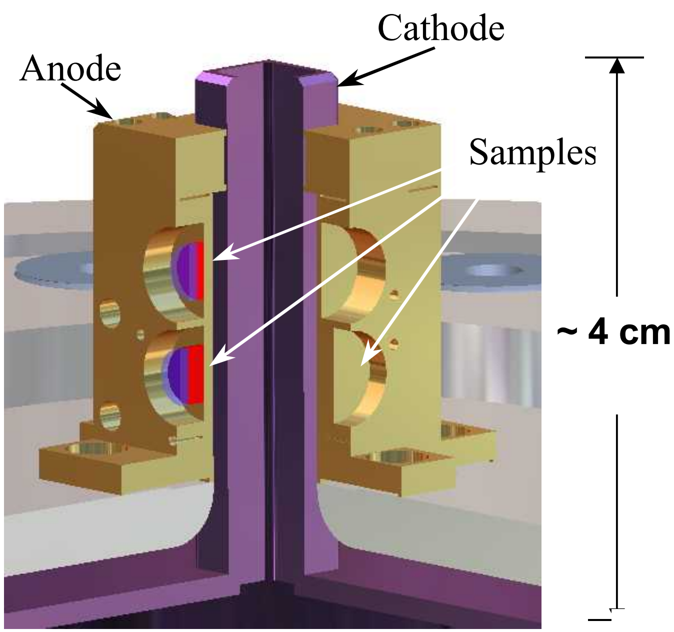


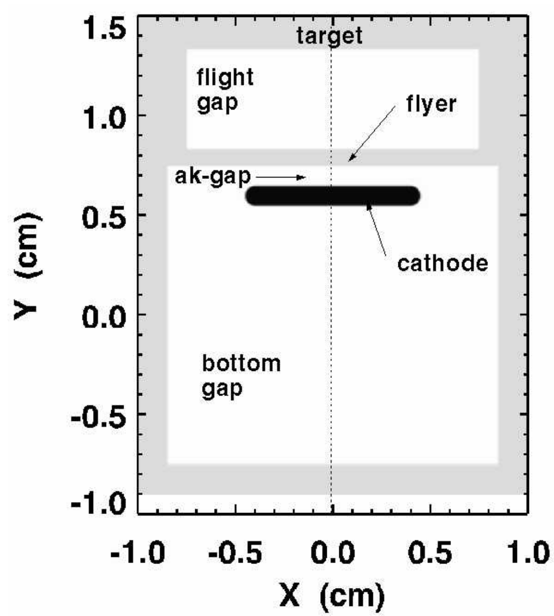


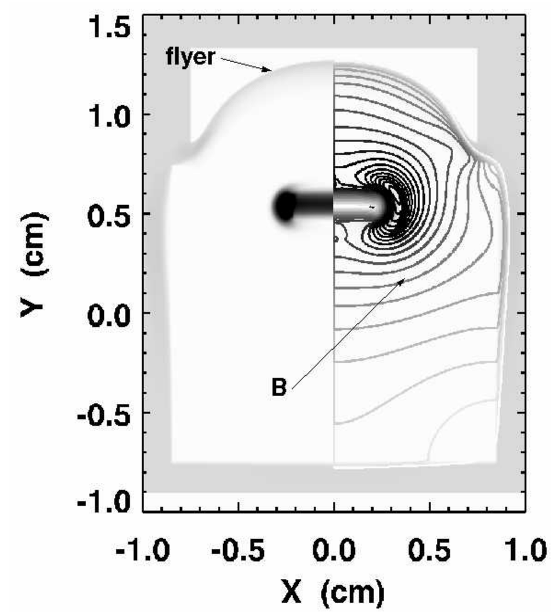


Electromagnetic Launch

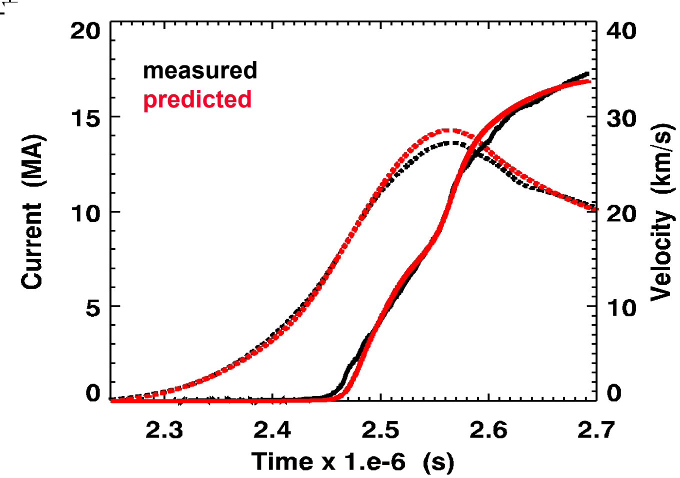
Predictive Capability
for Magnetically-Launched Flyers







Z-machine isentropic compression experiments (magnetic flyers)



Measured / predicted current & flyer velocity (850 μm Al)

