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Understanding Enhanced Blast Explosives: A Multi-Scale Challenge

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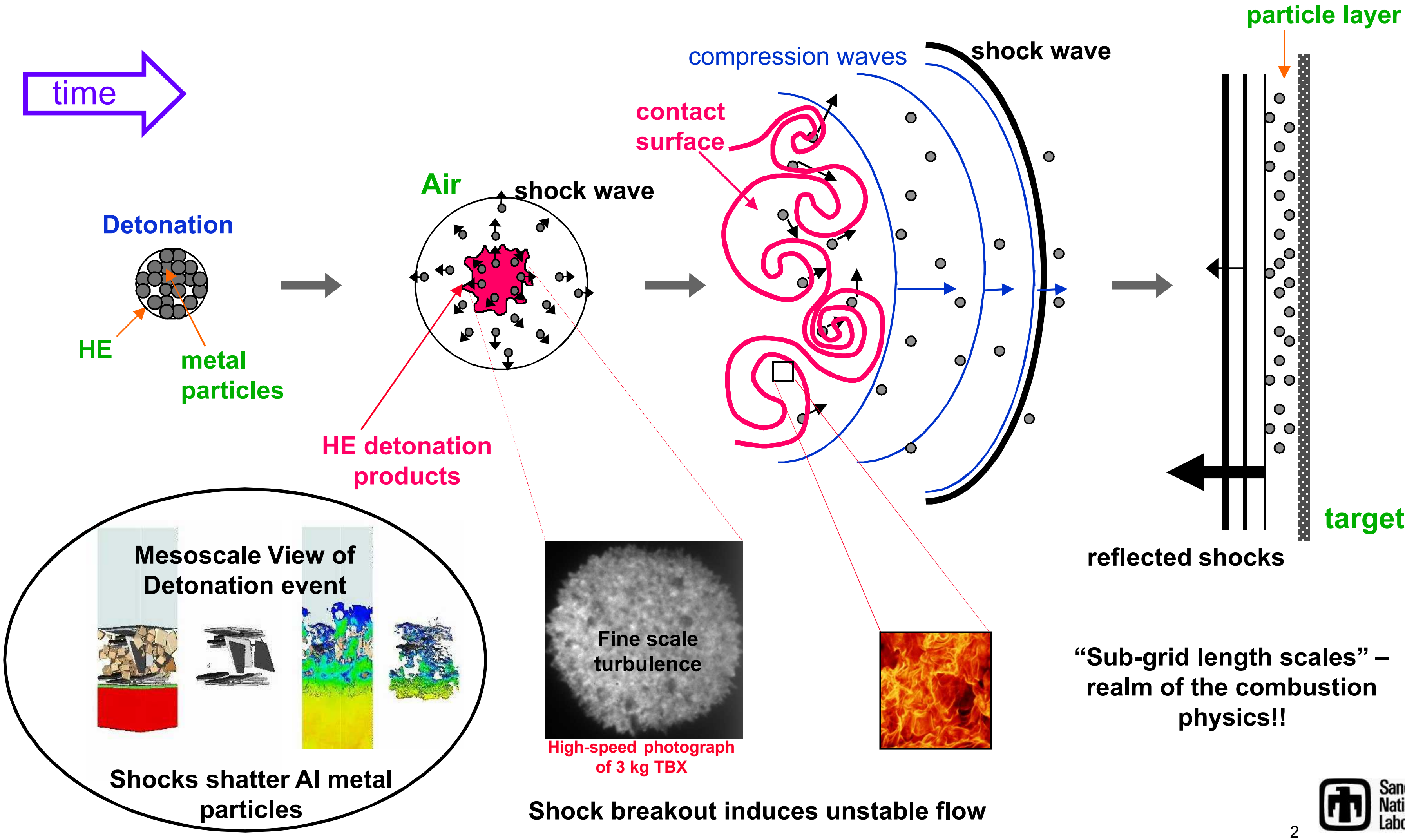
Sequence of “Events”

Flow instabilities induced by expansion / wave interactions and cascade to finer scales



Approach

- Linked modeling-experimental program at SNL
- Goal to develop predictive model of all processes
- Experimental program to
  - Support model development
  - Comparative testing
  - Development of novel diagnostics
- Objectives are coupled and overlapping
- Focus of this talk to highlight modeling efforts and supplement the discussion with examples from experiments

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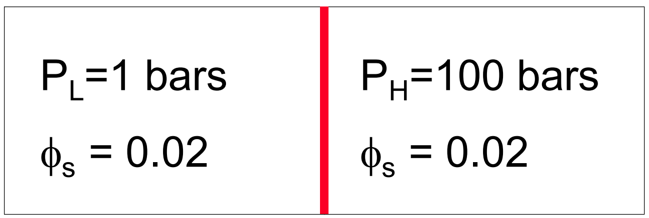
CTH: A Shock Physics Analysis Package

- **Eulerian shock wave physics computer code solving conservation equations of mass, momentum, & energy for multimaterials including gases, fluids, solids, & reactive mixtures**
  - Analytic & Tabular Equation-of-State representations
  - Advanced Strength & Fracture models
  - Adaptive Mesh Refinement
  - High Explosive models
  - Parallel and Serial platforms

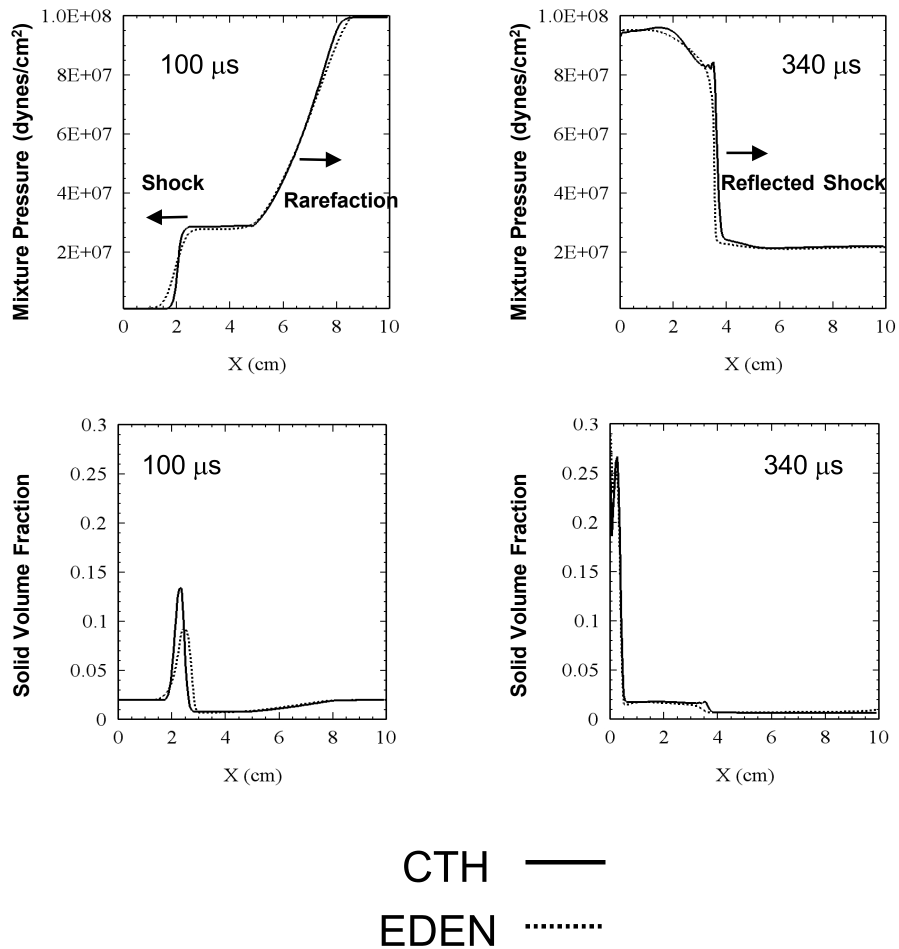
Shock Physics + CFD + Solid Mechanics with multi-material formalism

