Illinois Rocstar

Predictive modeling and simulation for industry, science, defense, and security

Physics-Based Modeling and Simulation of Shock-to-Detonation Transition in Energetic Materials

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NDIA National Defense Industrial Association — Promoting National Security Since 1919

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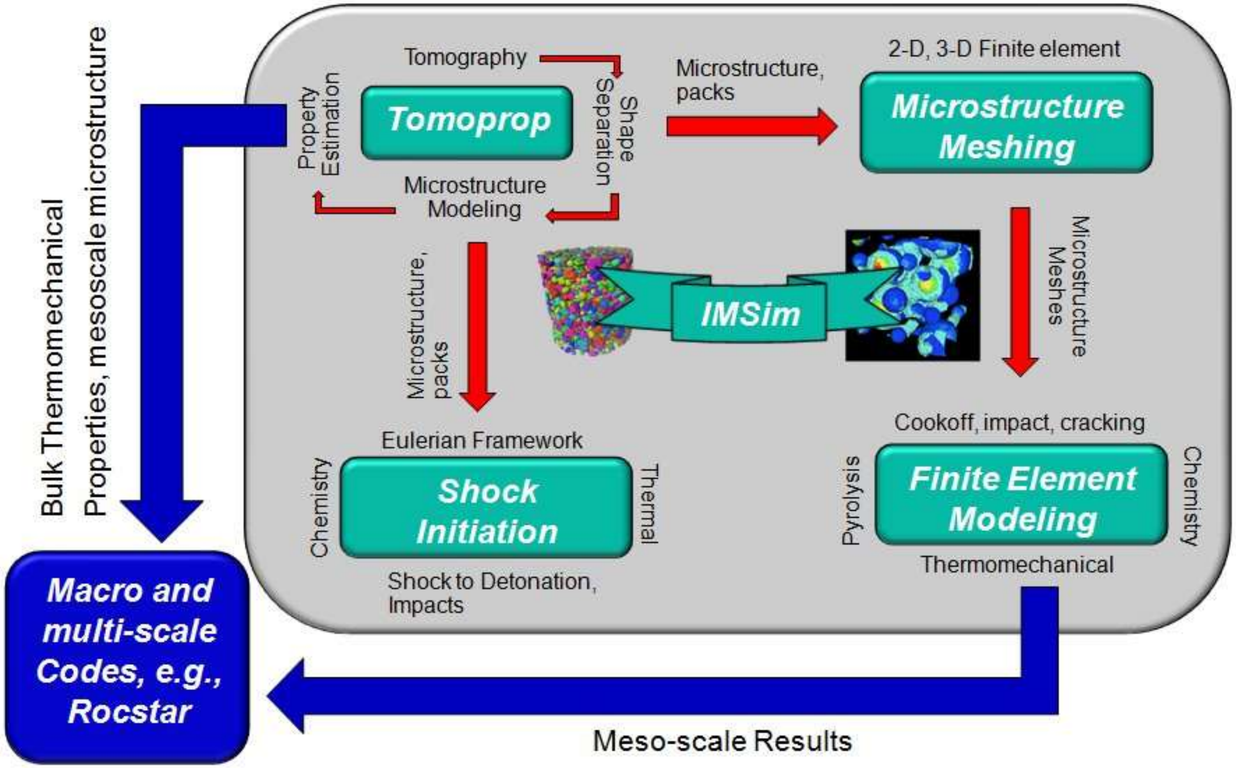
Outline

- *IMSim* Infrastructure
  - **I**nsensitive **M**unitions **Sim**ulation package
- *Rocpack*
  - Models the microstructure
  - Validation
- *RocSDT*
  - Shock-to-detonation physics code
  - Verification
  - Examples

Insensitive Munitions and *IMSim*

Characterization

Fast and Slow Cookoff

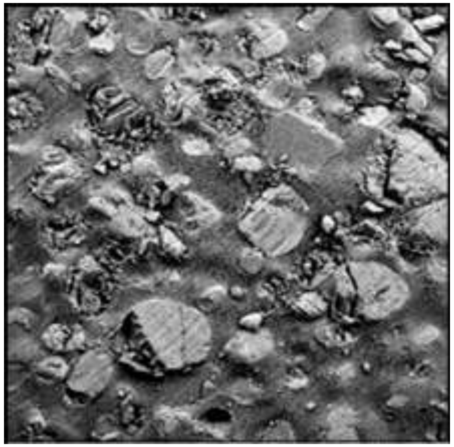


Bullet and Fragment Impact

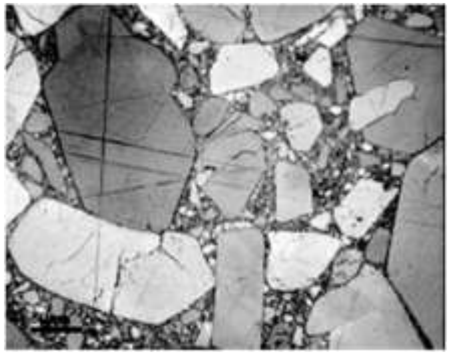
Aging

Issues with Energetic Materials

- Shock sensitivity of energetic materials
  - Material defects can augment shock sensitivity
  - Geometric effects (voids, crystal shape, binder) are important
- Modeling the microstructure is important for predictive simulations
  - Homogeneous modeling not predictive
- Difficulties at the mesoscale
  - Complex geometry
  - Multi-material interfaces
  - Complex chemical reaction pathways
- Goal
  - Develop virtual engineering infrastructure to predict properties and dynamics of shock-induced initiation in energetic materials



AP/HTPB Solid Propellant



PBX9501 (C. Skidmore, LANL)

Value Proposition

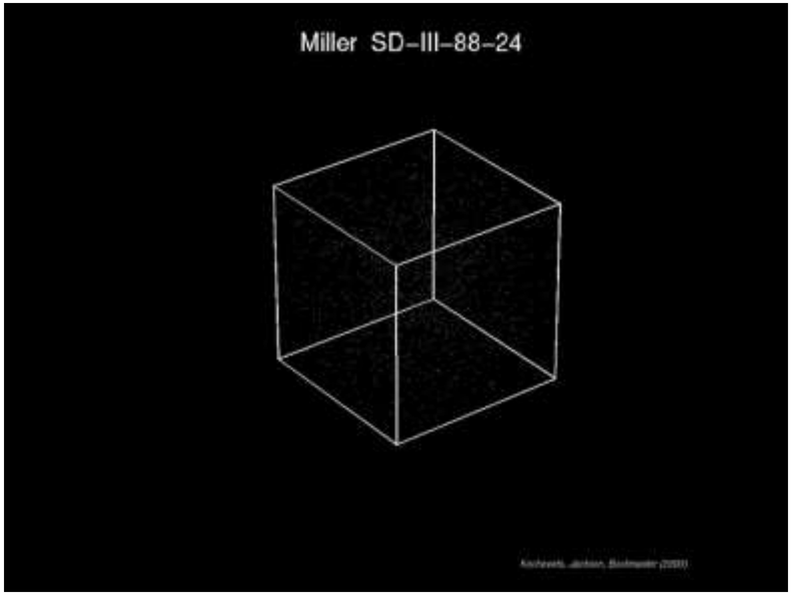
- Mesoscale structures and effects control the response of energetic materials
- IMSim tools, when complete will allow
  - Analyzing existing materials to explain observed effects
  - Designing new materials to tailor predicted properties and IM response before formulation and testing
- Replace "some" of the make-and-break cycle
- Produce detailed mesoscale response and effects for input to macroscale simulation tools
  - IllinoisRocstar's *Rocstar Simulation Suite*
  - Other shock physics, FEA, CFD codes

Microstructure Modeling

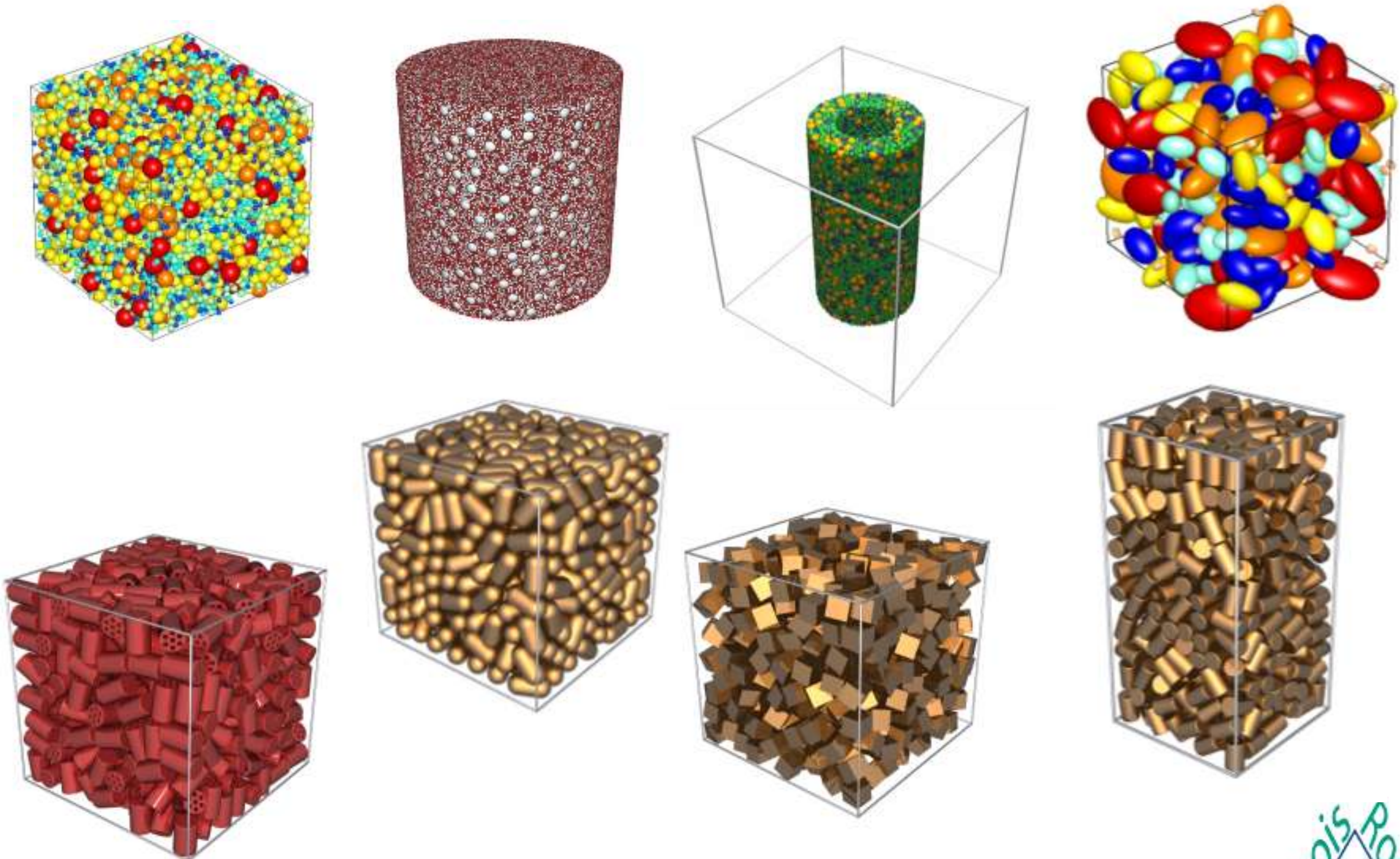
- Rocpack packing code
- Microtomography data for real energetic materials