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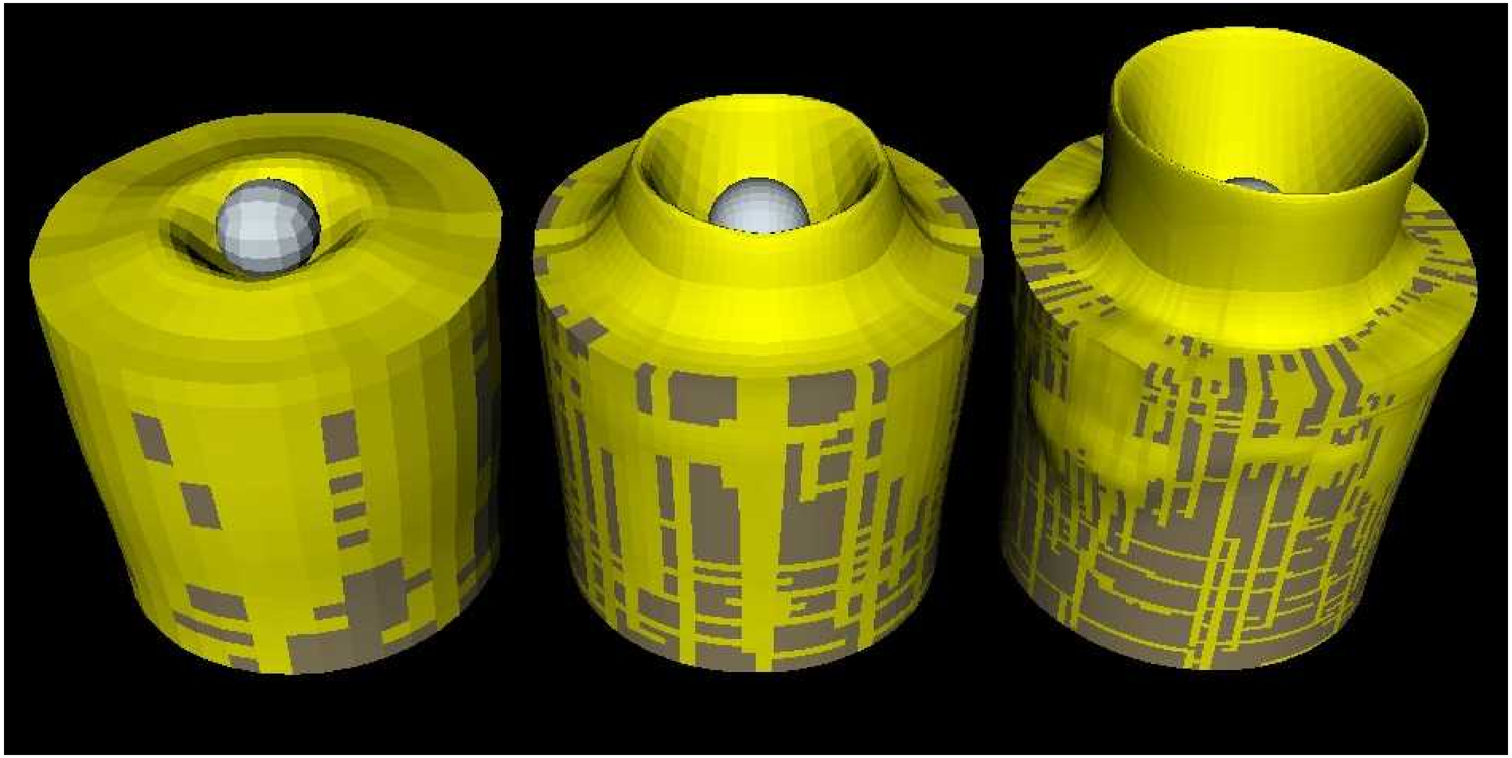
Ceramic Modeling: Addressing Mesh Dependence

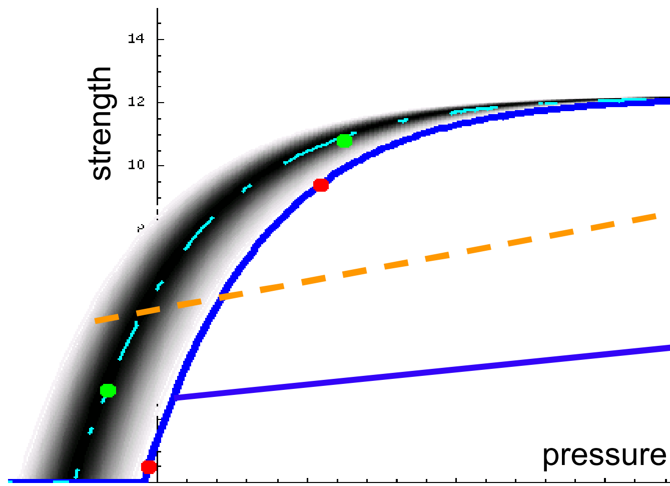
Ceramic mesh resolution studies – refinement to the right →

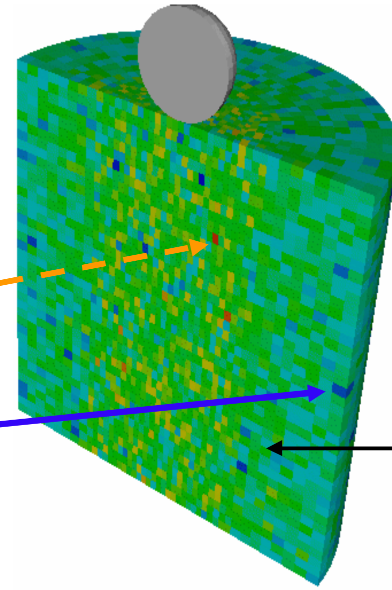


Dynamic Indentation of Silicon Carbide -- Sandia Model without Variability

Material Heterogeneity was Found to be Integral to Dynamic Failure

Spatially Variable Strength Profile for Ceramics

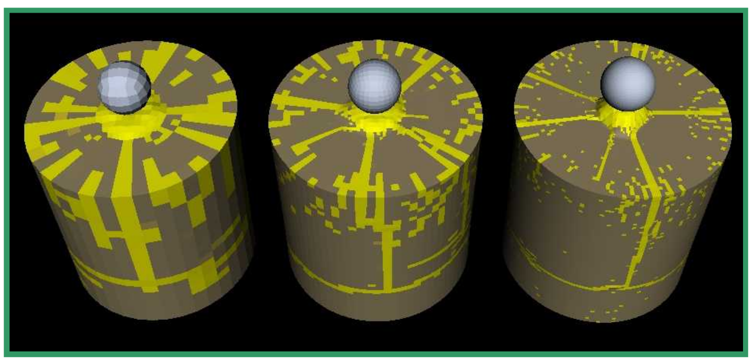




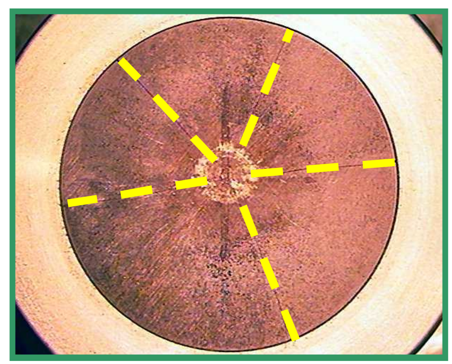
Initial state: small elements are stronger on average, but also more variable

