SAND2008-6386C

Multiphase and Reactive Flow Modeling

Gene Hertel, Sandia National Laboratories
Keo Springer, Lawrence Livermore National Laboratory
Alec Milne, Fluid Gravity Engineering

US UK PA Meeting
Huntsville, Alabama
September 30 and October 1, 2008

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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-AC04-94AL85000.

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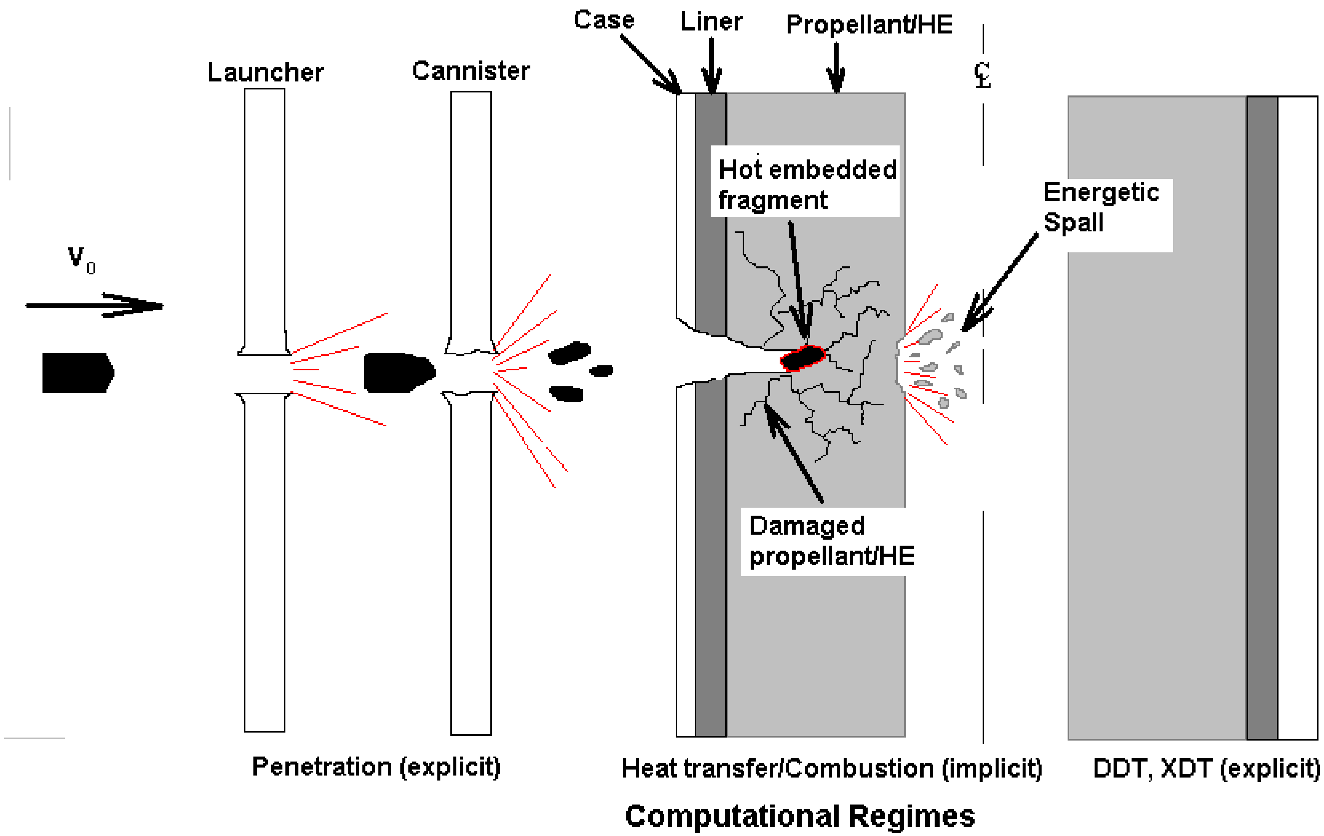
Simulate the Mechanical Insult of a Solid Rocket Motor



- Develop the technology necessary to simulate a mechanical impact into a cased rocket propellant
- AP/AL/HTPB propellant
- Threat typical of a fragment from a nearby explosion or a bullet
- Ultimate goal is to predict the resulting ignition and combustion dynamics leading to violent system response

Accurate prediction of the mass of propellant participating in the response from the mechanical failure of the rocket motor.