Rocpack

- *Rocpack* is based on the concurrent packing algorithm described by Lubachevsky and Stillinger, J. Stat. Phys. 1990
- Spheres of zero initial radius with random locations and velocities grow in a box at a prescribed growth rate a_i
- Stopping criterion
  - specified packing fraction
  - jammed

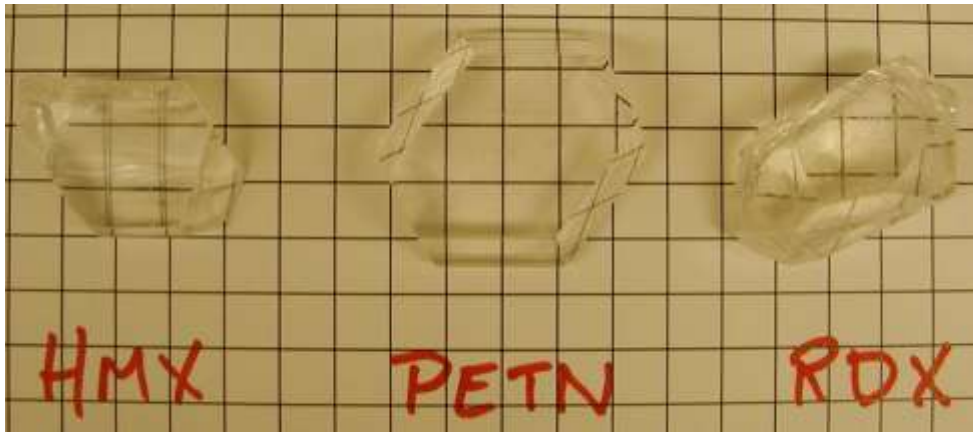


Shapes generated by *Rocpack*



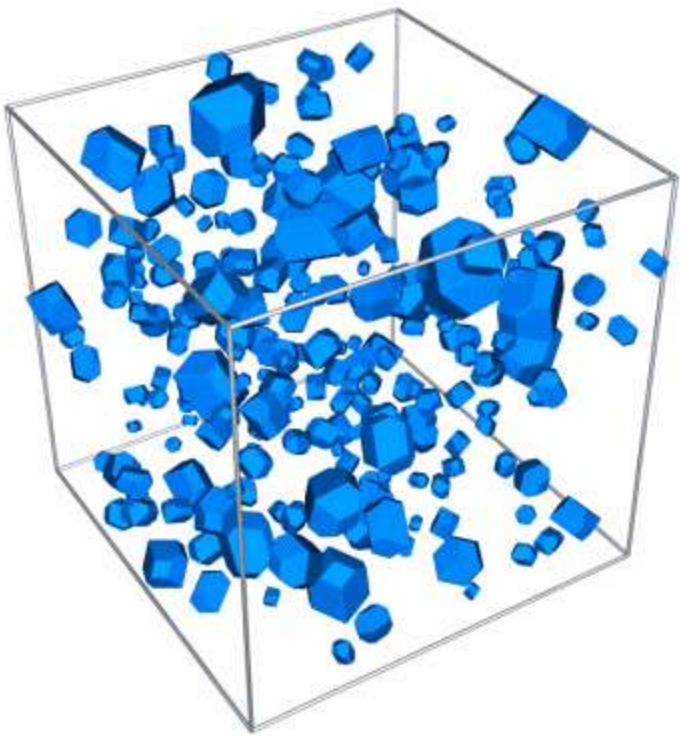
Modeling Crystals for Energetic Materials Using *Rocpack*

- Sphere packing algorithm extended to include crystals using level sets to describe the shapes



- *Stafford, D.S. and Jackson, T.L. (2010) Using level sets for creating virtual random packs of non-spherical convex shapes. Journal of Computational Physics, Vol. 229, pp. 3295-3315.*
- *Jackson, T.L., Hooks, D.E., and Buckmaster, J. (2011) Modeling the Microstructure of Energetic Materials with Realistic Constituent Morphology. Propellants, Explosives, Pyrotechnics (in press).*

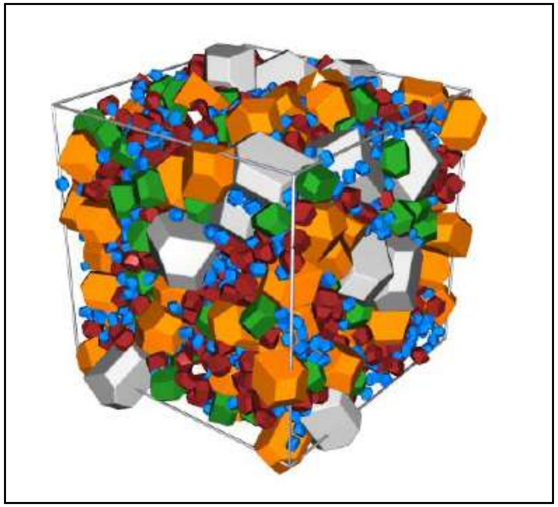
Rocpack Crystal Packing



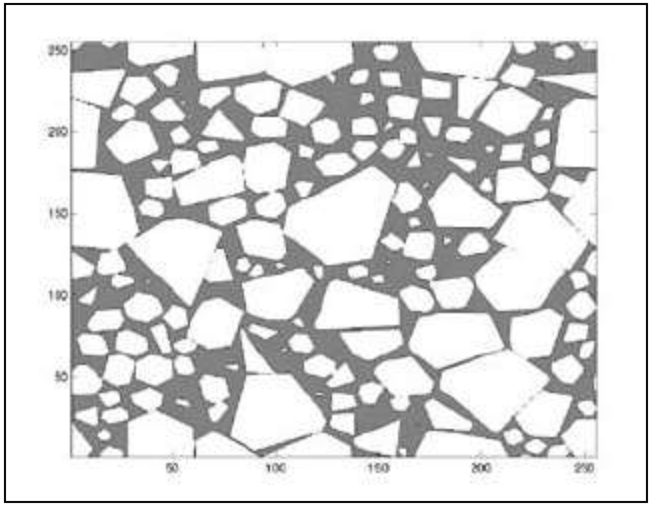
250 total HMX crystals
10 different particle sizes [55, 281] microns
Frames stopped at volume fraction 0.68

Computational Crystal Pack

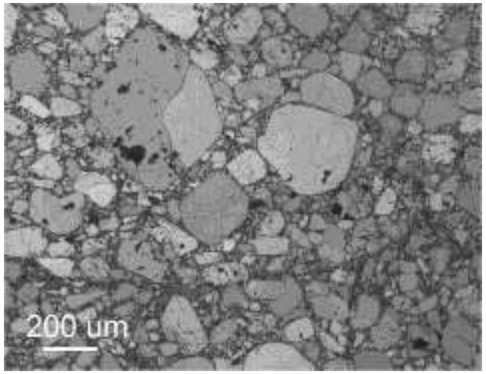
- Example: Low-density unpressed HMX (68%) pack
- Figure shows 3-D pack (each size colored differently) and a 2-D slice through the 3-D pack



3-D

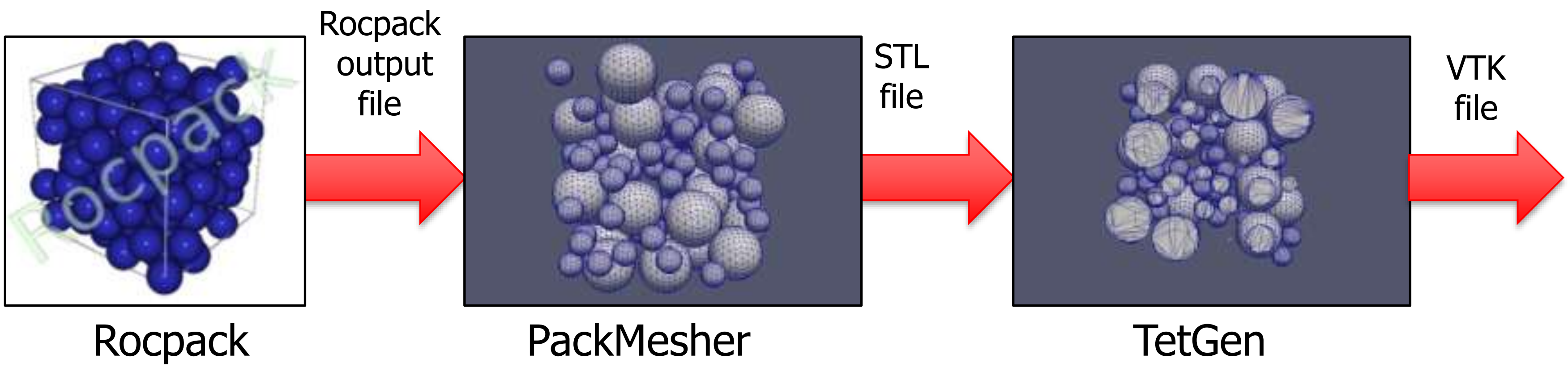


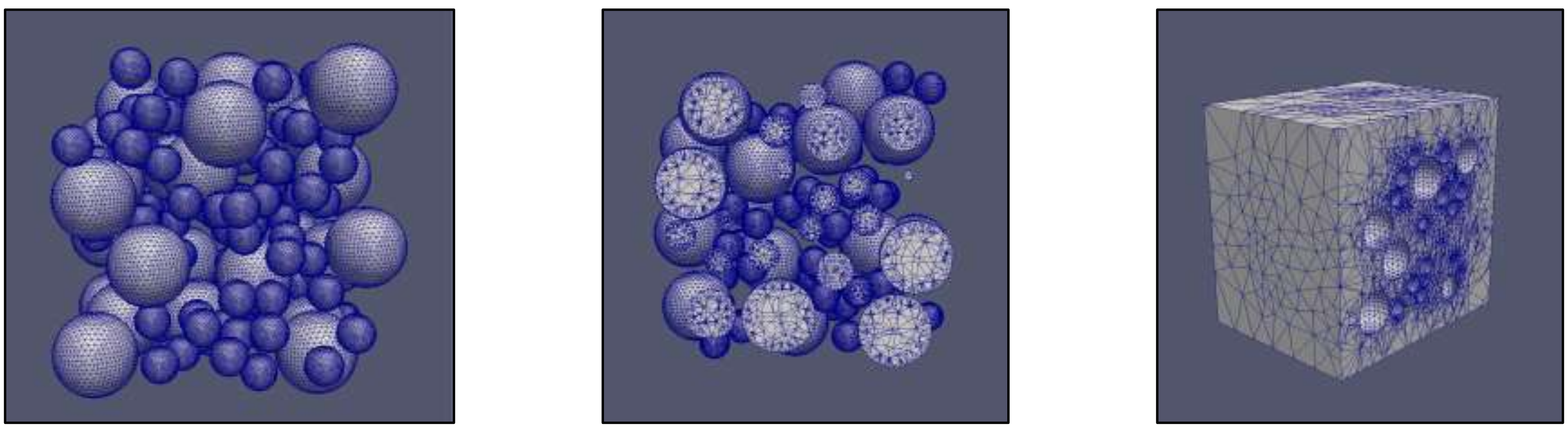
2-D slice



Plastic bonded explosive
(HMX 95%, 5% binder)