Weibull distribution of strength*:

$$\sigma = \bar{\sigma}\left[\frac{\bar{V}\ln R}{V\ln(1/2)}\right]^{1/m}$$



Reduced Mesh Dependence: Same Model with Uncertainty, Size, and Rate Effects



Comparison to Experiment

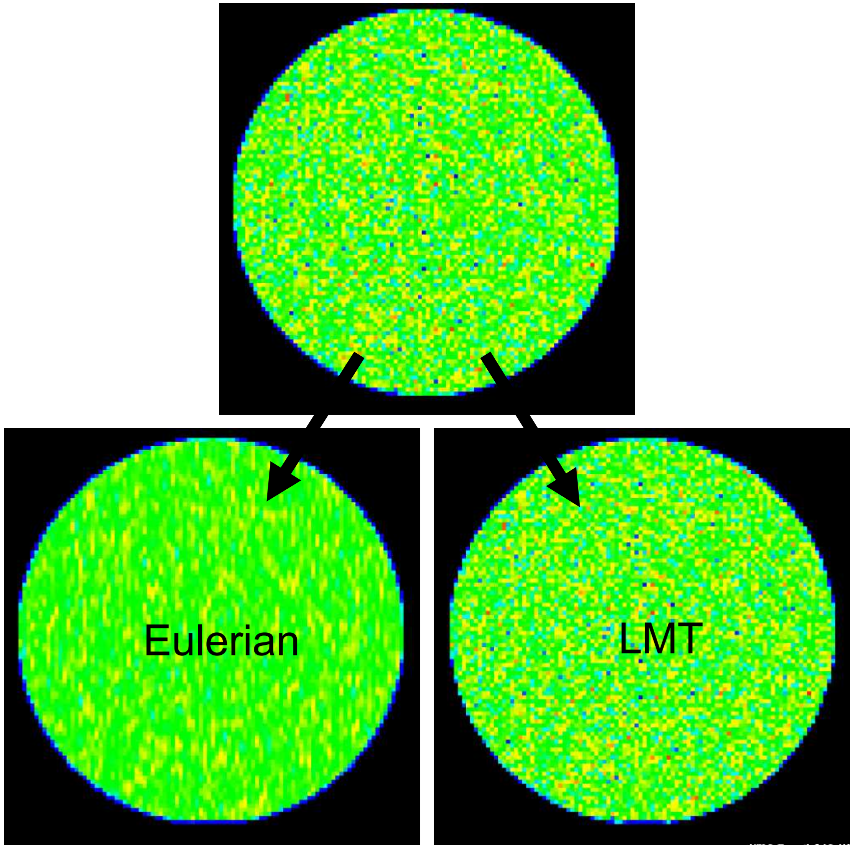
Similar crack morphology for different mesh sizes

Formal validation and uncertainty quantification will help identify remaining issues

*Brannon, RM, Wells, JM, and Strack, OE 'Validating Theories for Brittle Damage', Metallurgical and Materials Transactions A, 38A, p. 2861-8, 2007

Eulerian Codes Need Enhancements to Support Heterogeneity

Initial State



After Remap

Heterogeneous Cylinder Dropping Vertically

Lagrangian Material Tracking (LMT):*

- Standard Eulerian momentum solver (in contrast to other particle methods)
- Variable material properties reside on Lagrangian tracers
- Dramatic improvement in preservation of properties

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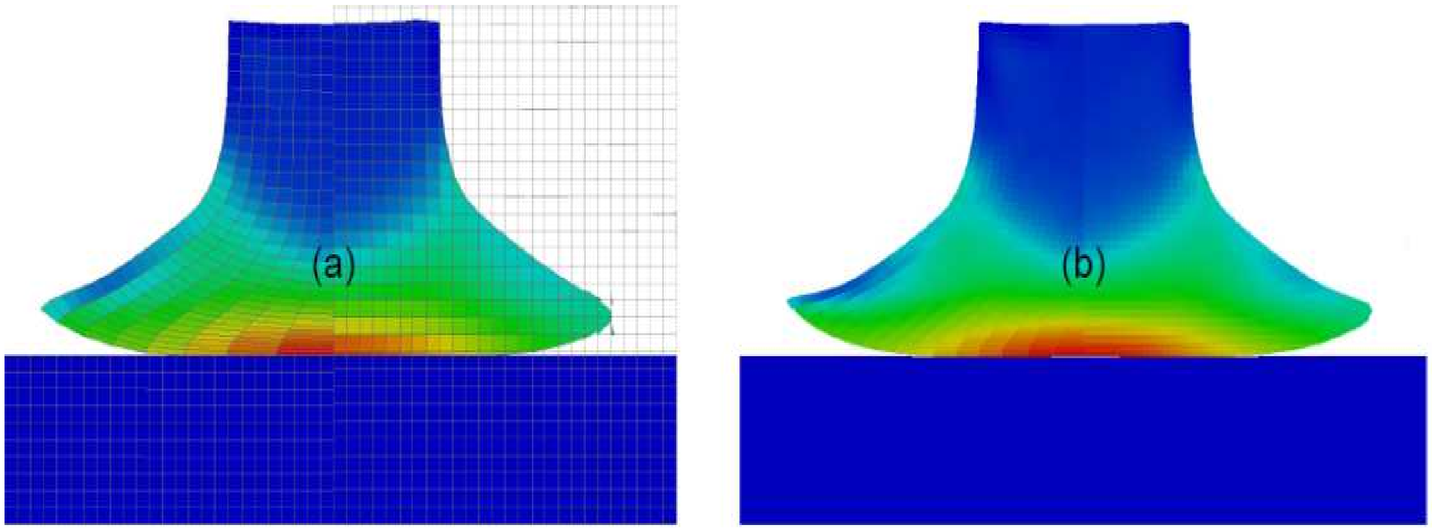
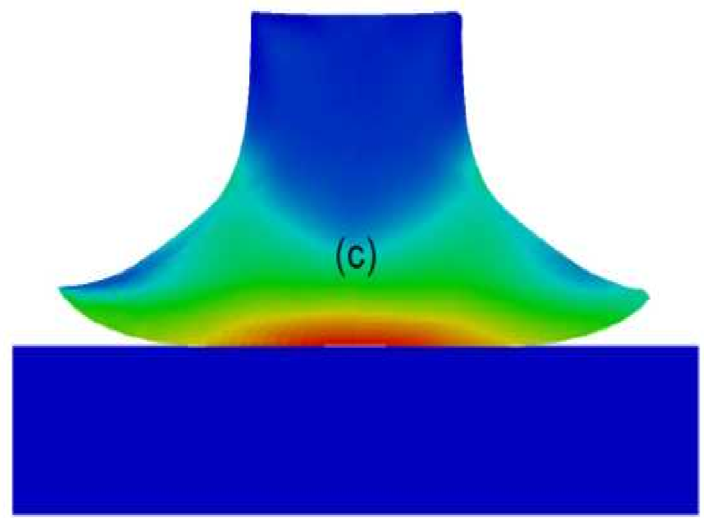
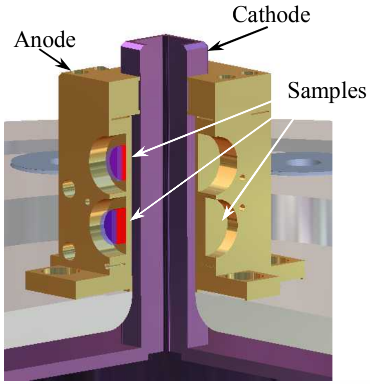
Eulerian XFEM is a Promising New Method