- **Applications (CTH licensed to over 300 organizations including DOE, DoD, NASA and government contractors)**
  - large strain and/or high strain rate dynamics
  - multiphase interactions
  - examples include: high speed impact, blast-structural loads and deformations, armor/anti-armor, explosive detonation

Dilute Multiphase Shock Tube (1D)



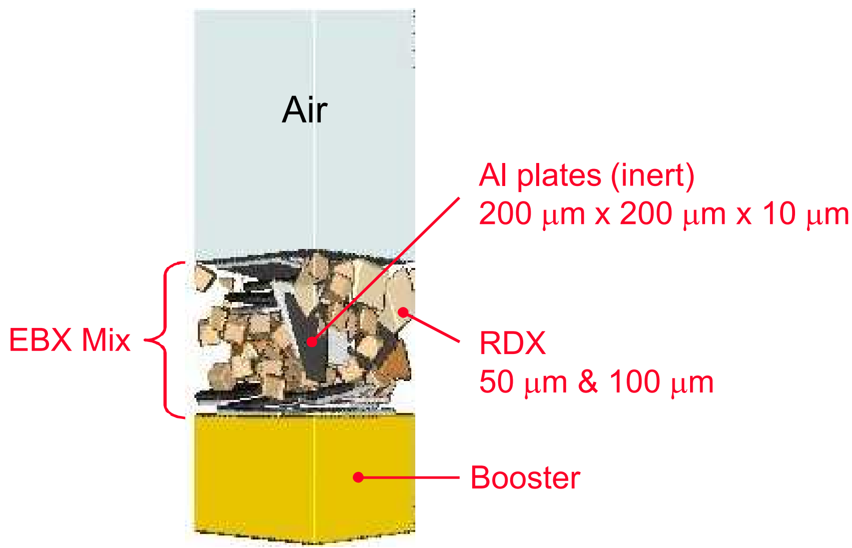
- Multiphase Riemann problem
- EDEN (UK) comparison
- Stiffness issues
- Stability issues
- Similar results observed with 2D example

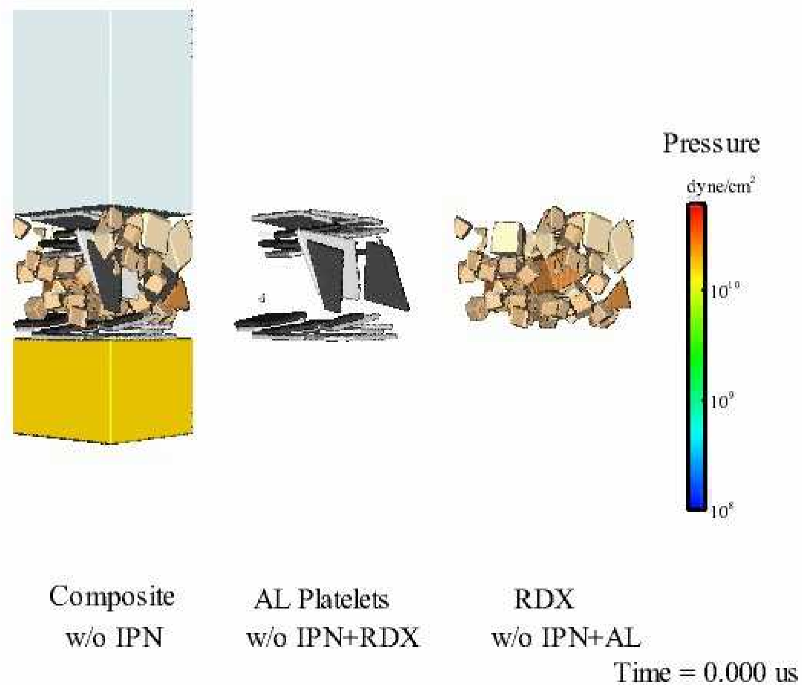


"Initial" Conditions
Detonics Regime (μs's)

- Nonideal detonation state
  - PVT state + initial KE + how much metal reacts prior to breach of confinement + role of constituents
  - partition of energy and dissipation due to case effects (case breakup, localization jetting effects, etc.)
- EOS + detonation wave data for shock physics analysis
- Geometry / properties drive the later stages
- *Combustion dictated by the shocked material characteristics*
- *Morphology and specific surface area of dispersed materials likely to be changed during detonation*

Mesoscale Modeling of an EBX





– Mixture of IPN/RDX/Al, typical composite explosive

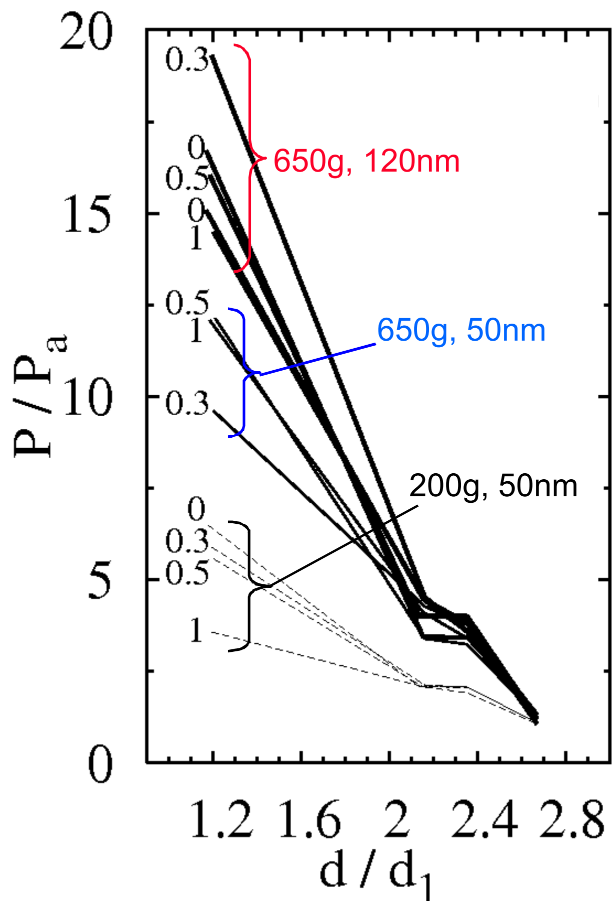
– Shock-induced reaction rates determined by impact testing