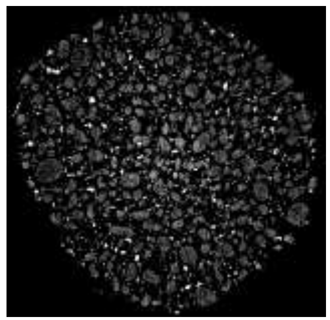
PackMesher





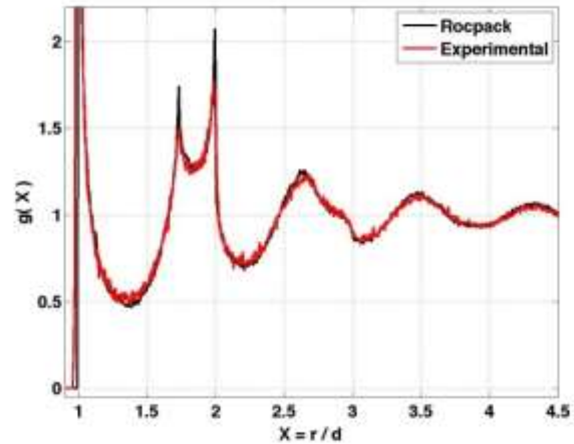
- Currently supports separated spheres and tetrahedral mesh
- Extending to all other *Rocpack* shapes and shapes that touch

Validation of *Rocpack*



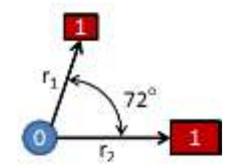
Tomography

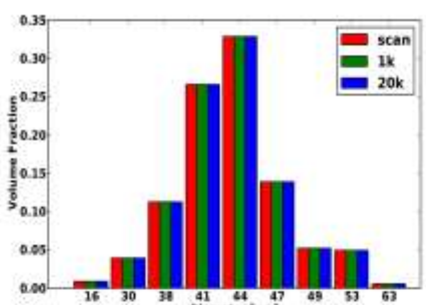
Validation data or directly for packs

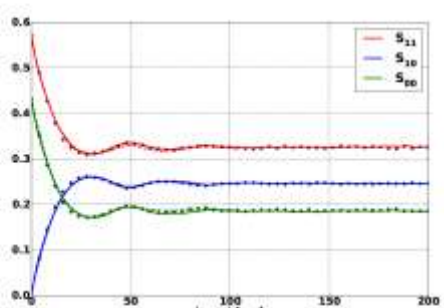


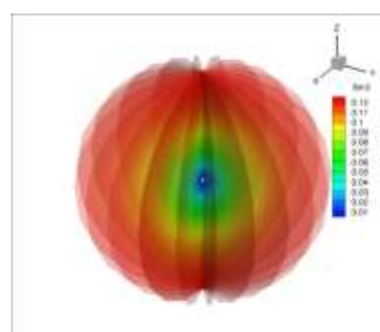
Radial distribution function

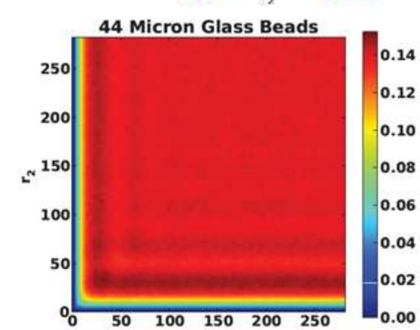
Compare first, second, and third-order statistics