Impact Hazards

- **Bullet/fragment impact (SDT, XDT, DDT, and potential thermal ignition)**
- **Develop capability to accurately simulate impact response of energetic materials**
  - **Mechanics and damage models are needed that couple to reactive behavior**
  - **Complex combustion phenomena possible**
    - ***SDT, DDT, XDT, enhanced surface area combustion***
- **SNL JMP tasks are focused on getting SDT right first and then moving to more complicated phenomena for high explosives and propellants**
  - **SNL focus is on Continuum Mixture Theory (CMT) framework for SDT and beyond**
  - **Appropriate physics-based coupled models are being developed and implemented in CTH and the Sierra suite**
- **LLNL JMP tasks are focused on the sub-detonative response of energetic materials, as this area is relatively immature compared to detonative response**
  - **Physics- and chemistry-based models of ignition, damage, combustion, and flame spread are being implemented and integrated within the multi-physics code, ALE3D**
  - **LLNL has developed a multiphase framework within ALE3D for the detailed burning of damaged energetic materials**

Detonations

A detonation is a shock wave supported by exothermic chemical reactions directly behind the shock front

An ideal detonation exhibits a nearly planar wave structure with all of the energy release occurring within the sonic surface

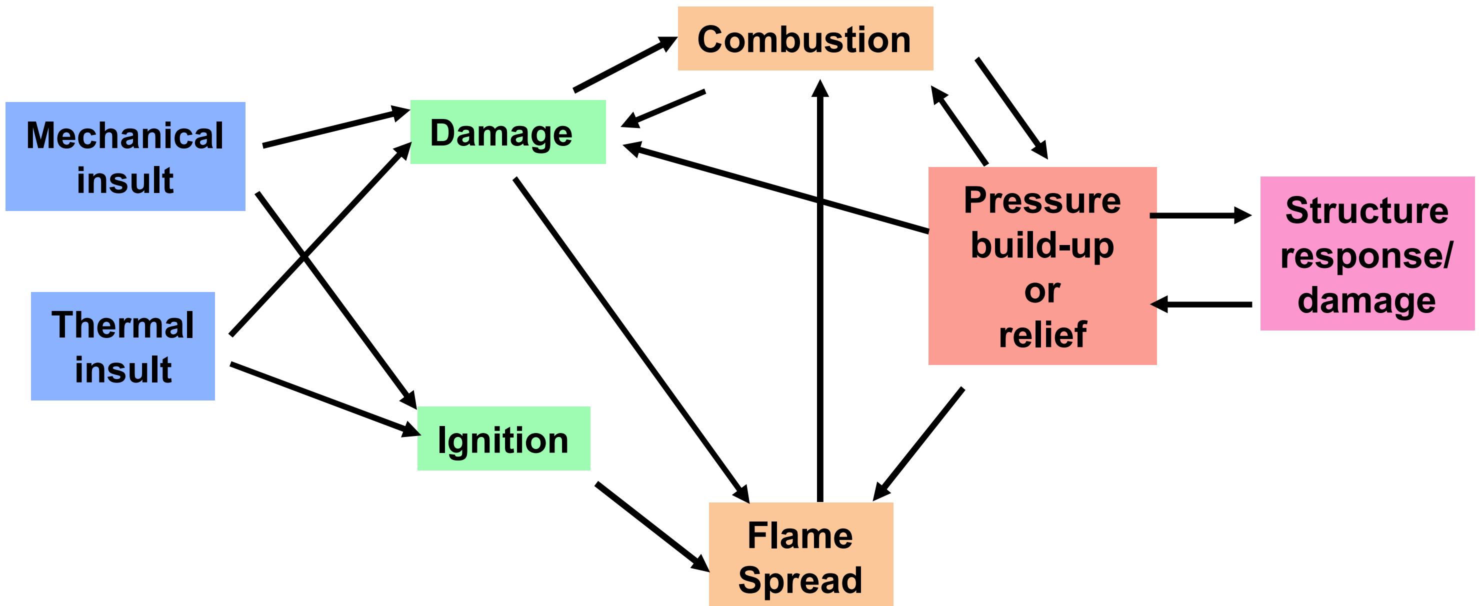
A non-ideal detonation exhibits non-planar wave structure with extended energy release occurring behind the sonic surface