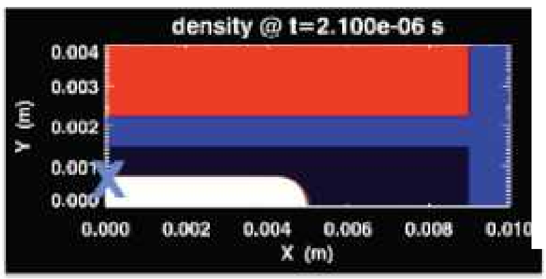


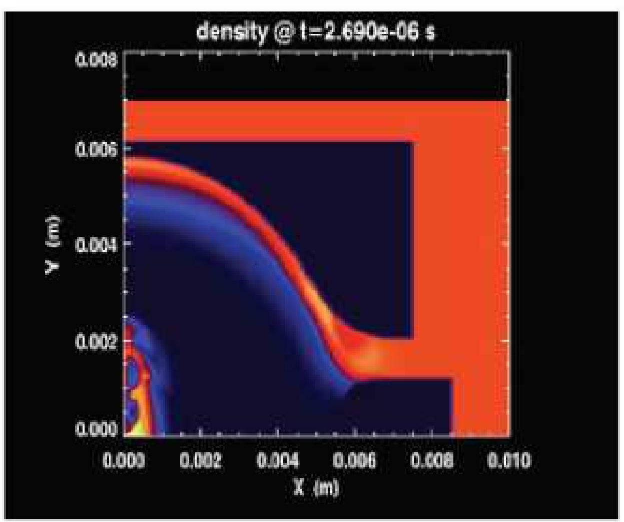
EQPS on (a) coarse (b) medium and (c) ifi ne meshes. Lagrangian (left) and X-FEM Eulerian (right).

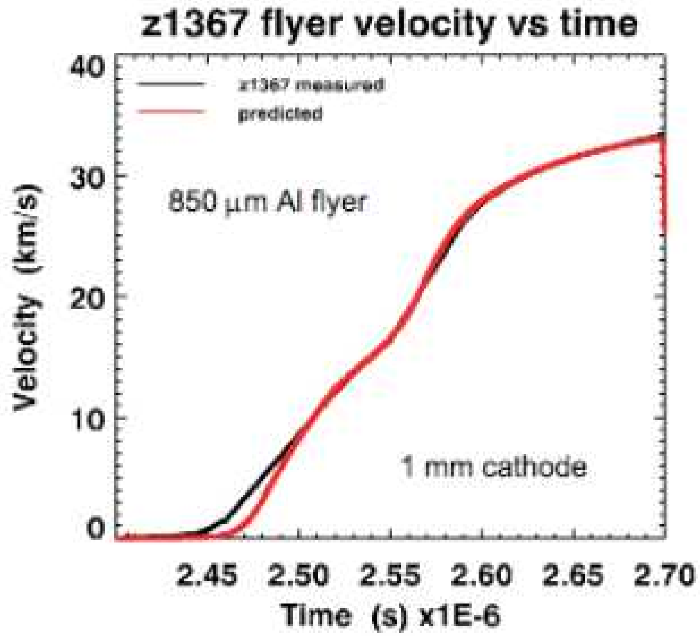


New Method for Mixed Element (Eulerian) Advection

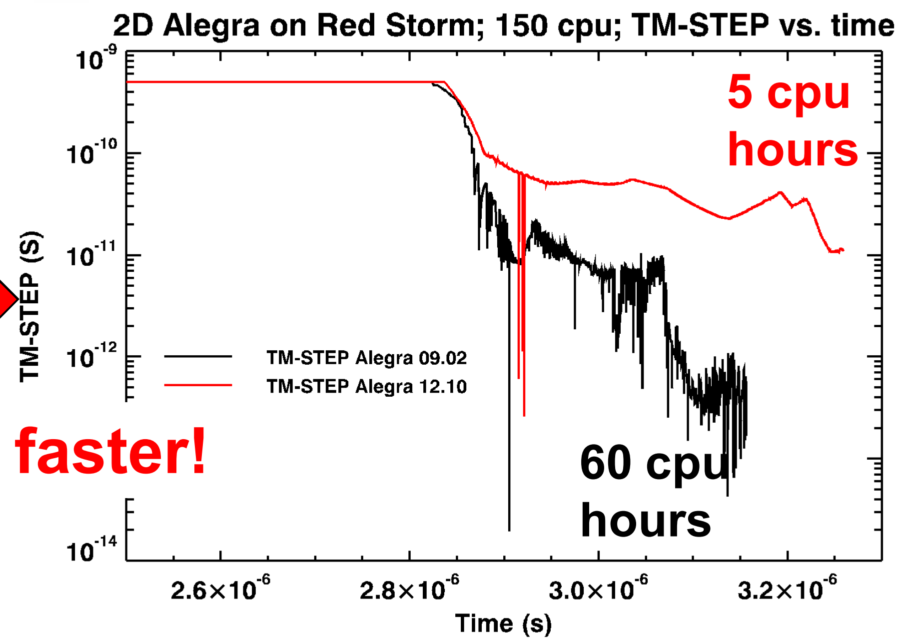








The better multimaterial remap allows work on the “physics” to proceed, so the improvement is due to both remap and the material dynamics.



>12 times faster!