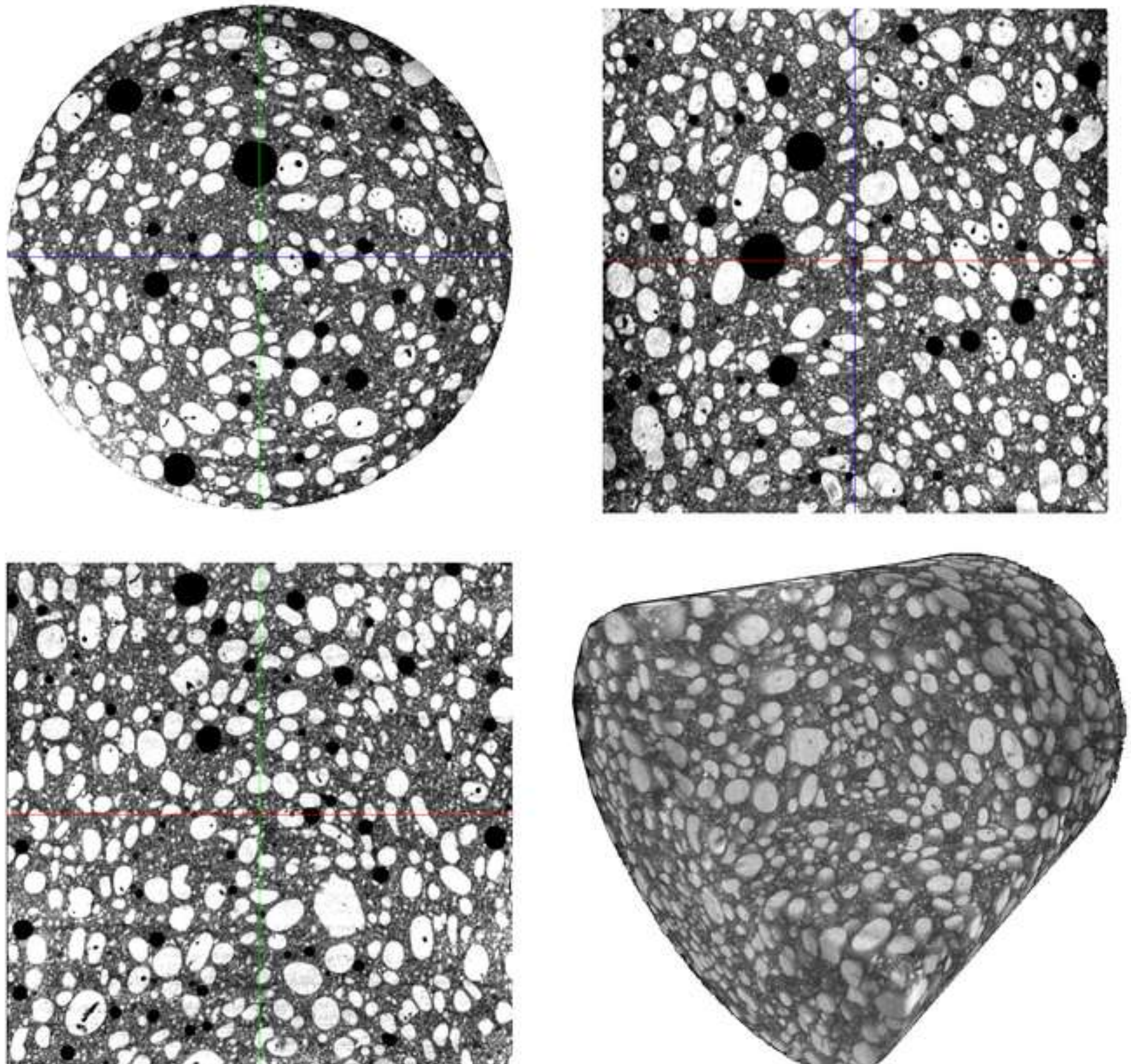






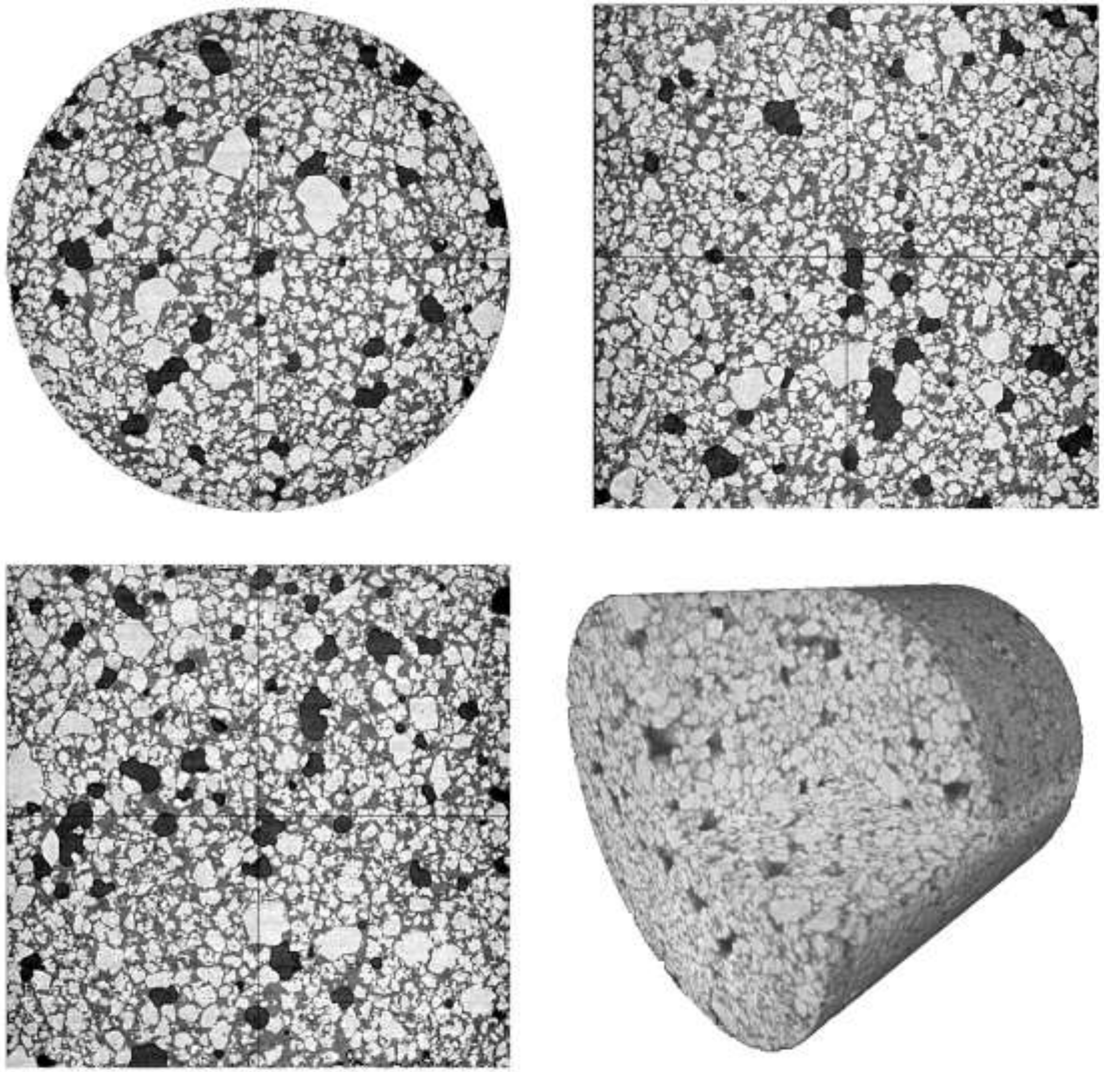
AP/HTPB

80% 200 micron AP; 1:1 fine to coarse; 20% HTPB



CL20/HTPB

80% 200 micron AP; 1:1 fine to coarse; 20% HTPB

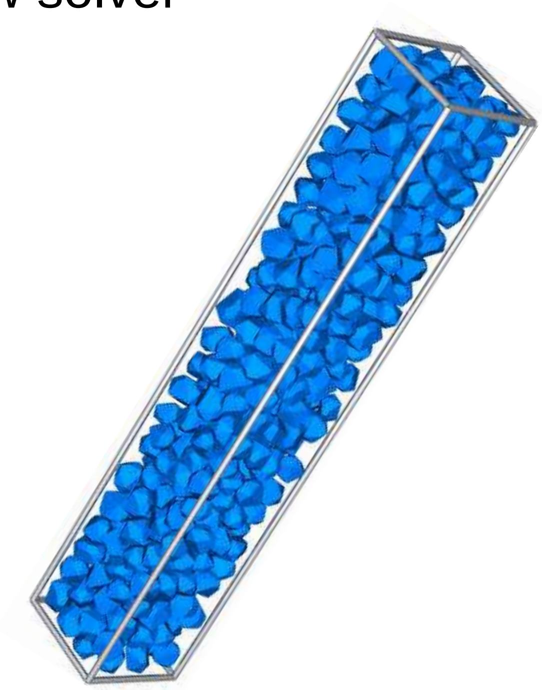


Shock to Detonation Modeling

- Code status
- Background
- Verification
- Borne data comparison

RocSDT

- Three-dimensional compressible reactive flow solver for explosives
- Current characteristics of *RocSDT*
  - Strong shocks ✓
  - Sharp material interfaces ✓
  - High density ratios (voids) ✓
  - Multiple EOS ✓
  - Kinetics/Chemistry
  - Microstructure from *Rocpack* ✓
  - Material deformation
  - Three-dimensional ✓
  - Parallel using MPI ✓



Pack of HMX crystals produced by *Rocpack*

Zhang, J, Jackson, T.L., Buckmaster, J.D., and Freund, J.B (2012) "Numerical Modeling of Shock-to-Detonation Transition in Energetic Materials," recently accepted in *Combustion & Flame*.

Governing Equations

- Reactive Euler equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$
$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla p + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = 0$$
$$\frac{\partial E}{\partial t} + \nabla \cdot ((E + p)\mathbf{u}) = Q\Omega$$
$$\frac{\partial (\rho Y)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y) = -\Omega$$
$$\Omega = Da \rho Y e^{-E_a/R_u T}$$
$$E = \rho \left(e + \frac{1}{2}\mathbf{u} \cdot \mathbf{u} \right)$$

- Multiple Equations of State (ideal, stiffened, Mie-Gruneisen)

Maintain Sharp Interfaces

- Interface capturing method; Φ is a material marker
  - Changes over small number of mesh points near interfaces

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0$$

Move interface using this…

$$\frac{\partial \phi}{\partial \tau} = \mathbf{n} \cdot \nabla (\epsilon_h |\nabla \phi| - \phi(1-\phi))$$

Correct interface position each timestep using this…
τ=pseudo time
n=normal vector

- Density compression:

$$\frac{\partial \rho}{\partial \tau} = H(\phi)\mathbf{n} \cdot (\nabla(\epsilon_h \mathbf{n} \cdot \nabla \rho) - (1-2\phi)\nabla \rho)$$

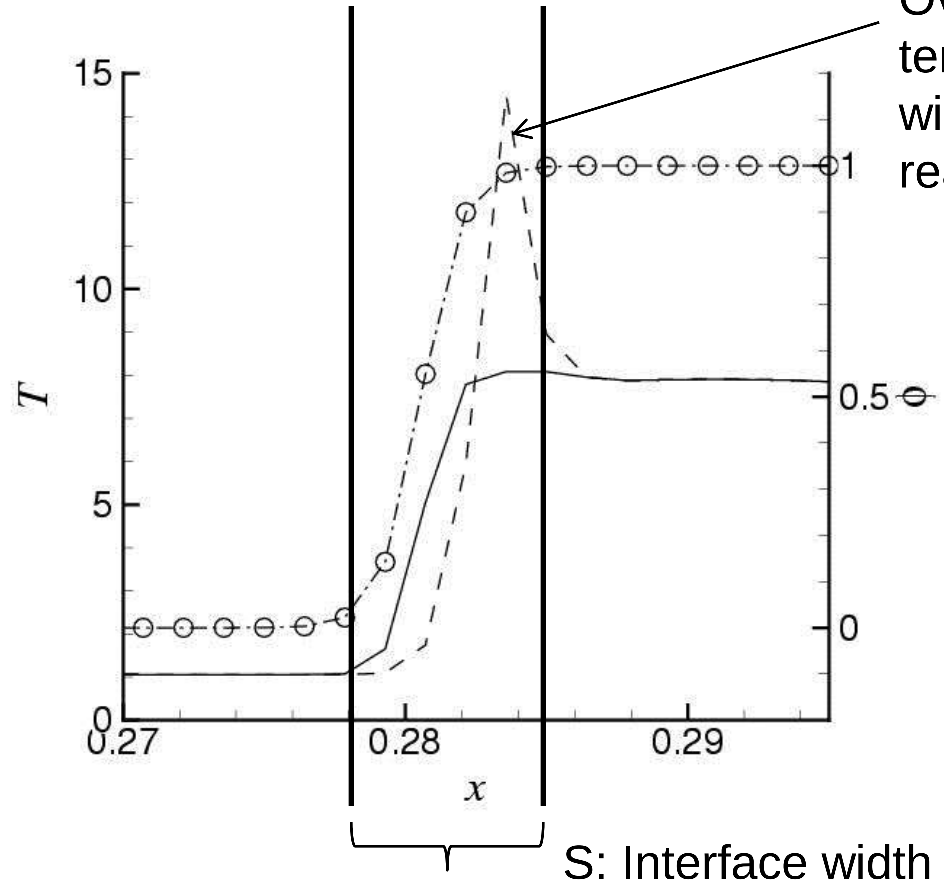
- Temperature and mass fraction compressions:

$$\frac{\partial T}{\partial \tau} = H(\phi)\mathbf{n} \cdot (\nabla(\epsilon_h \mathbf{n} \cdot \nabla T) - (1-2\phi)\nabla T)$$

$$\frac{\partial Y}{\partial \tau} = H(\phi)\mathbf{n} \cdot (\nabla(\epsilon_h \mathbf{n} \cdot \nabla Y) - (1-2\phi)\nabla Y)$$

Temperature Correction

- Comparison of temperature profile with (solid) and without (dash) temperature correction
- Dash/circles denote location of material interface ϕ

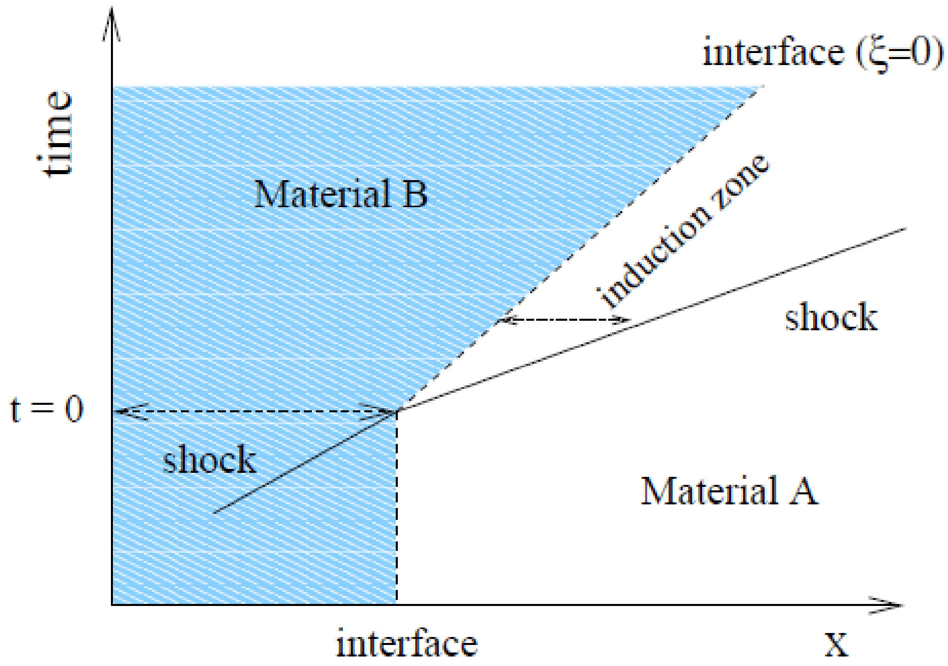


Overshoot without temperature correction will cause spurious reactions to occur.