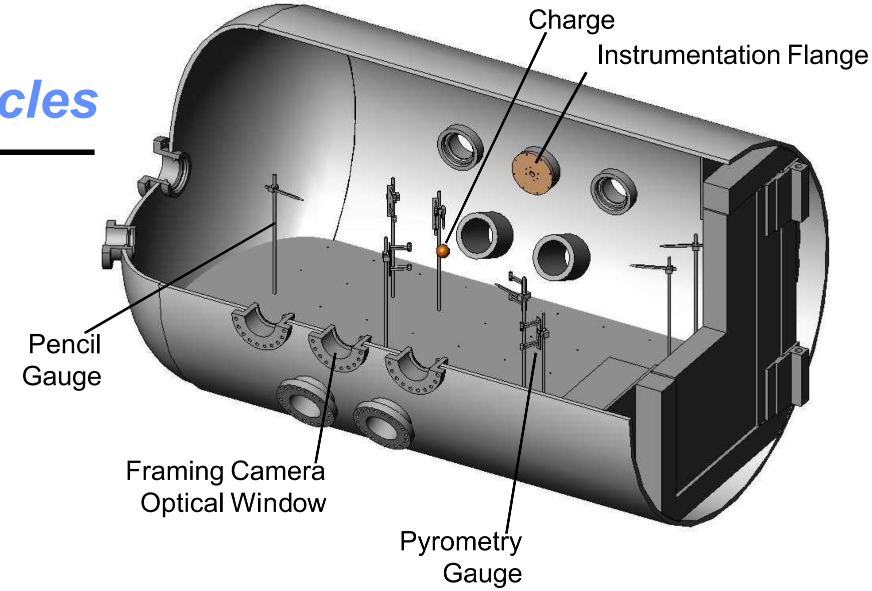
– Shock loading during detonation produces high local stress/strain/fracture

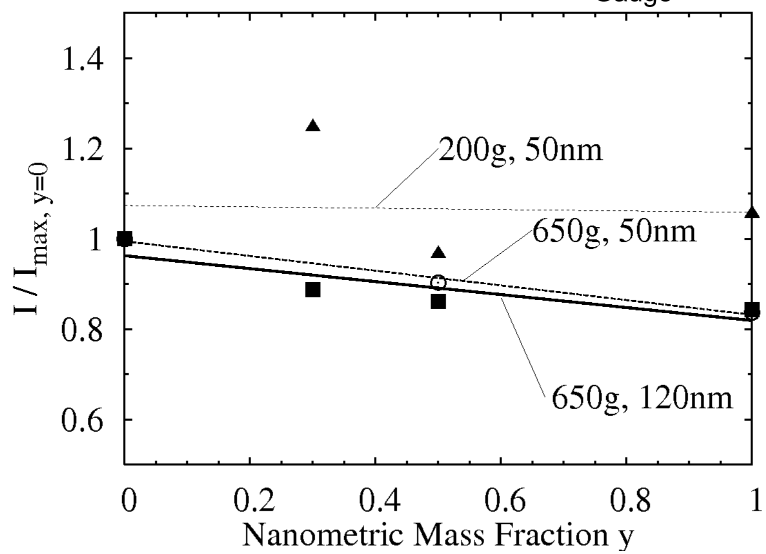
– Al morphology and surface characteristics likely change during detonation

– Prediction of early-time expansion rate

Experiments with Al nanoparticles





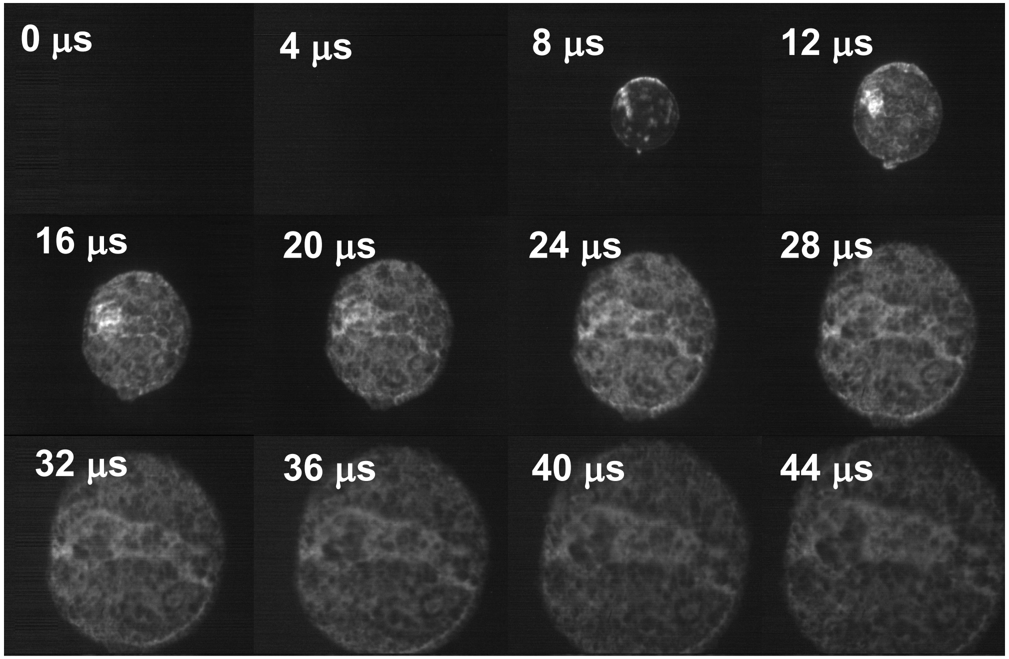


- Varying Al particle size shows differences in blast pressure at early times and impulse at late times