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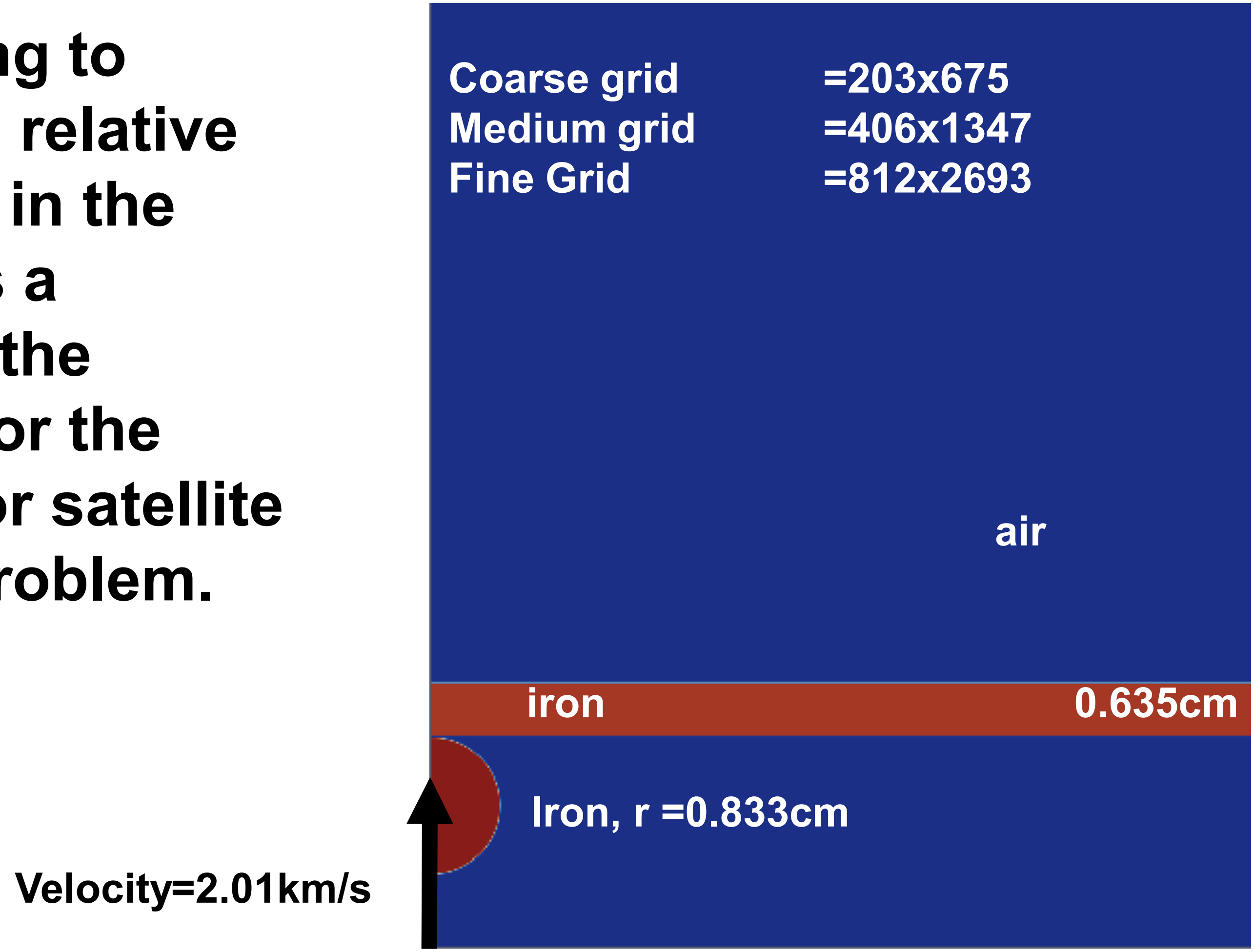
The New Method can Improve Physical Results in Substantial Ways

- **We are going to discuss the relative differences in the methods as a function of the advection for the "whipple" or satellite shielding problem.**



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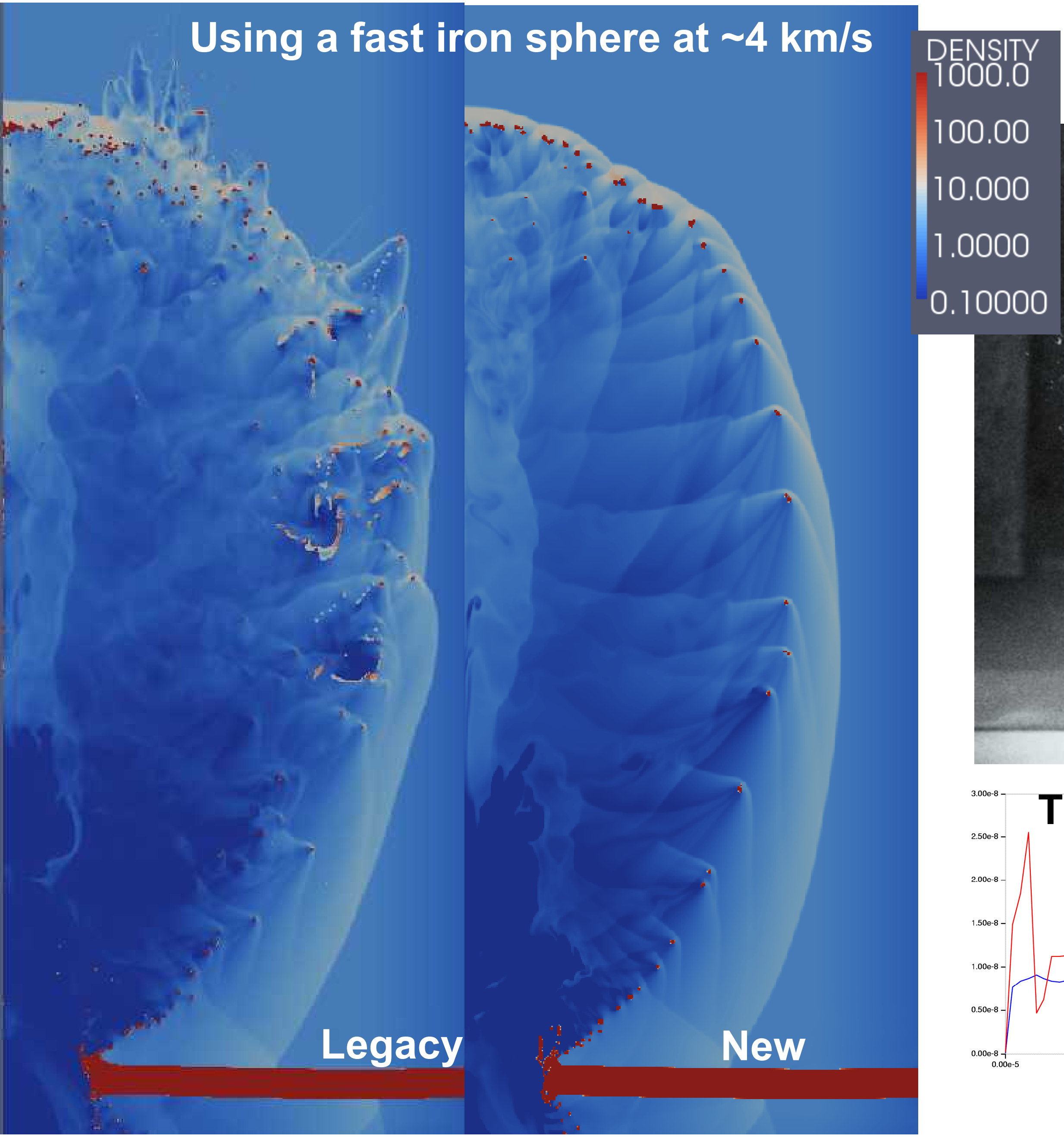
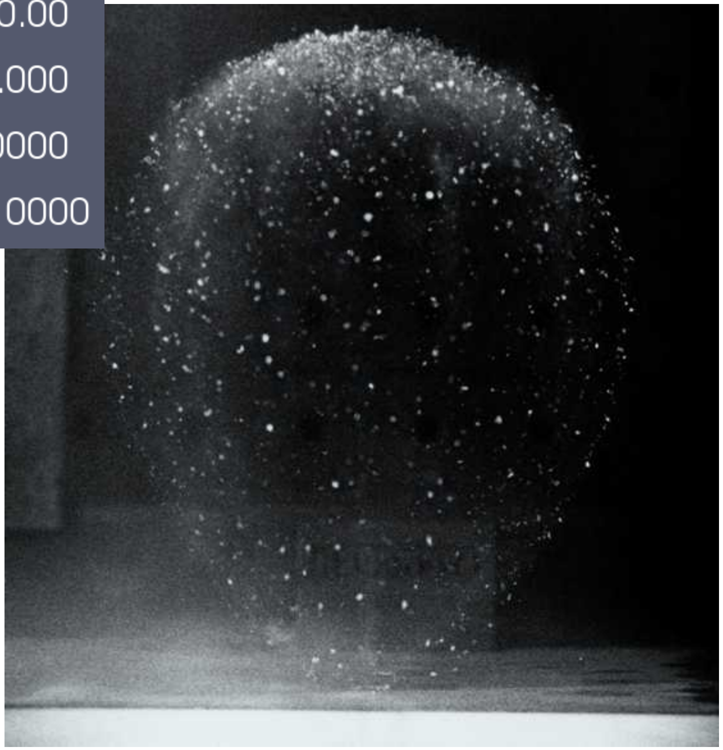
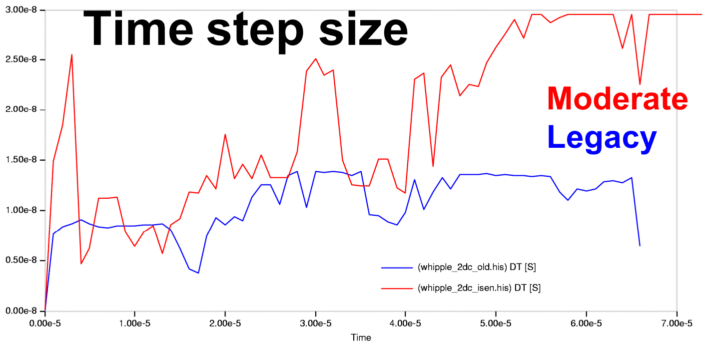
Using a fast iron sphere at ~4 km/s