S: Interface width

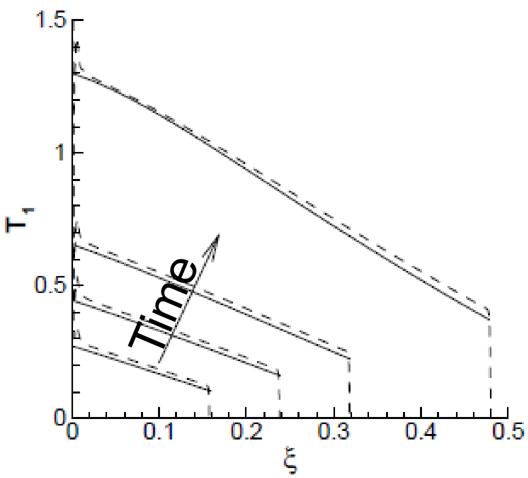
Verification of *RocSDT* Shock-Material Interface

- Assume shock is strong enough to raise temperature between shock and interface to an ignition temperature T_0, thereby switching on chemical reaction
- The induction zone defined to lie between the shock and the (moving) material interface

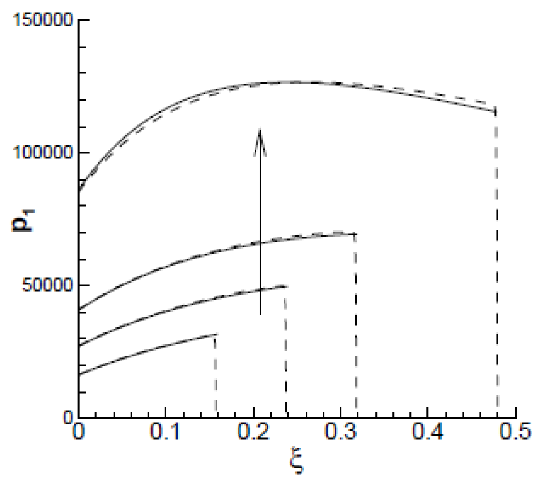


Results for Shock-Material Interface (1)

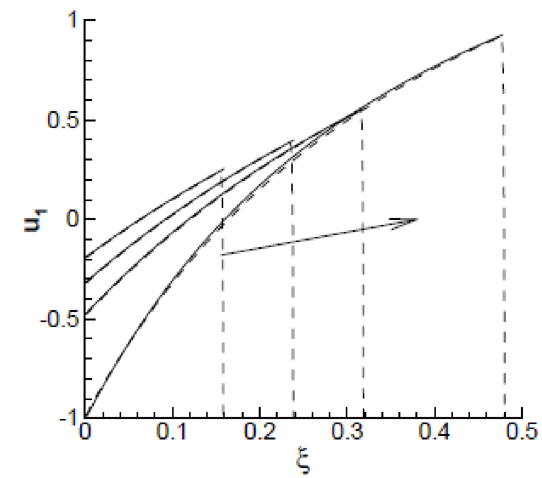
- Form non-dimensional perturbation solution
- Comparison of perturbation temperature, pressure, and velocity in the induction zone using stiffened EOS
  - Asymptotic solutions: solid
  - RocSDT: dash
  - ξ = non-dimensional interface position



(d) Stiffened; Temperature



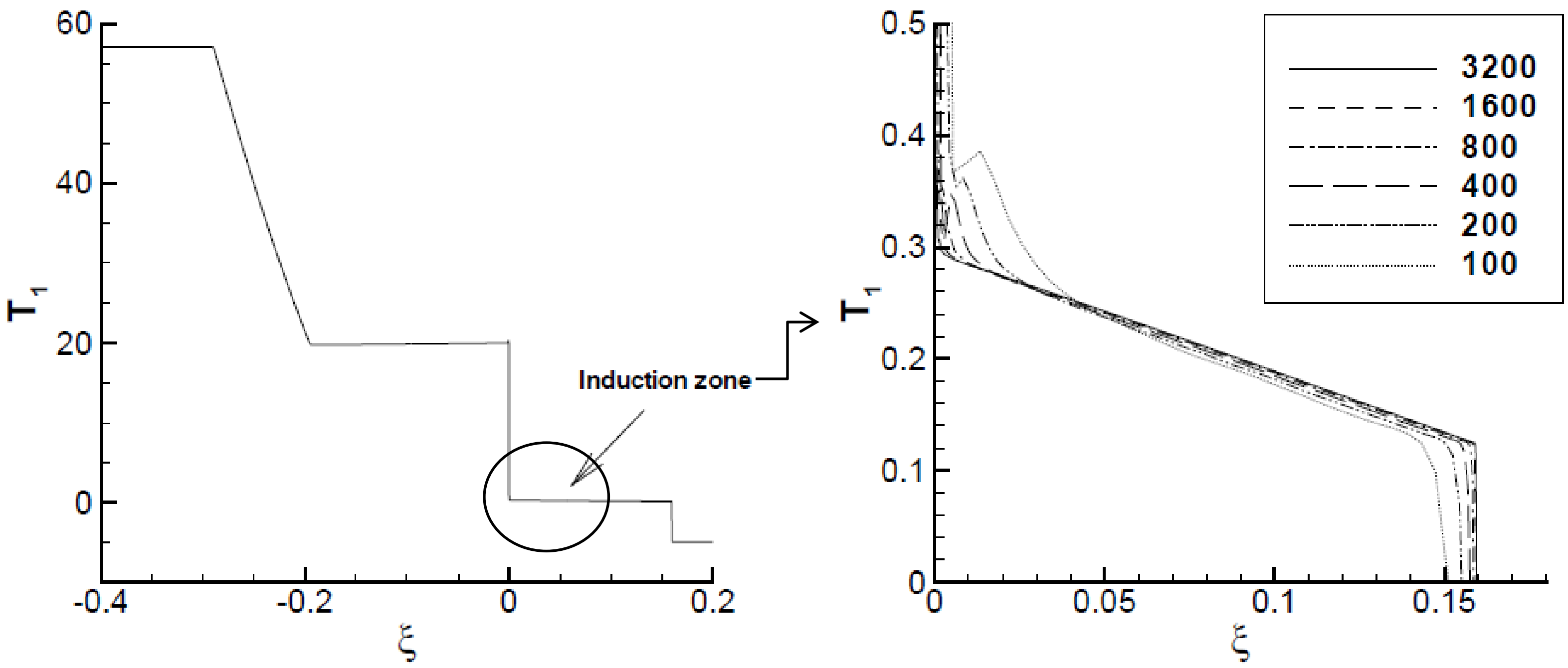
(e) Stiffened; Pressure



(f) Stiffened; Velocity

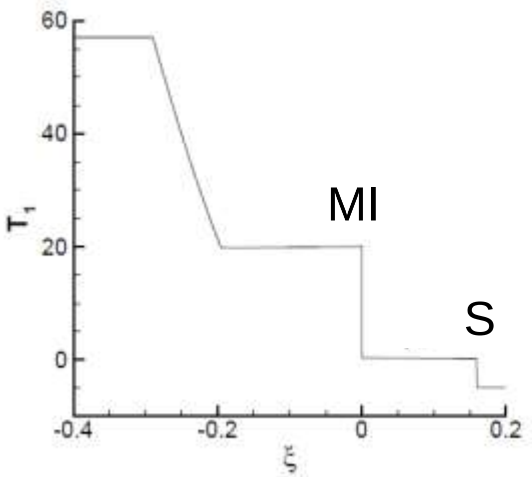
Results for Shock-Material Interface (2)

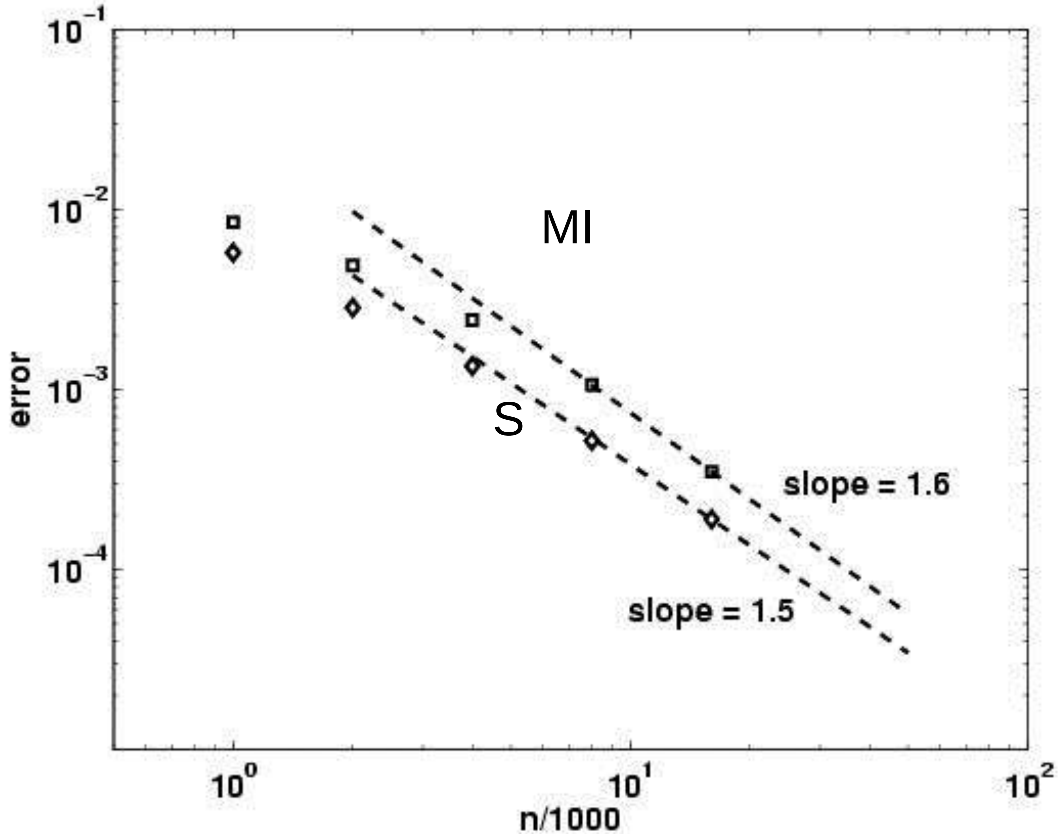
- Grid resolution study showing grid convergence of perturbation temperature
- T_1 is the perturbation temperature



Results for Shock-Material Interface (3)

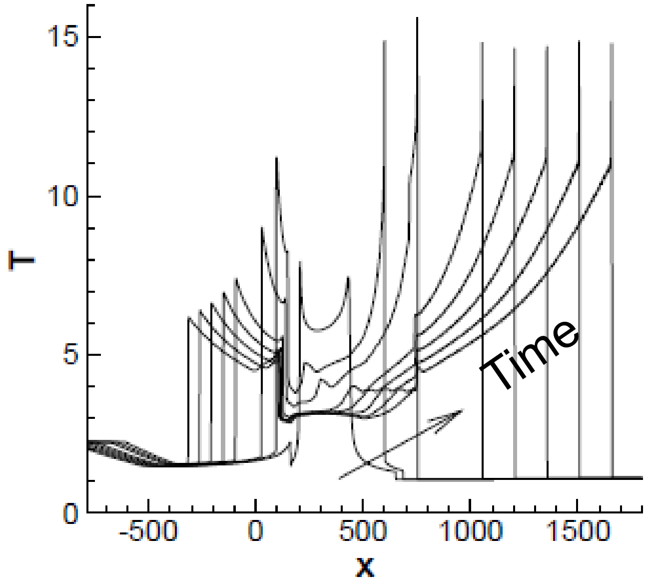
- Convergence rate of perturbation temperature as a function of n (number of grid points) at material interface (square) and shock location (diamond)
- Relative error in maximum perturbation temperature