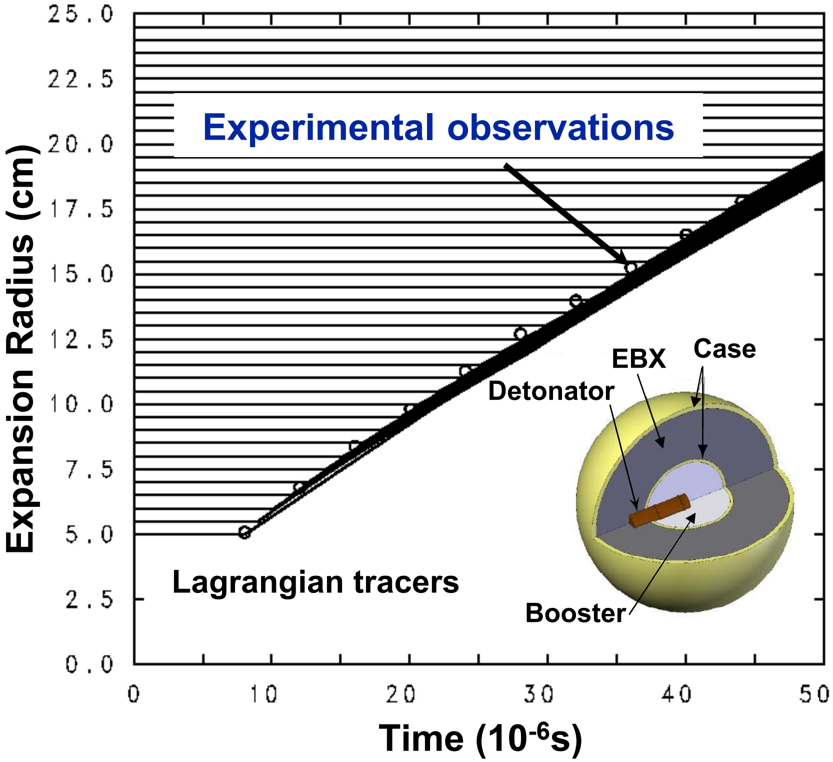
- Impulse decrease with decreasing particle size attributed to increased oxide layer

Spherical Charge Expansion

High speed photography of spherical expansion

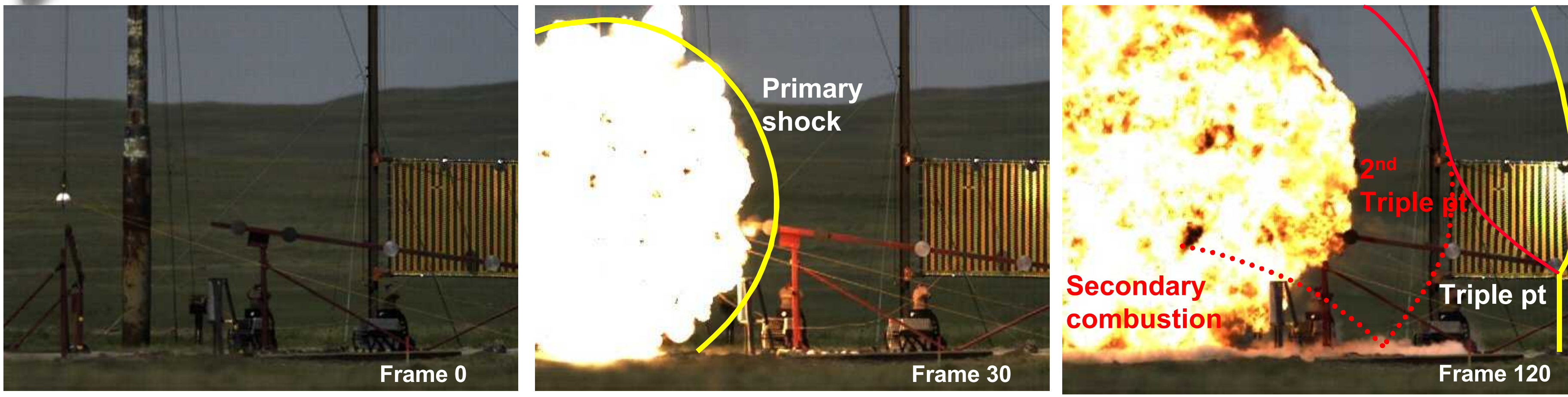


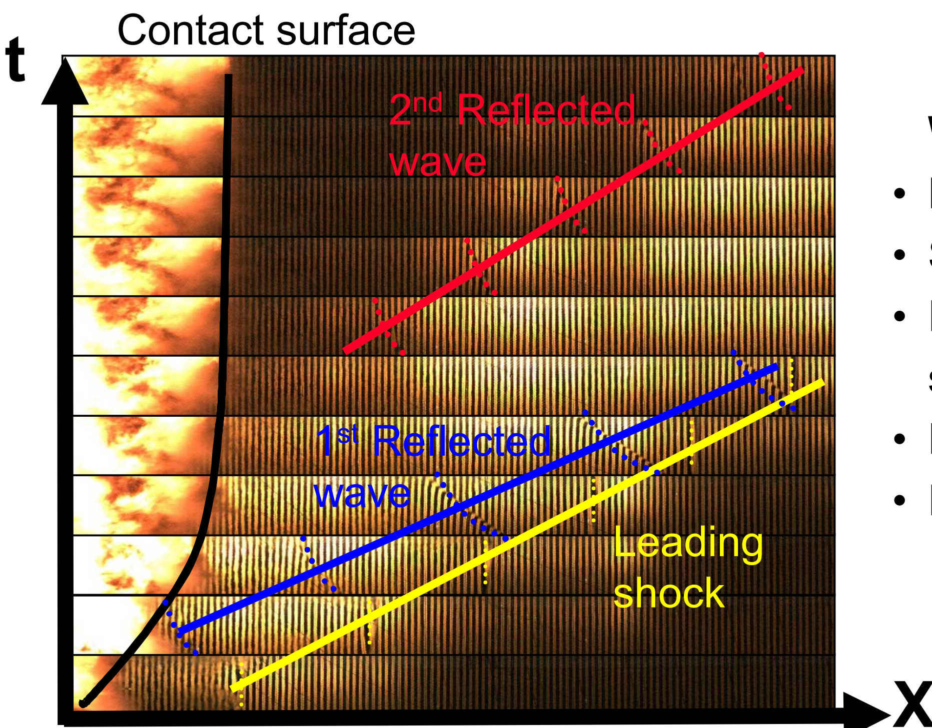
CTH calculation



Detonation modeling predicts early expansion

Post Detonation Secondary Combustion





Wave Features:

- Deceleration of gas expansion products
- Separation of dispersed phase materials
- Formation of large scale jets and turbulent structures
- Heat transfer and reactions with entrained air
- Formation of secondary shocks

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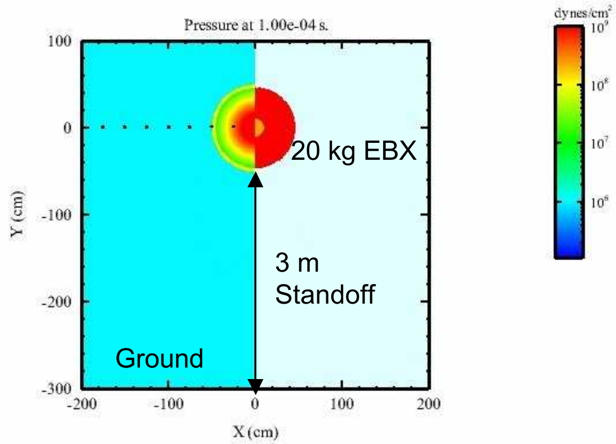
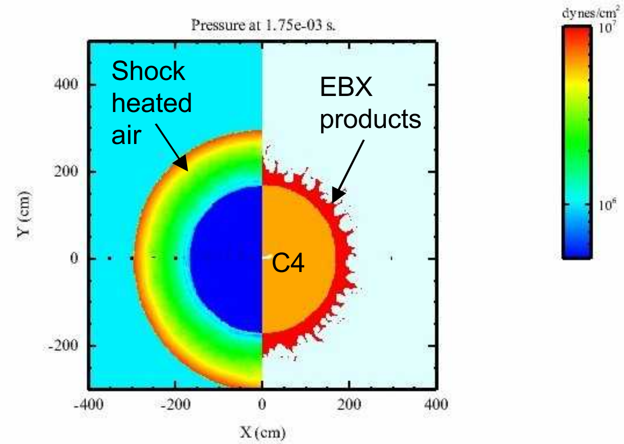
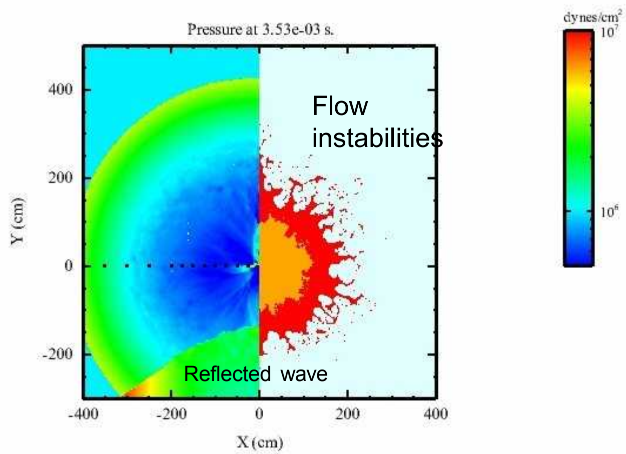
CTH calculation of 20 kg EBX Charge



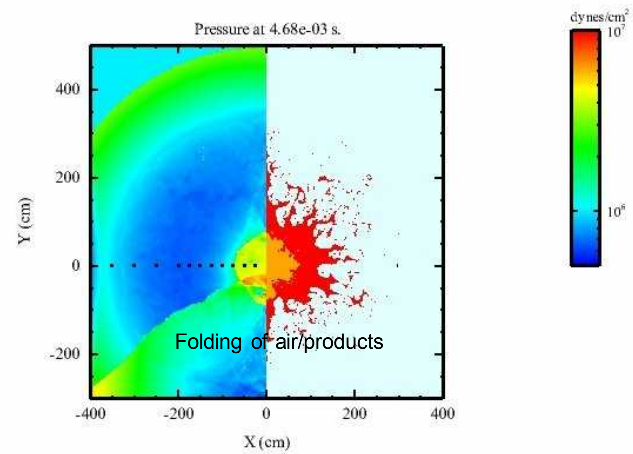
- EBX Detonation
- Shock loading of mixture



- Onset of reflection with ground
- Expansion of booster charge



- Booster collapse
- Onset of reflected waves



- Rebound of booster products
- Shock folding of expansion products

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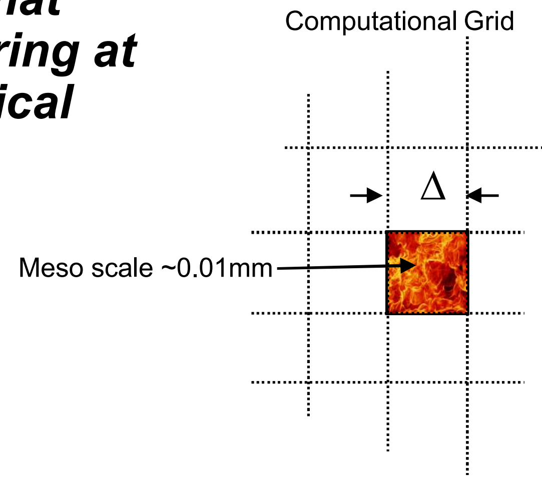
Turbulent Combustion Modeling
PDF formalism

- ***Central idea: define an "averaging" method that extracts relevant combustion physics (occurring at small scales) that can be applied to the practical computational scales***



- A "point" means a distribution of states

  - *i.e.* $\langle\psi\rangle = \int_{\Omega_\psi} f_\psi \psi \, d\Omega_\psi$

  where f_ψ is the probability of the state Ψ in the space $d\Omega_\psi$ such that: $\int_{\Omega_\psi} f_\psi \, d\Omega_\psi = 1$

"The devil is in the details!"

- Description includes species transport and reaction, *i.e.:*

$$\left\langle \frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i \vec{u}) = \nabla \cdot (\rho D \nabla Y_i) + \dot{m}_i''' \right\rangle$$

Key aspect is defining f_ψ

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Overall Modeling Approach

CTH Phase-Averaged Transport Equations

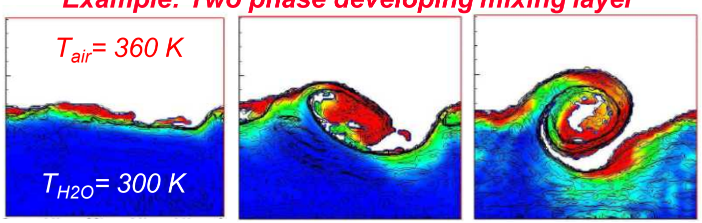
Specify PDF's and define mean and variant states in terms of transport relationships

Moments of multiphase PDF transport equation

PDF SGS Modeling

Solution to full and presumed multiphase PDF for use with LES using Monte Carlo techniques