A non-ideal detonation can also have non-steady reactive wave speeds, strong geometric dependencies, different scaling laws (blast versus cratering), etc

Phenomena

- **1.3 propellants do not support ideal detonations**
  - **That's why the were placed in the 1.3 hazard class!**
  - **They can release a substantial amount of total energy under hazards conditions**
    - ***Energy release of 1-10% from a 10,000 lb motor can really spoil your day!***
- **All current reactive flow models (HVRB, PMOD, IG, PERMS, …) are not predictive for energy release simulations for propellants**
  - **All current reactive flow models can be correlated to any single experiment but not to multiple experiments**
  - **All current reactive flow models are not based on the right physical processes for propellants reactions due to impacts**
    - ***Substantial energy release occurs behind the sonic surface (delayed in time and space)***
    - ***The energy release can't be correlated to only pressure***

Physical and Chemical Processes Critical to Understanding Impact Response



Predicting system response requires an understanding of each process and the coupling between processes – basis of the multi-physics model development

Technical Challenges

- Combustion dynamics
  - Models/theory and dynamics of various modes of combustion
  - Normal surface regression (conductive)
  - Enhanced surface area combustion (convective)
  - Enhanced volumetric combustion modes
- Ignition Criteria
  - Models/theory/algorithms and numerics
  - Energy localization leads to Hot Spot formation
  - Hot-spot growth/coalescence leads to ignition
  - Statistical representation of temperature and chemistry
- Flame spread
  - Models/theory/numerics
  - Transition of ignition into flame propagation
  - Transition into combustion dynamics regime

Technology Gaps

- **Experimental diagnostics**
  - **Necessary for development of understanding and models**
- **Mechanistic understanding of processes**
  - **Mechanics, localization, ignition, growth, decay**
- **Appropriate mechanics and chemistry models**
  - **Composites and energetics**
- **Numerical algorithms and models**
  - **Hydrocode models and assumptions**
  - **Implementation details**
  - **Processes are complex and coupled**
  - **Hybrid numerical algorithms with multiscale technology**
    - ***Resolution of appropriate length and time scales***
- **Methodologies/strategies for verification/validation/confidences**
  - **Statistical response requires probabilistic interpretation of experimental data and numerical simulation**

Modeling Paradigm

- Capability to treat multiphase reactive flow
  - Thermodynamic consistency
  - Combustion dynamics
- Coupled mechanics/damage/reactivity
  - Mathematical formulations
  - Appropriate constitutive models
  - Processes inherently coupled and models must be developed with this in mind!
- Sub-grid scale technology
  - Resolution of appropriate time and length scales
- Numerical algorithms, mathematics and models
  - Models and assumptions
  - Codes: shock physics, transient dynamics, quasi-static mechanics, heat transfer, various coupled physics applications
- Critical need for phenomena discovery
  - Translation into appropriate theoretical models
  - Implementation into appropriate code suite

Modeling Tasks

- Multiple computational/numerical frameworks
- Coupled mechanics, damage, and chemistry
- Statistical representation of key processes

- SNL plans on using multiphase and continuum mixture concepts but the focus is a physically based model(s) for reactive wave phenomena in AP/Al/HTPB propellants
- LLNL plans on using the multiphase framework for the propellant burn-to-violent reaction (BVR)
  - Initially synchronize the multiphase model to PERMS for a generic AP/Al/HTPB propellant
  - Long-term: Development of energetic material BVR model within multiphase model framework that includes Al after-burn (with in-line Cheetah)