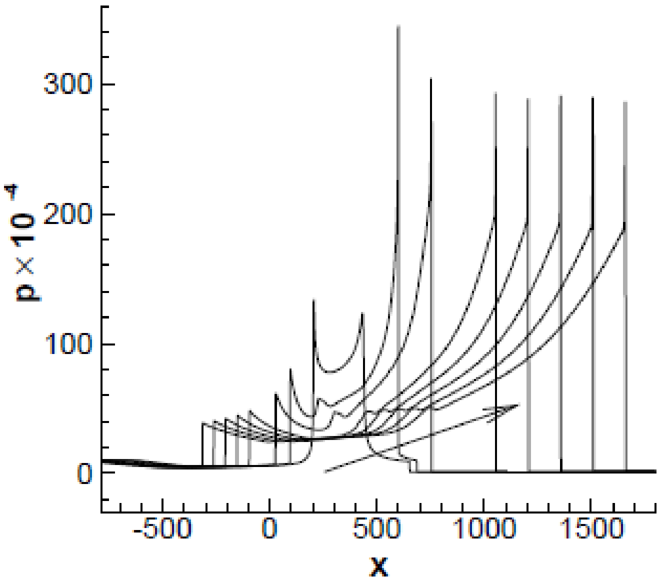


Results for Shock-Material Interface (4)

- Transition to detonation
  - The peaks are within 4% of those obtained on a grid with four times the resolution
  - CJ states captured to within 1%
  - Transition to detonation around x=600



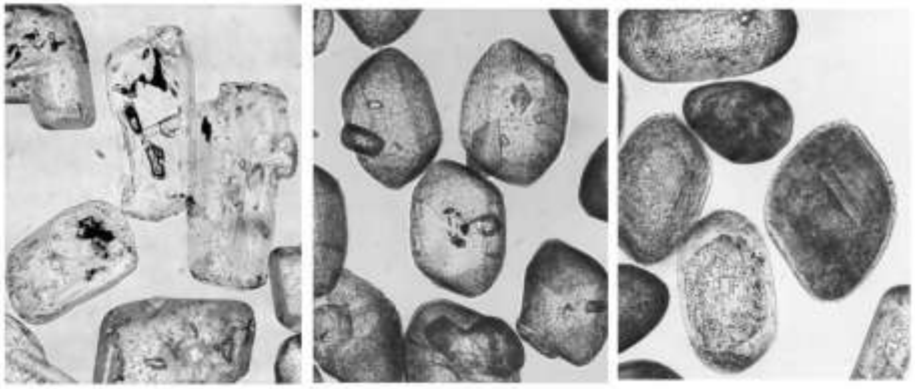
Temperature



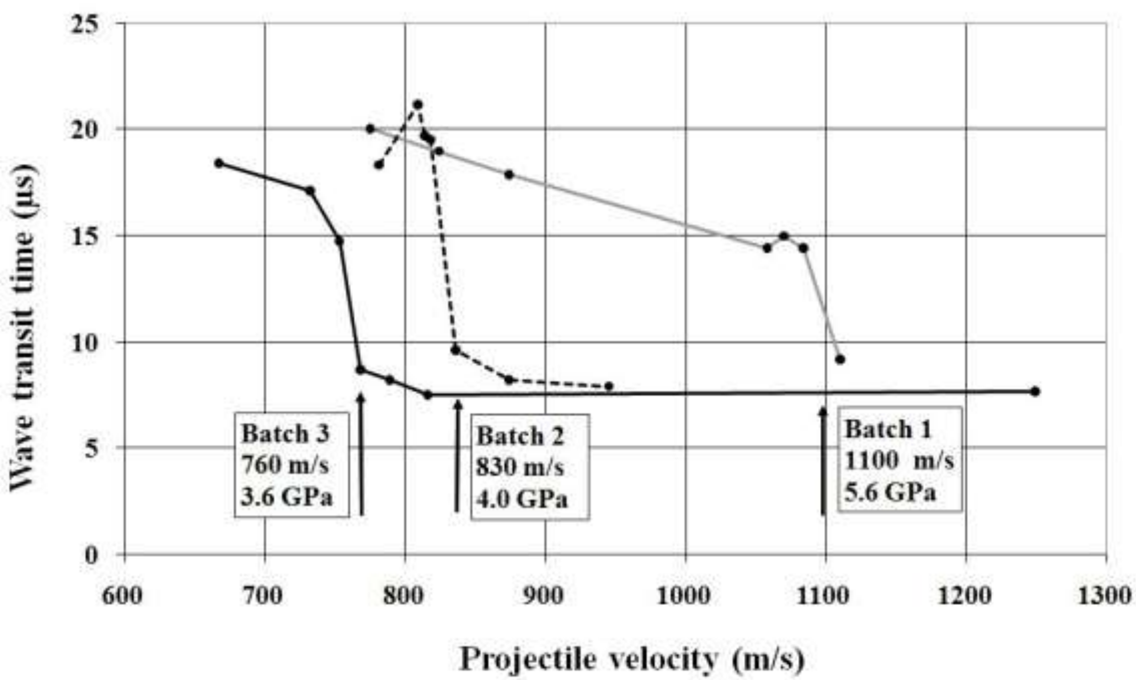
Pressure

Example: Borne Experiment

- Borne (1982)
  - Experimental investigation of HMX crystals in wax
  - Projectile against plate to introduce shock

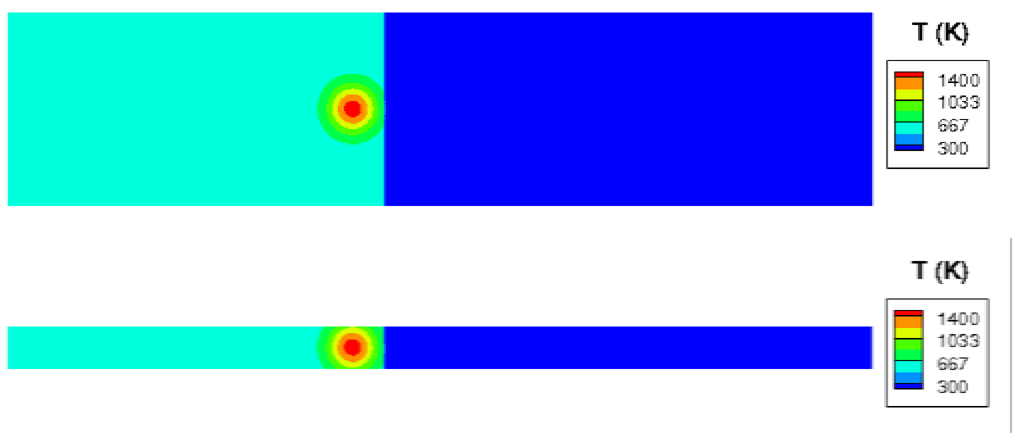


  - Void content varied
    - 0.1% (Batch 1)
    - 0.5% (Batch 3)
  - Experimentally measured velocity threshold for detonation; function of crystal impurity



Periodic Single Void Model

- Borne’s experiments suggests that hot spot formation due to void collapse is an important ingredient for transition to detonation
- Numerical experiment with current capabilities
  - One-step global kinetics
  - We mimic the experiment by modeling hot spots as a periodic array in an infinite slab of HMX
  - Vertical distance between hot spots corresponds roughly to volume percent of voids in HMX crystals
  - 2 μm diameter hot spot

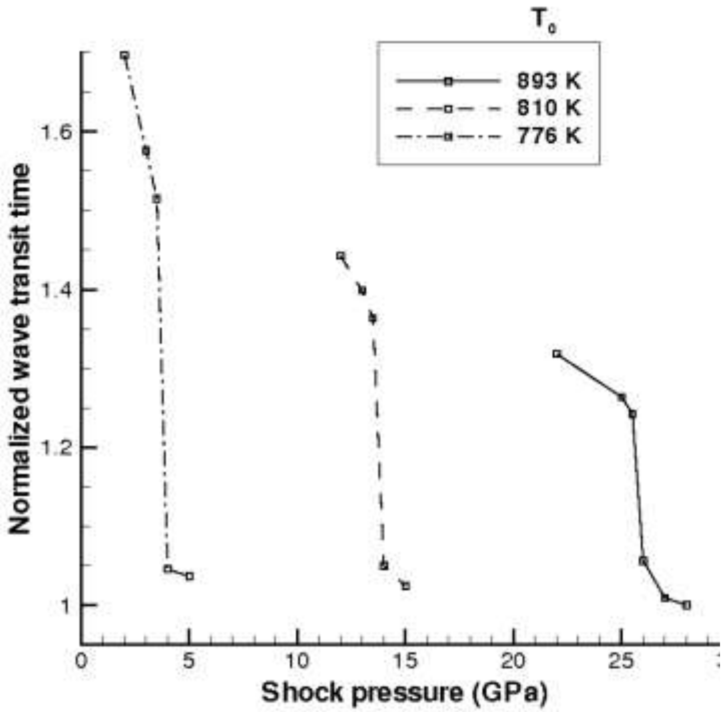


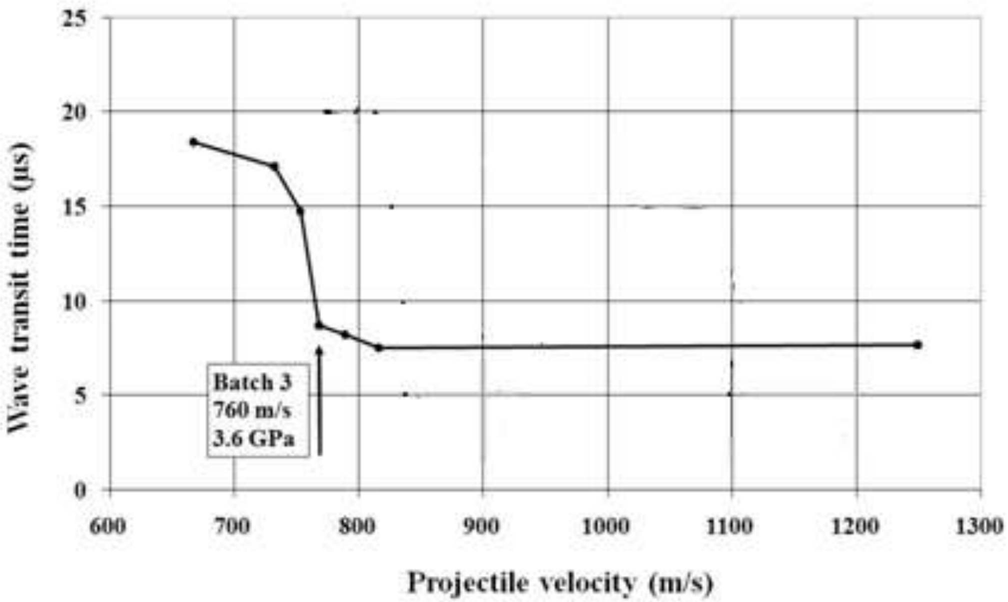
Batch 1

Batch 3

Example: Borne Experiment (1)