Example: Two phase developing mixing layer



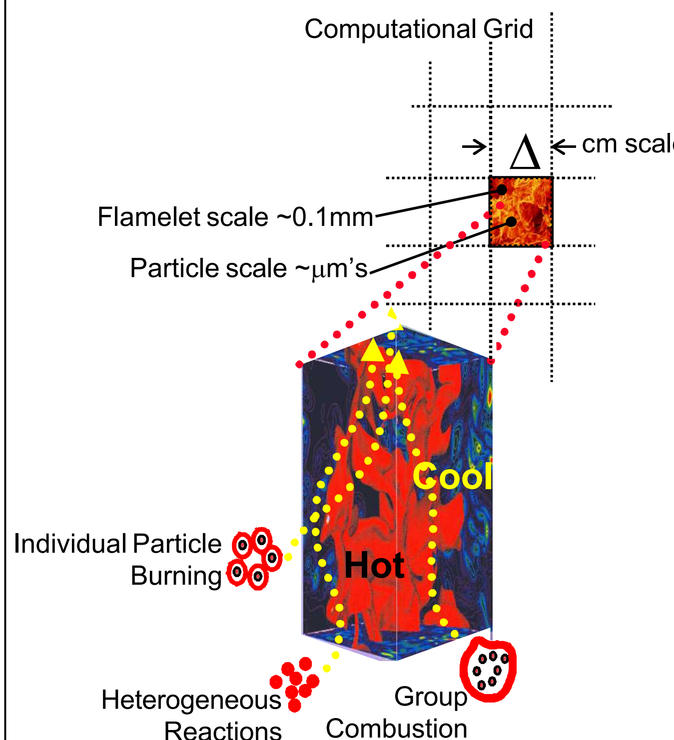
0.125 sec **0.375 sec** **0.75 sec**

Improved single-point micro-mixing models

LEM/ODT Simulations

"DNS-like" information

Mechanistic and Detailed Models of Al Combustion



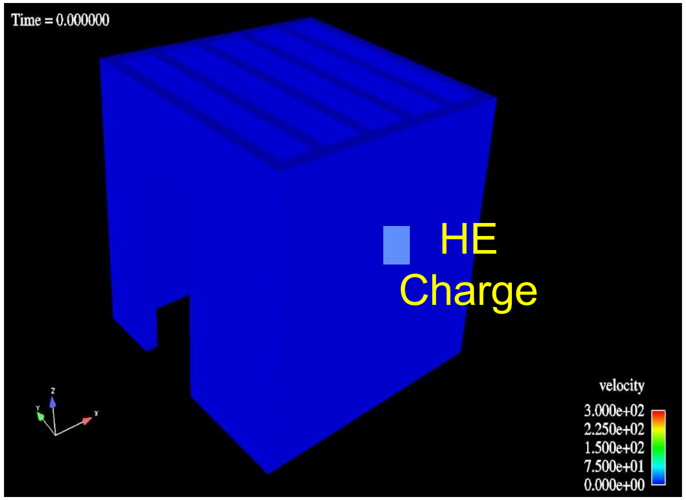
Increasing geometrical complexity

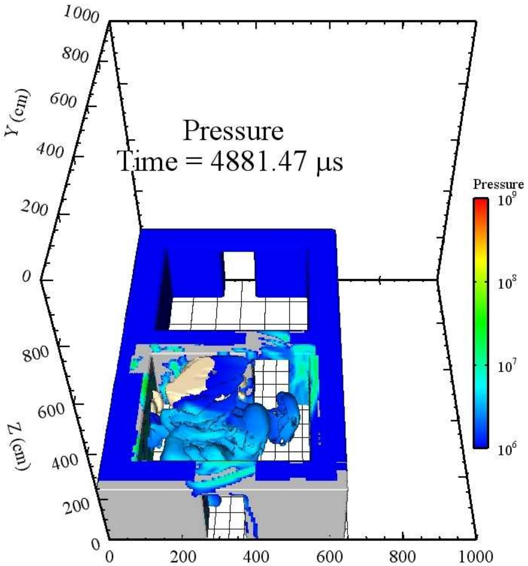
Coupling to Structural Analysis

PRESTO

- Fully Three-Dimensional
  - Massively Parallel
    - Thousands of processors
  - Nonlinear
    - Complicated material response
    - Large deformations
    - Complex interaction of components in contact
  - Solution Method
    - Explicit central-difference integrator
    - Durations of interest: ms

Blast onto single room structure





- Target Modeling
  - Expansion of particle methods (GPA, HPM)
  - Element-to-particle conversion
  - EPIC material models
- Explosive Modeling: CTH
- Coupling Strategies:
  - One-way transfer of pressures from CTH to PRESTO
  - Two-way coupling

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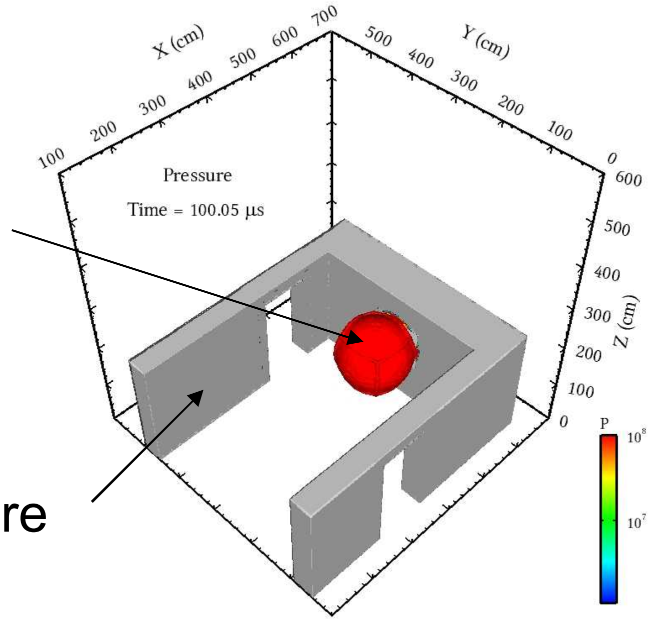
6 Kg Explosive
1.5 m standoff from window plate