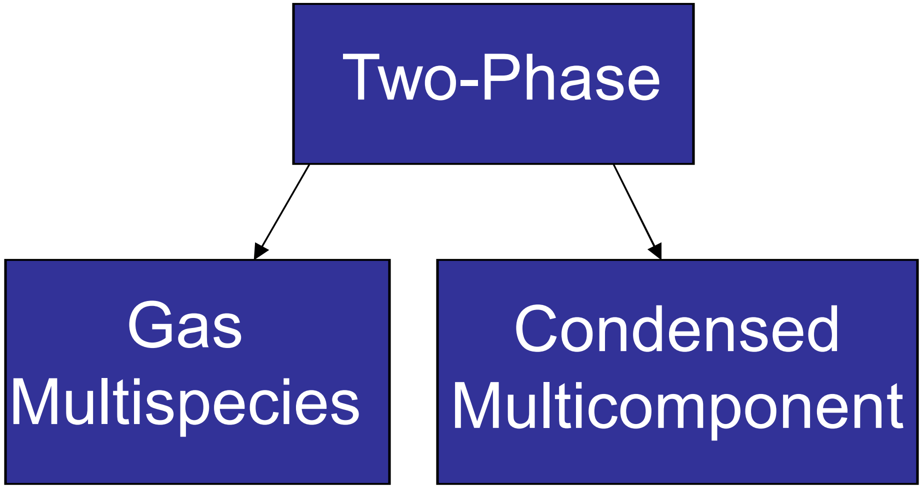
SNL Propellant Modeling Program

SNL PA Modeling Task

Task	Status	Date
PMOD model development	Complete	
Initial CDAR model development	Complete	
N9 SITI experiments	Complete	
Initial multiphase flow model development	Complete	
HPP samples to SNL	At Risk	ASAP
SITI experiments on HPP	At Risk	9/1/2008
HPP characterization experiments	On Track	10/1/2008
Initial CDAR-K model development complete	On Track	10/1/2008
CDAR-K into production CTH	On Track	11/1/2008
HPP parameters for CDAR-K	On Track	12/1/2008
CDAR-K simulation of single BFI into HPP analog motor	On Track	12/1/2008
CDAR-K simulation of single BFI into HPP motor	On Track	12/1/2009
CDAR-K simulation of multiple BFI into HPP motor	On Track	12/1/2009
Coupled thermal/mechanical/chemical/flow model for energetic materials	On Track	9/1/2010

SNL Propellant Modeling Overview

- **Multiphase is really two-phase Baer-Nunziato**
- **Goal is to enhance modeling capabilities for reactive wave phenomena in propellants**
- **Also used as a framework for development of physically based initiation/detonation models**
- **Approach is to use the two-phase treatment and expand the capabilities by adding multispecies and multicomponent Equations of State**



Multiphase Flow Phenomenology

- ***Applications driving investment are:***
  - *IM/Hazards; modeling initiation and growth of reaction front in energetic materials*
- ***Capability must include:***
  - *All aspects of reactive wave development in energetic material where strength and damage state of solid phase must be physically modeled*
  - *Break-out of reaction wave and formation of steady state behavior with appropriate sub-grid chemistry and physics*