Experimental Image





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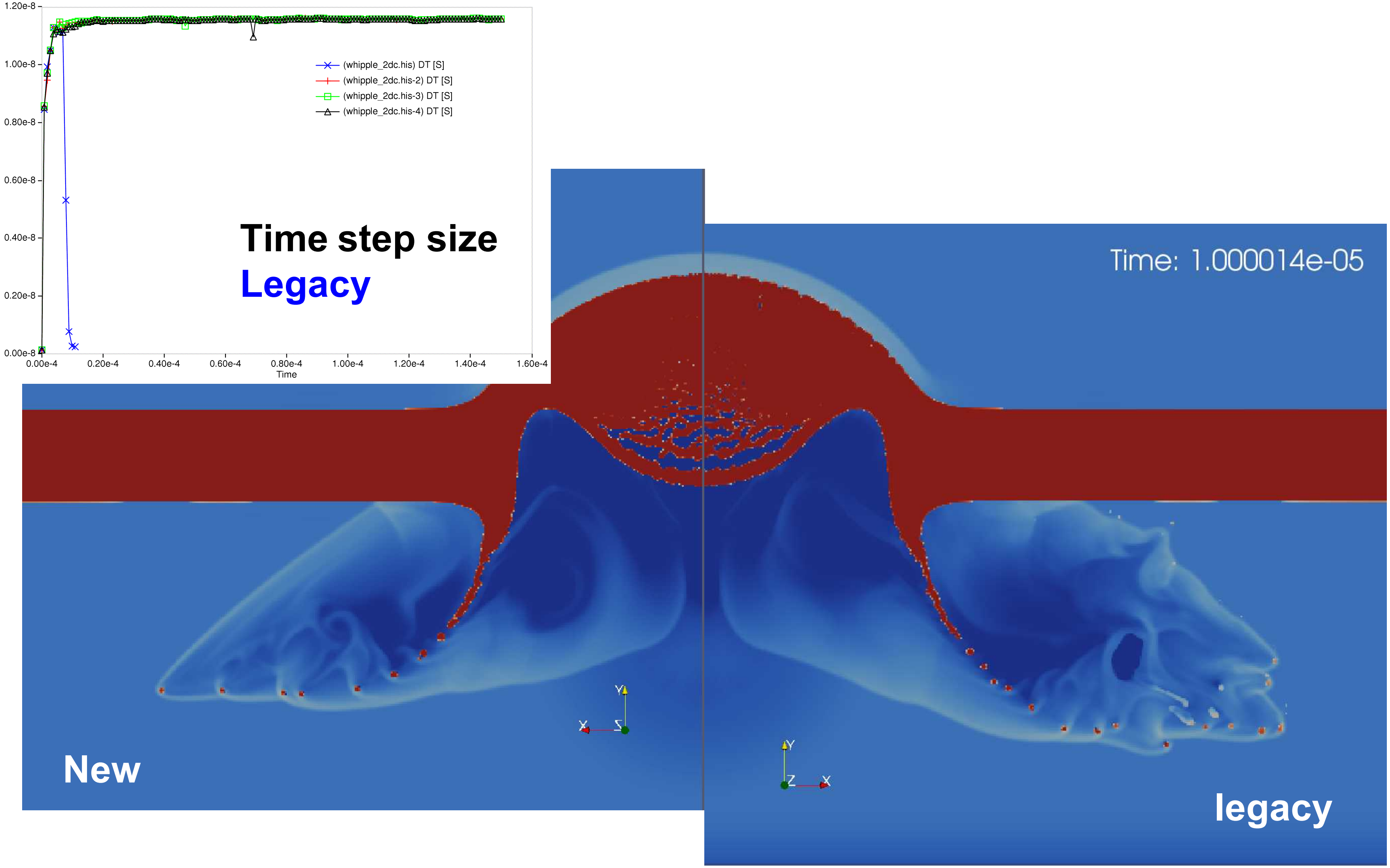
The Legacy Method Fails on the Fine Grid due to a Time Step Crash