- T_0 (the ignition temperature) is calibrated for Batch 3; held fixed for batches 1 and 2

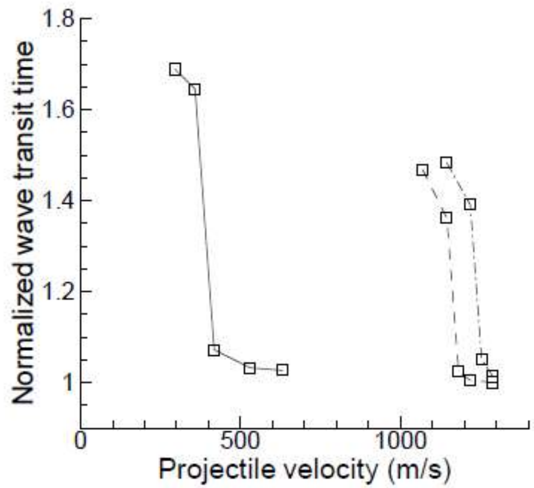


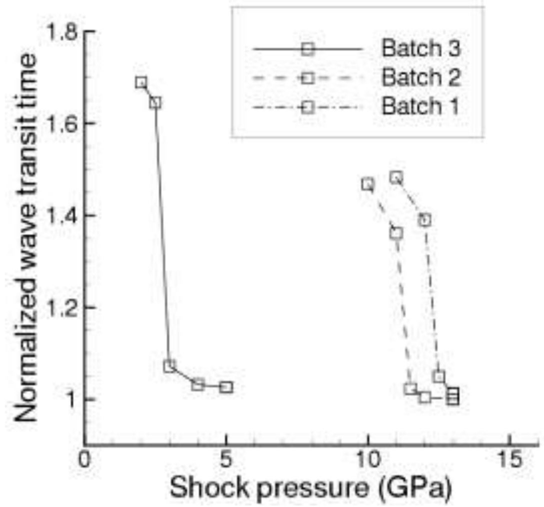


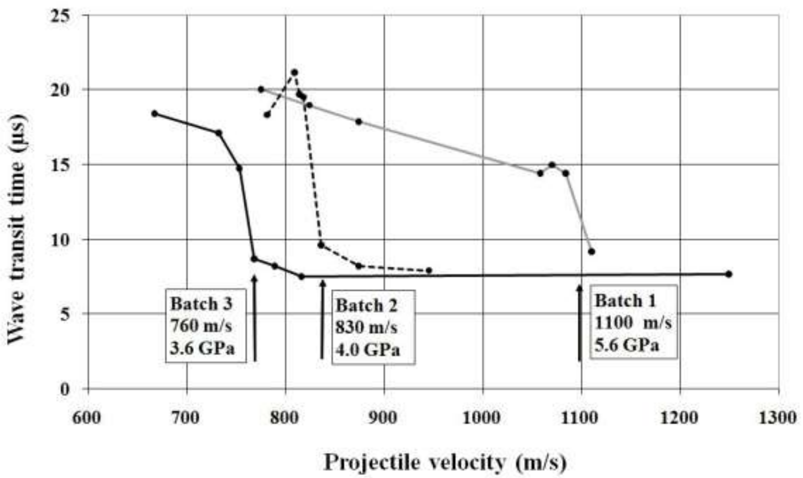
Results for Batch 3
Effect of changing T_0

Example: Borne Experiment (2)

- Numerical simulations qualitatively reproduce experimental trend

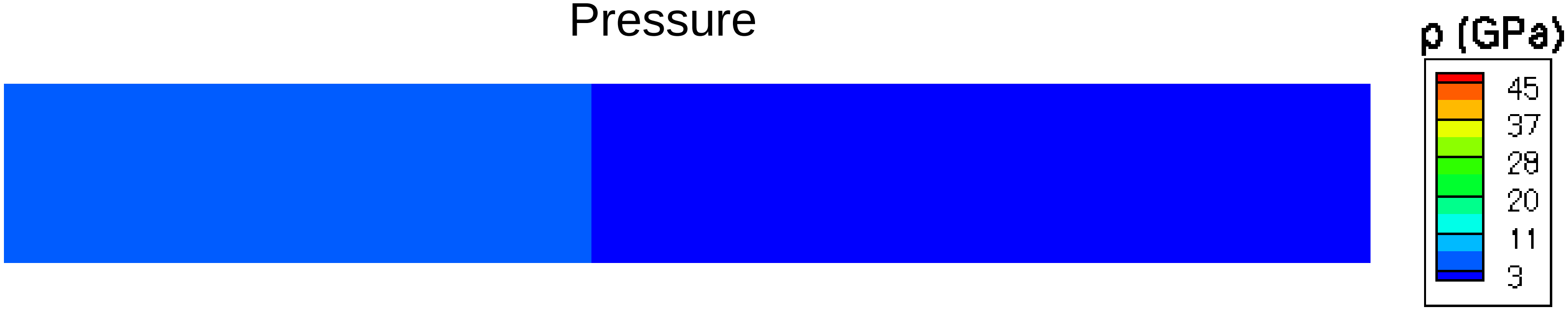






Pressure and Species Contours for Batch 3

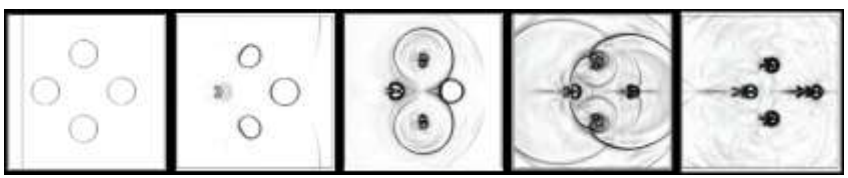
Pressure



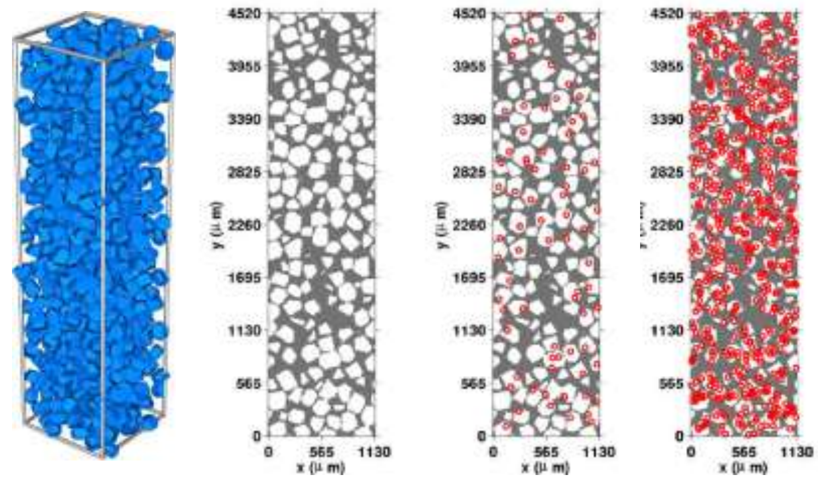
Fraction of reactants remaining

Example: Statistical Hot Spot Model

- Due to grid considerations, it is not possible to resolve both void collapse and heterogeneity at the same time
- Adopt a subgrid modeling approach
  - Subgrid : Simulate a small collection of voids
  - Mesoscale: Use data as input for a statistical hot spot model at the crystal/grain level

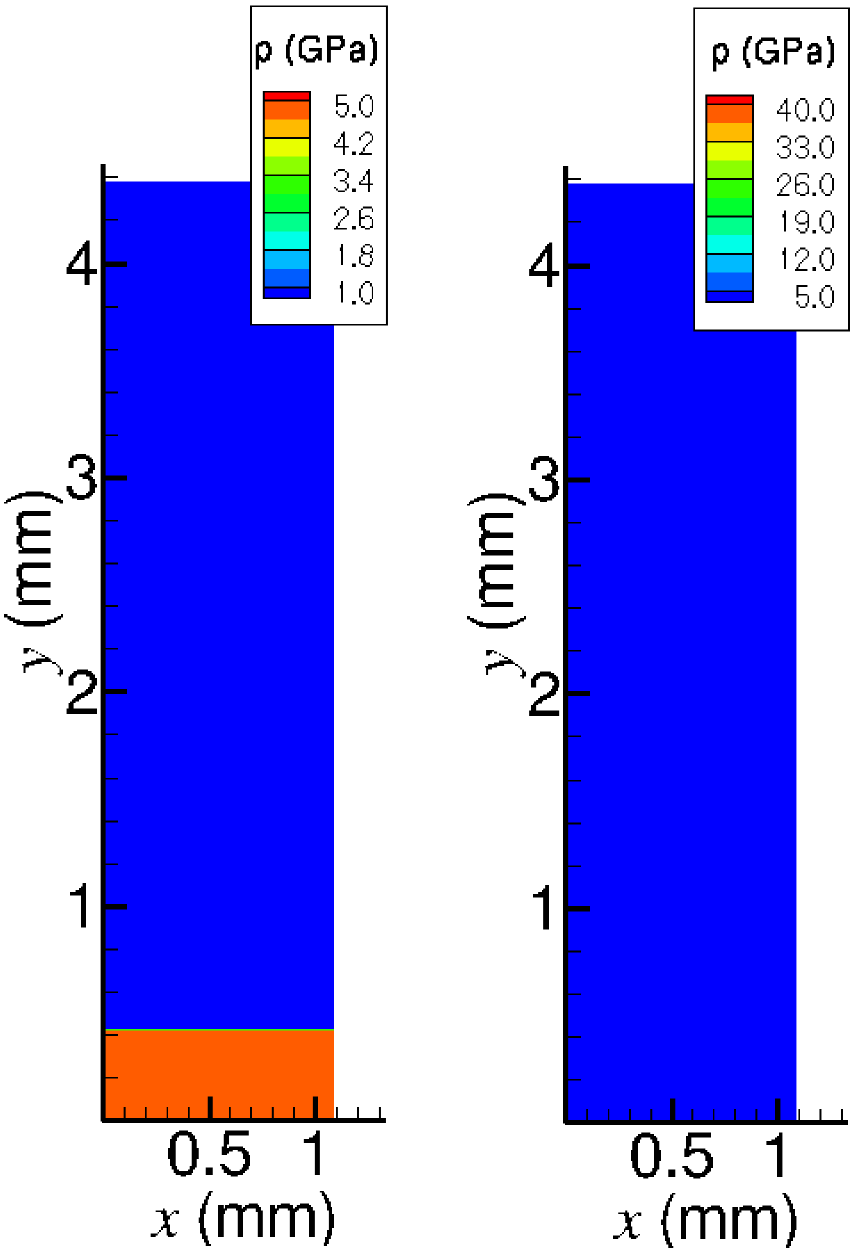


Collapse of four air-filled "voids" by a shock in a stiffened-EOS medium. Numerical Schlieren are plotted.