Detonics and Non-Ideal Behavior

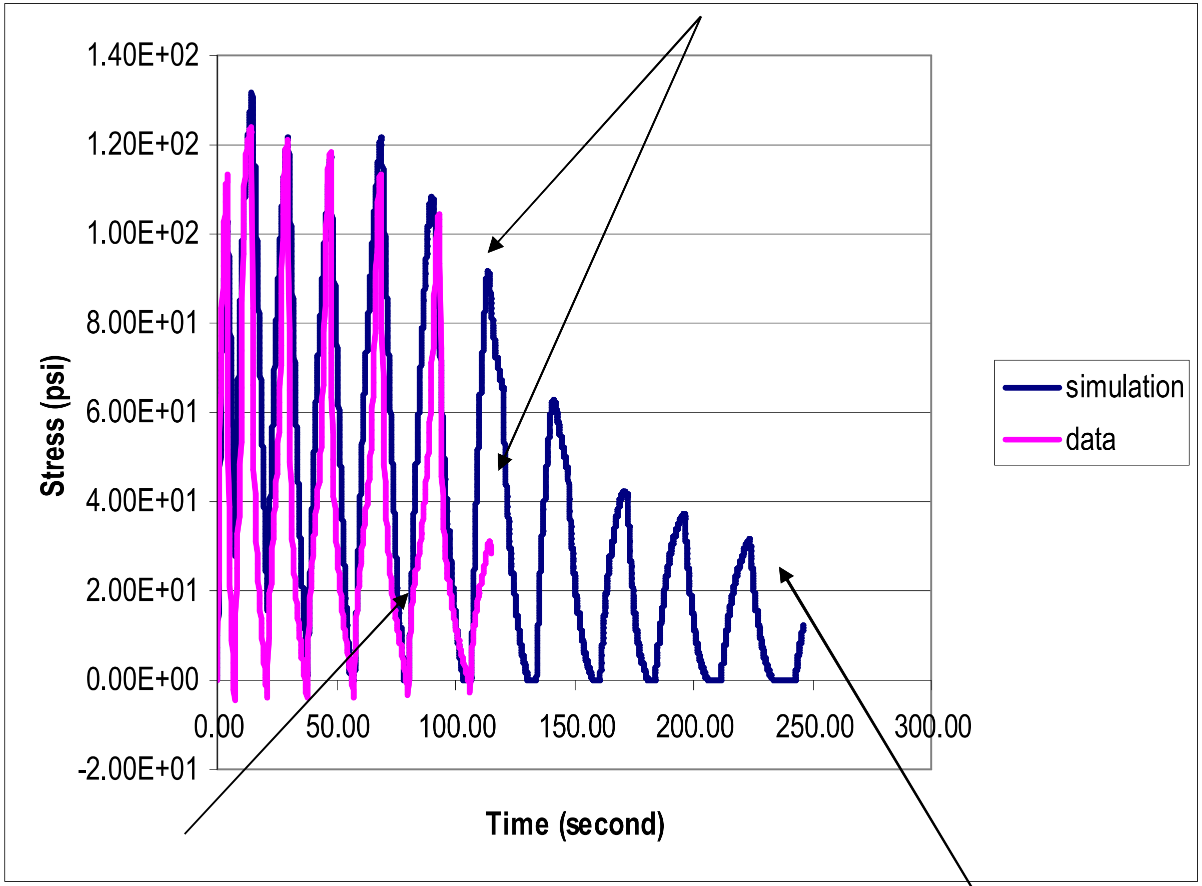
- ***Eulerian formulation for solid and gas***
- ***Model reactions from detonations to highly non-ideal sub-detonation***
- ***Physically represent solid phase(s) EOS, strength and damage evolution from mechanical or thermal insult***
- ***Couple solid mechanics (stress tensor and damage state) to the initiation and subsequent growth of chemistry including kinetics***
- ***Represent sub-grid physics and chemistry from the reaction front to the late time reactions behind the reaction front***

SNL Propellant Modeling

- **Coupled Damage and Reaction Model with Kinetics (CDAR-K)**
- **Multiphase reaction response**
  - Grain burning
  - Gas generation
- **Clearly demonstrated capability to capture:**
  - Hypervelocity impacts on rocket motors
  - Complex response of various materials
  - Damage modes unique to solid propellants
- **Damage algorithms in CDAR-K have been updated**
  - Matches stress history data for the cyclic test
  - Additional cycles beyond the actual test cycles were added demonstrating how the stress drops as propellant is damaged
  - Wave profile and spall tests correlations completed
  - Taylor test shows damage as observed in the data
  - Damage algorithms/parameters unchanged from those for the cyclic test
  - CDAR-K correlated to a sequence of shadowgraphs showing overall deformation in the Taylor rod experiment
- **An initial calibration of the CDAR-K fragmentation algorithm against shotgun/combustion bomb data has been completed**
  - Matches the experimental fragment specific surface area data from shotgun/combustion bomb data