H-G Structure



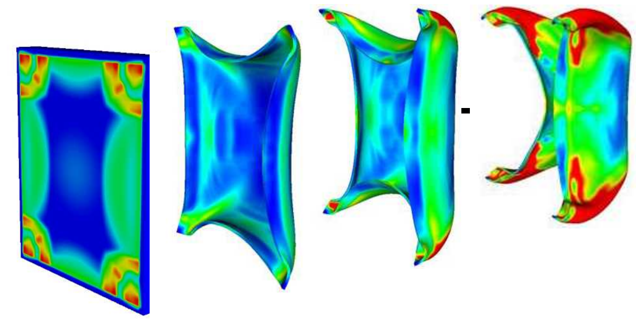
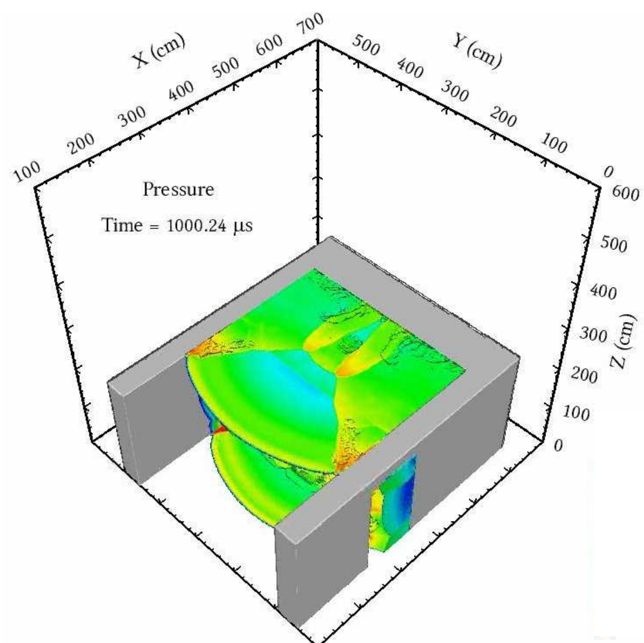
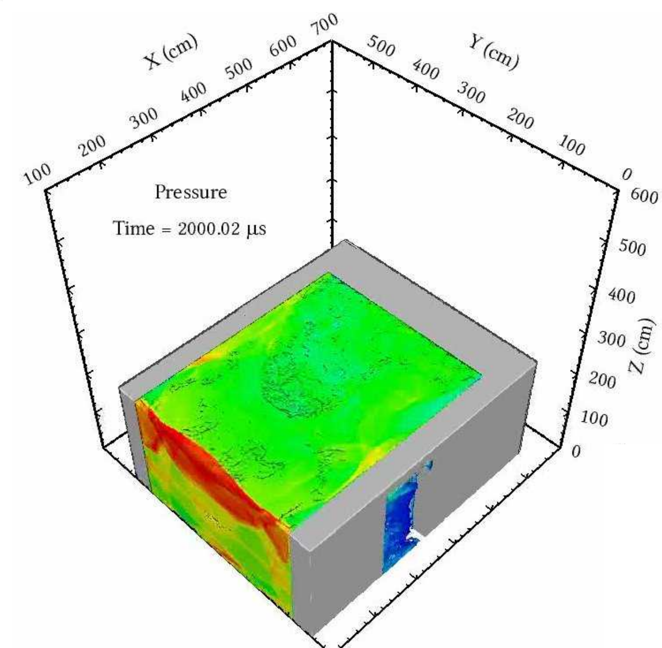


Plate response to blast

(PRESTO calculation)





(CTH calculation)

Reflected blast waves in structure

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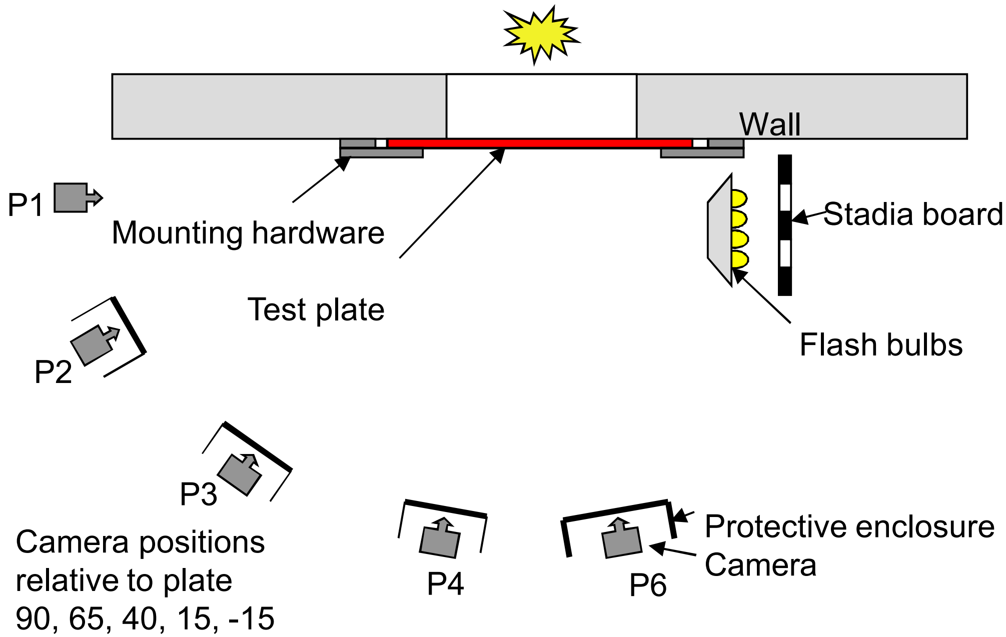
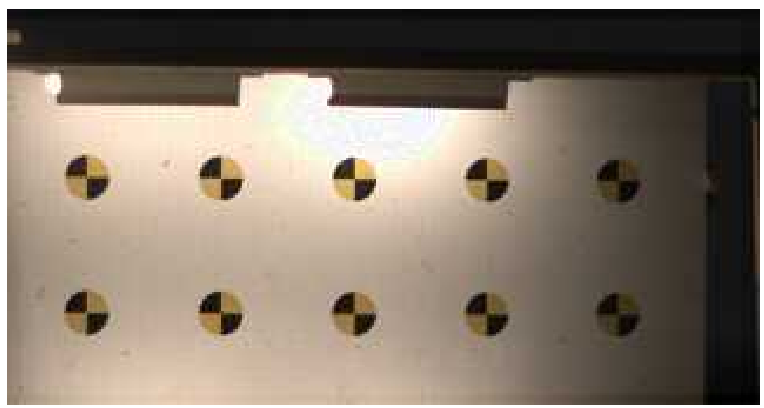
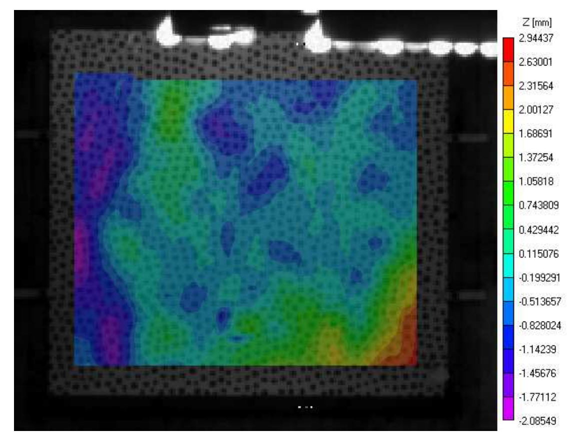
General overhead view of test area