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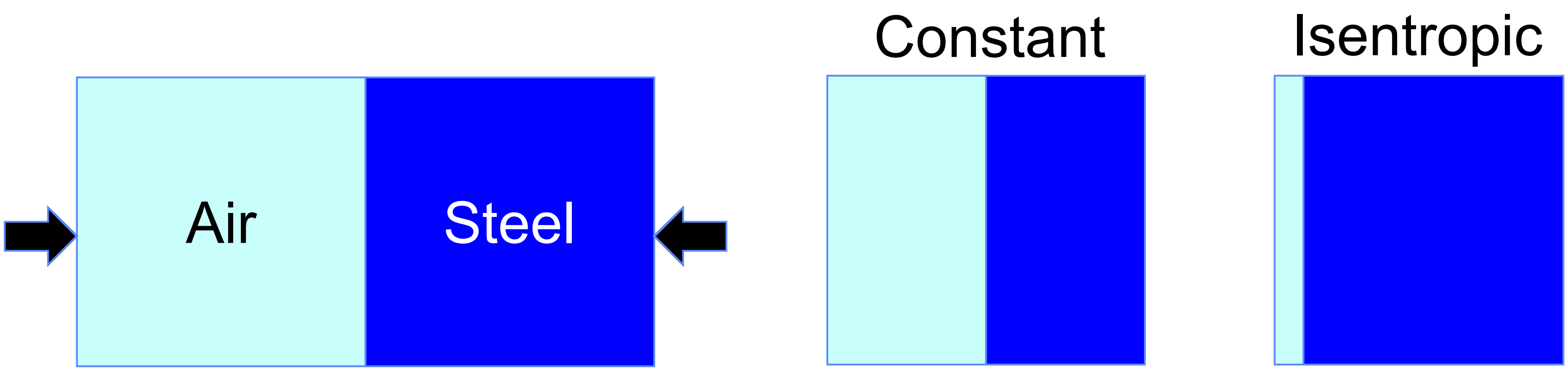
Material Mixture Models

- **Needed for ALE or Eulerian (mixing) simulations**
- **Legacy constant volume algorithm:**
  - **The relative volumes remain constant**
  - **Can lead to some obviously unphysical results**
- **Isentropic respects differences in material compressibility – compress softer materials first.**



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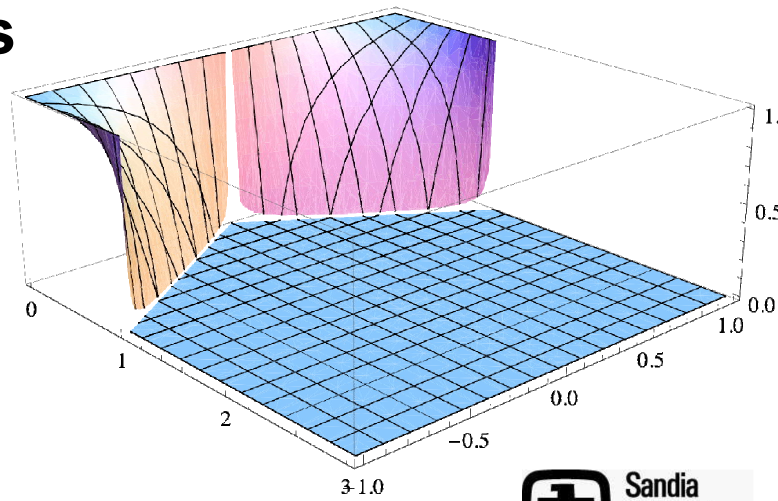
The stability of Isentropic Methods

- The isentropic equations when integrated using the explicit Euler method are unstable under the standard CFL condition.
- The stability was analyzed using techniques taken from ODE's
- Problems were found if one of the volume fractions approaches zero or if the bulk modulii of the materials are sufficiently different.



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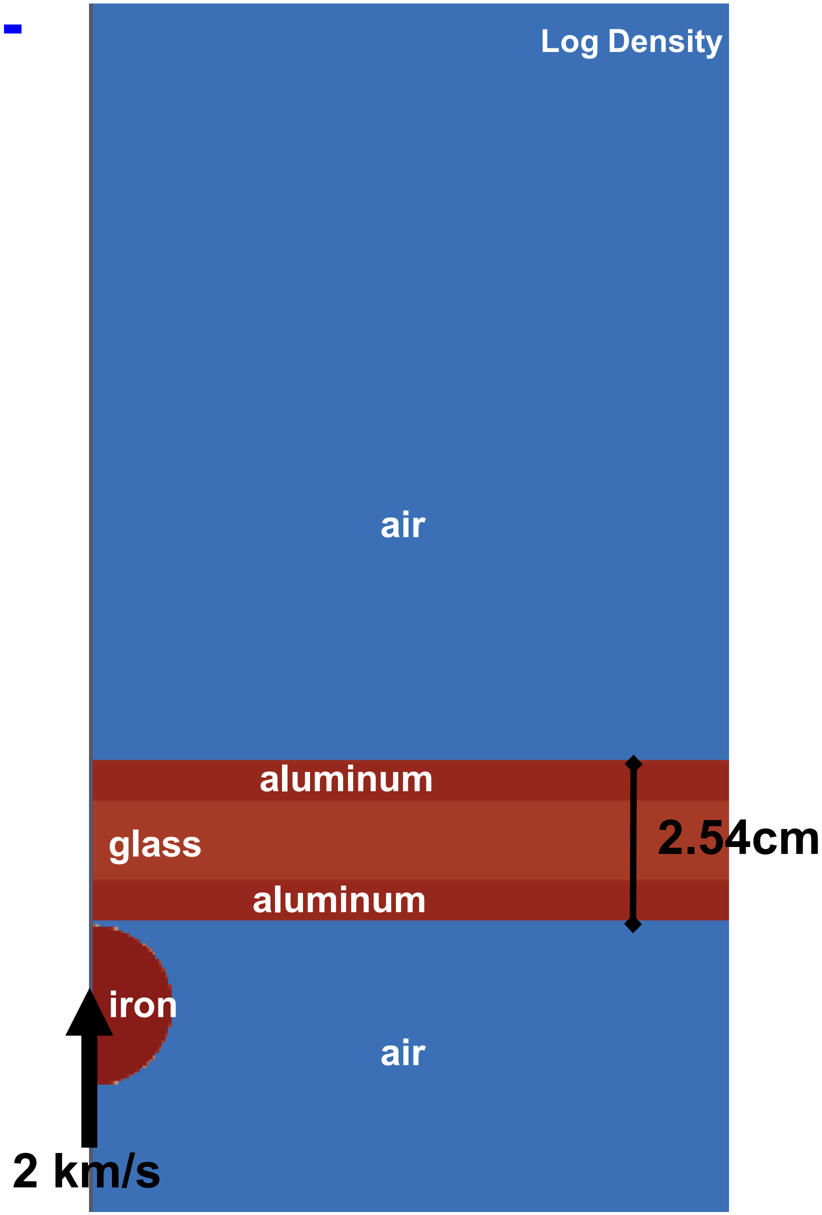
Application of the Isentropic Multi-material Method (IMM)