3-D pack of HMX and corresponding 2-D slices. Also shown are hot spot locations (red circles) for 0.1% and 0.5% voids.

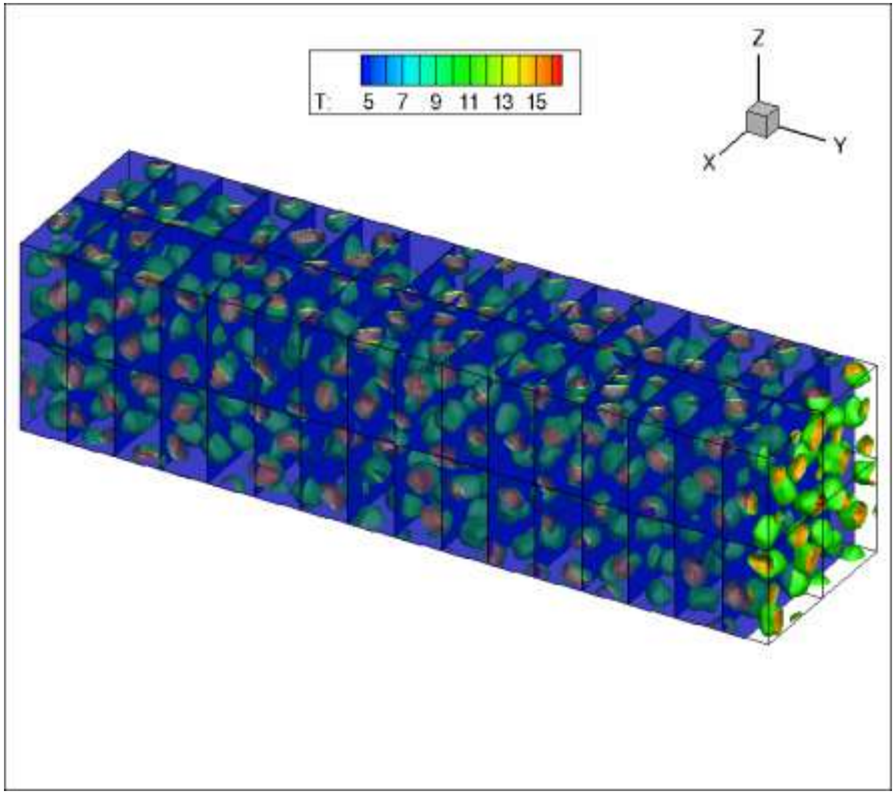
2D Example: Statistical Hot Spot Model



- Pressure fields for 0 (left) and 0.1% (right) void content
- Initial shock 5 GPa
- Sample with higher void content transitions to detonation, in general agreement with Borne (1988)
- Sample without voids does not transition
- Beginning to rerun with new 3-D code

Summary

- Realistic mesoscale microstructures are important for predictive simulations
  - *Rocpack* packs or tomographic scan data may be used
- 2-D *RocSDT* simulations with basic chemistry show qualitative agreement with data
- Interface capturing, density and temperature compression critical to maintaining sharp and stable solution
- 3-D, parallel *RocSDT* under production – will be a core component in *IMSim* infrastructure



Early non-reacting 3-D simulation

Acknowledgements

- This work has been supported by several organizations over 10 years;
  - Department of Energy through the University of Illinois Center for Simulation of Advanced Rockets (Rocpack)
  - An Air Force SBIR through Buckmaster Research (RocSDT)
  - An Air Force SBIR to IllinoisRocstar (RocSDT)
- Continuing work funded by a Phase II SBIR to IllinoisRocstar through Eglin AFB

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Modeling of Void Collapse as Subgrid Component of Mesoscale Simulations

- Mesoscale simulations require the dynamics of void collapse be treated as a subgrid component due to grid resolution constraints
- Goal: Develop a subgrid model for hot spot dynamics that can be incorporated in mesoscale simulations
  - Hot spot model parameters:
    - Ignition delay time
    - Pressure and temperature
    - Time and length scales
    - Void diameter
    - Porosity
    - Etc.
- As an initial effort, we have recently developed a 2-D flow solver with deformation for collapse of single or multiple voids

- Example 1: Wave propagation in heterogeneous medium
  - Propagation of shock through aluminum medium
  - Reflected and transmitted shear and pressure waves observed without spurious oscillations at copper-aluminum interface

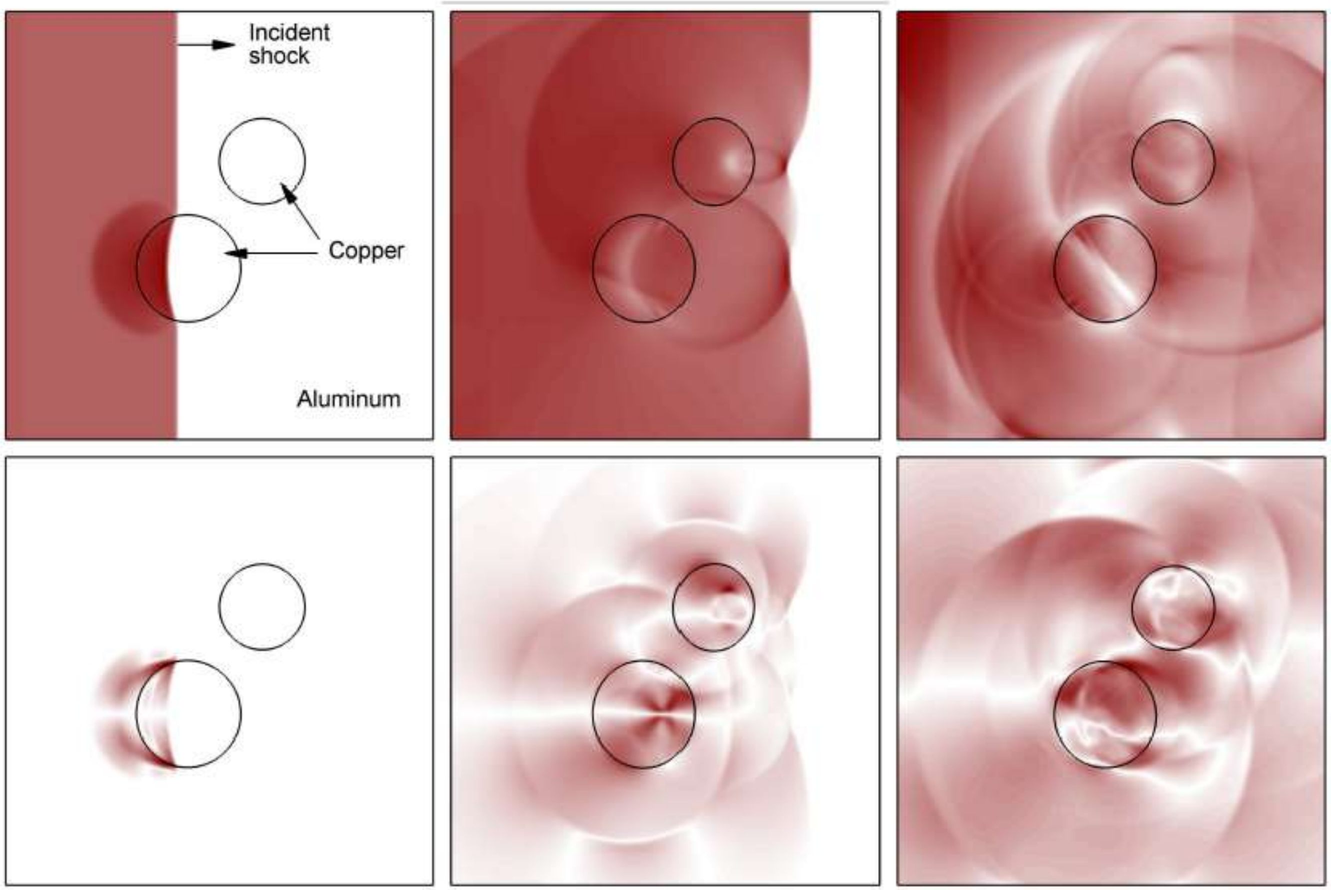

Fig. 1: (Top) Pressure ($P = -(1/3)tr(\sigma)$) and (bottom) shear stress as a function of time.

- Example 3: Two-dimensional void collapse
  - Figure shows collapse of void (air) in copper medium
  - Numerical method stable for high density ratios (~ 10^4) and different EOS
  - Strong pressure and shear waves observed in final stages of collapse

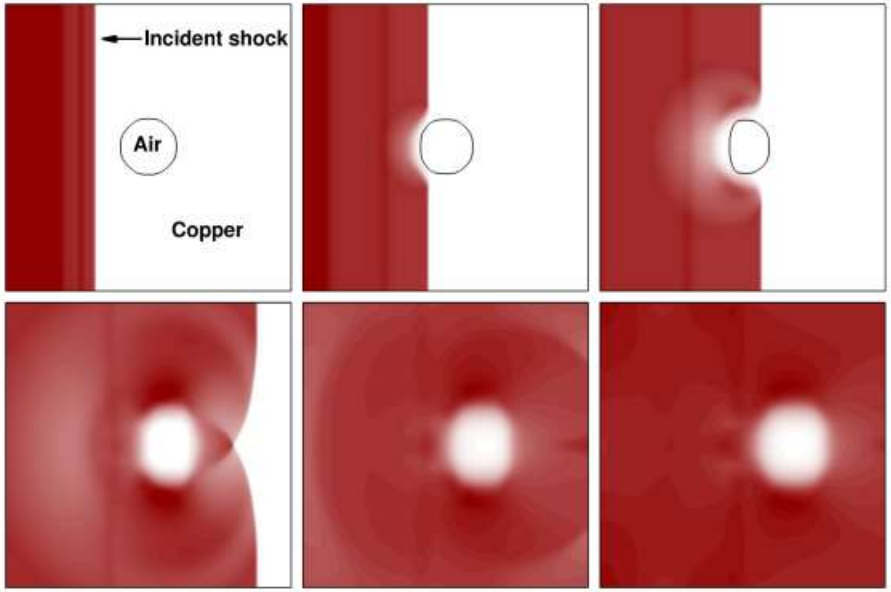

Fig. 4: Pressure contours and $\phi = 0.5$ iso-contour (solid line) as a function of time for two-dimensional void collapse.