Side view at P3 of plate with spackle pattern



Oblique view at P1 showing reflection and blow by of detonation products



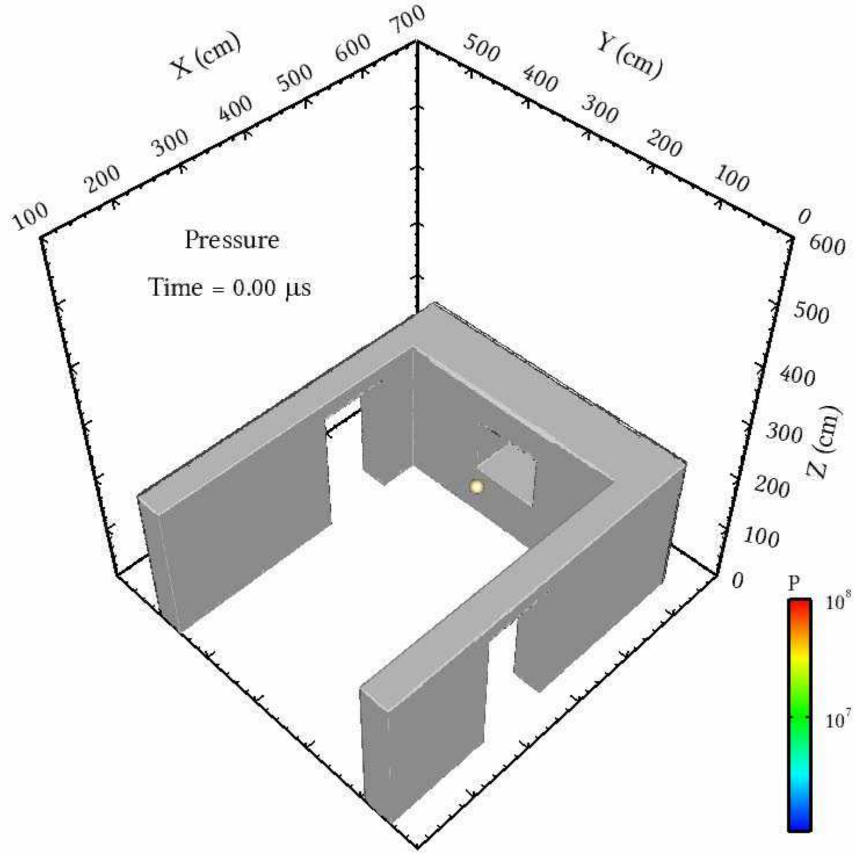
Deformation contours from image post processing

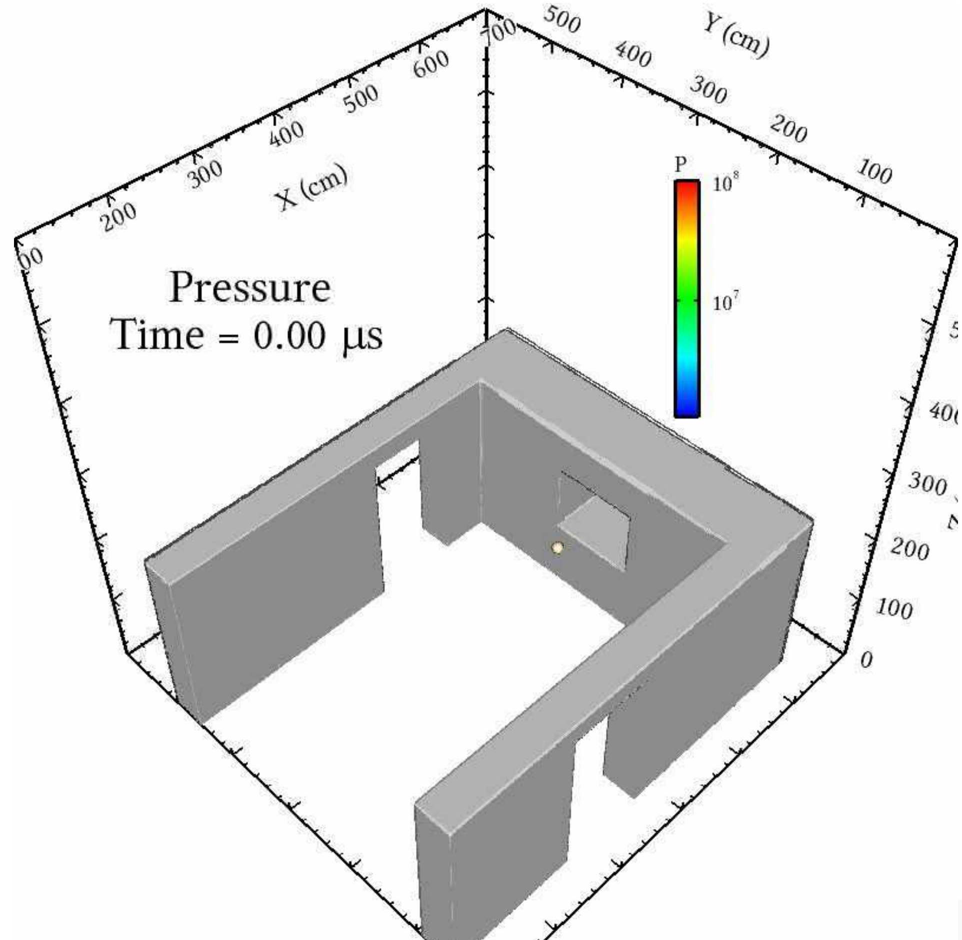
Summary

Multiphase modeling implemented into CTH for dense to dilute flows

- Benchmarking shock tube problems
- Mesoscale modeling suggests that detonated materials are distinctly different than pre-detonated materials
  - Dispersed particulate probably have different particle sizes, morphology and surface characteristics
  - Ignition and combustion characteristics are likely to be different than those associated with a propellant environment
  - Experiments with different metal particle sizes show no significant differences
- Dispersal occurs in shocked heated air – non-ideal real gas effects
- Turbulent flow is induced near the detonation front
  - Jetting and flow instabilities are observed
  - Localization is the nature of multiphase flow
- First generation model applied to chamber and open field tests
- Continuing development of PDF reactive flow for secondary combustion effects
- Coupling to structural analysis (PRESTO) for target assessment

Modeling is still work in progress





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