- Simple problem – a steel sphere impacting a shield comprised of aluminum sheets encasing glass.
- The multimaterial treatment changes the physical state achieved by material adjacent to the impact and puncture of the plates.
  - Temperature will matter for softer materials
  - 203x402 mesh



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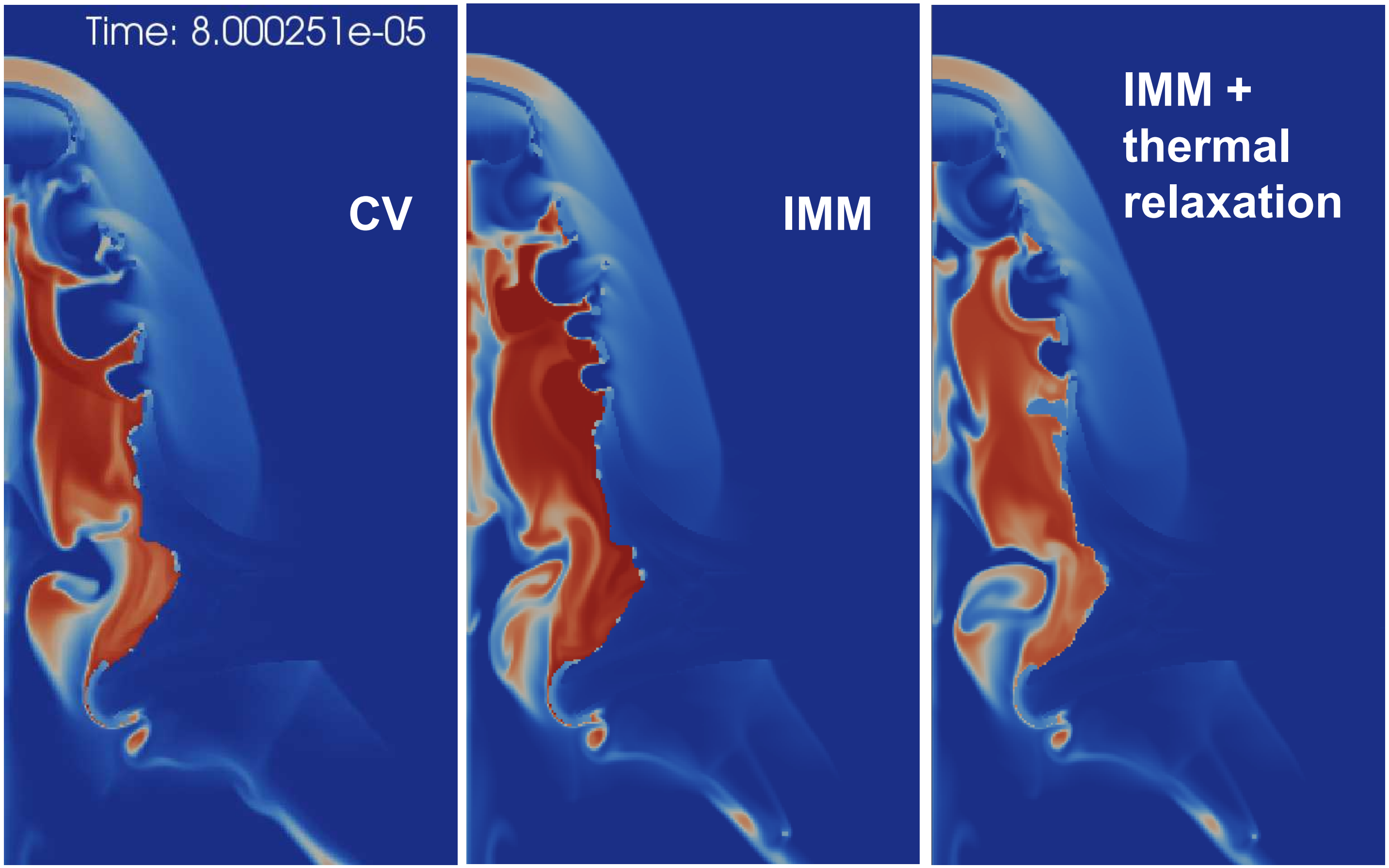
Example results with the shield simulation



CV	IMM	IMM + thermal relaxation
T_{max} = 3608K	**T_{max} = 5803K**	**T_{max} = 3001K**
T_{max} = 5392K @42μs	**T_{max} = 6355K @42μs**	**T_{max} = 3537K @42μs**

Temperatures in region behind sphere

Current Shock Physics Software R&D

- Coupling
  - Presto-CTH (Lagrangian-Eulerian)
  - ALEGRA-Presto (Lagrangian-ALE)
- Solution handoff (output from one code as input to another)
  - Lagrangian → Eulerian
  - Eulerian → Lagrangian
- Material model consolidation
  - common interface, material libraries, behavior and look & feel available to all Sandia shock codes.
- Statistical-based fracture and fragmentation

Current Shock Physics Software R&D (cont.)

- Improved EOS representations
  - better SESAME interpolation
  - adaptive tabular representations
- Improved non-ideal explosive descriptions
- Various ongoing projects to understand the relationship between mechanical damage and reaction kinetics in energetic materials.
- Code usability improvements:
  - context sensitive editor
  - common look & feel input deck improvements
  - common on-the-fly visualization
  - coordinated training

For more information

ALEGRA

- project lead: Allen Robinson (acrobin@sandia.gov)
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CTH

- project lead: David Crawford (dacrawf@sandia.gov)
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Presto

- project lead: Martin Heinstein (mwheins@sandia.gov)
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