Cyclic Test Stress History

End of data/
beginning of artificial cycles

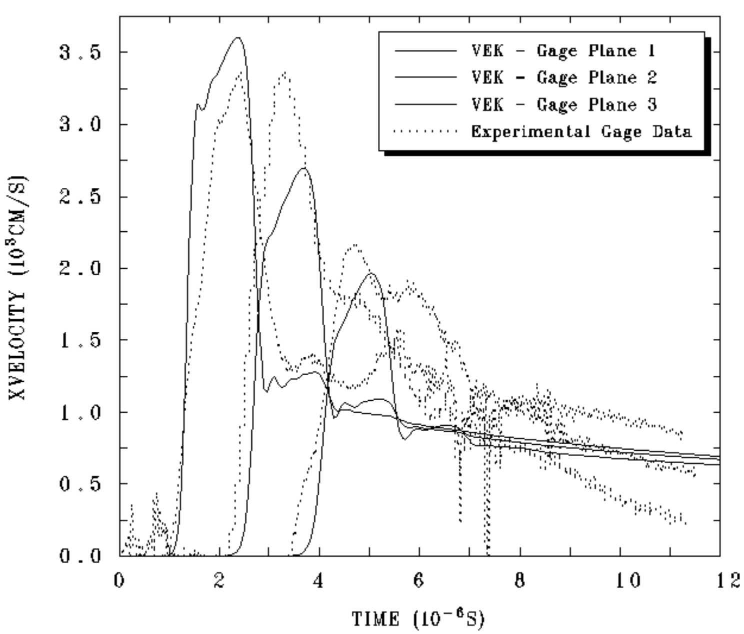


Scission damage starts
at this point in the test

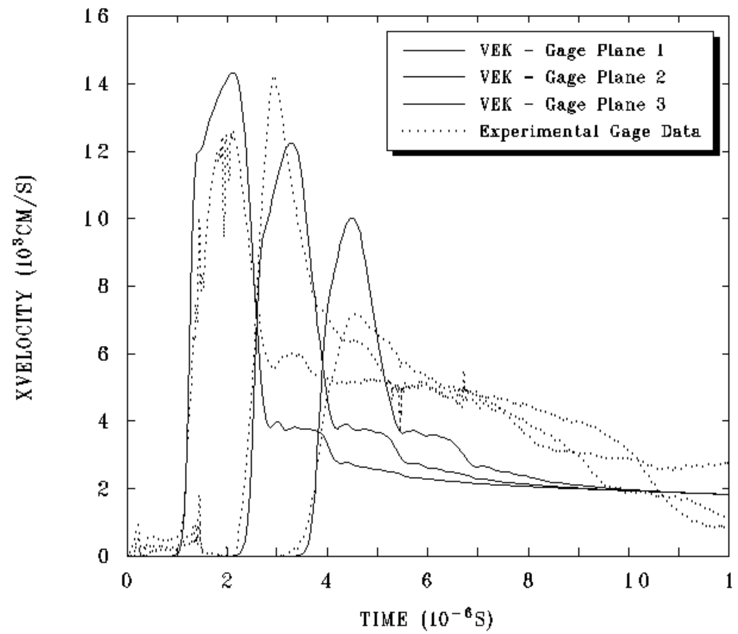
Stress drops as material
is damaged

Wave Profile Tests

Model matches at two different velocities

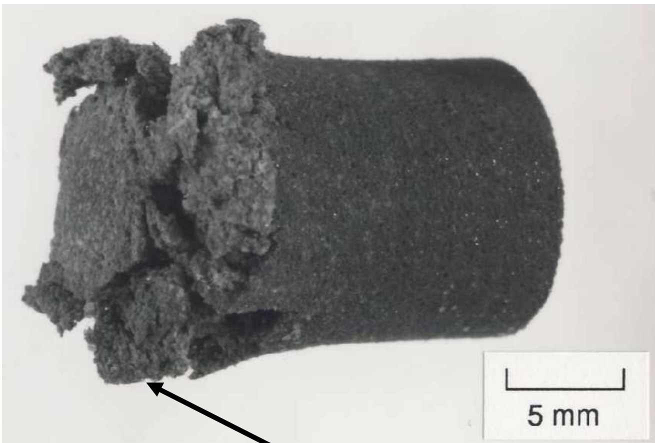


1D Wave Profile Test Simulation for HTPB 76 m/sec
KZJBGK 11/26/07 09:14:05 CTH



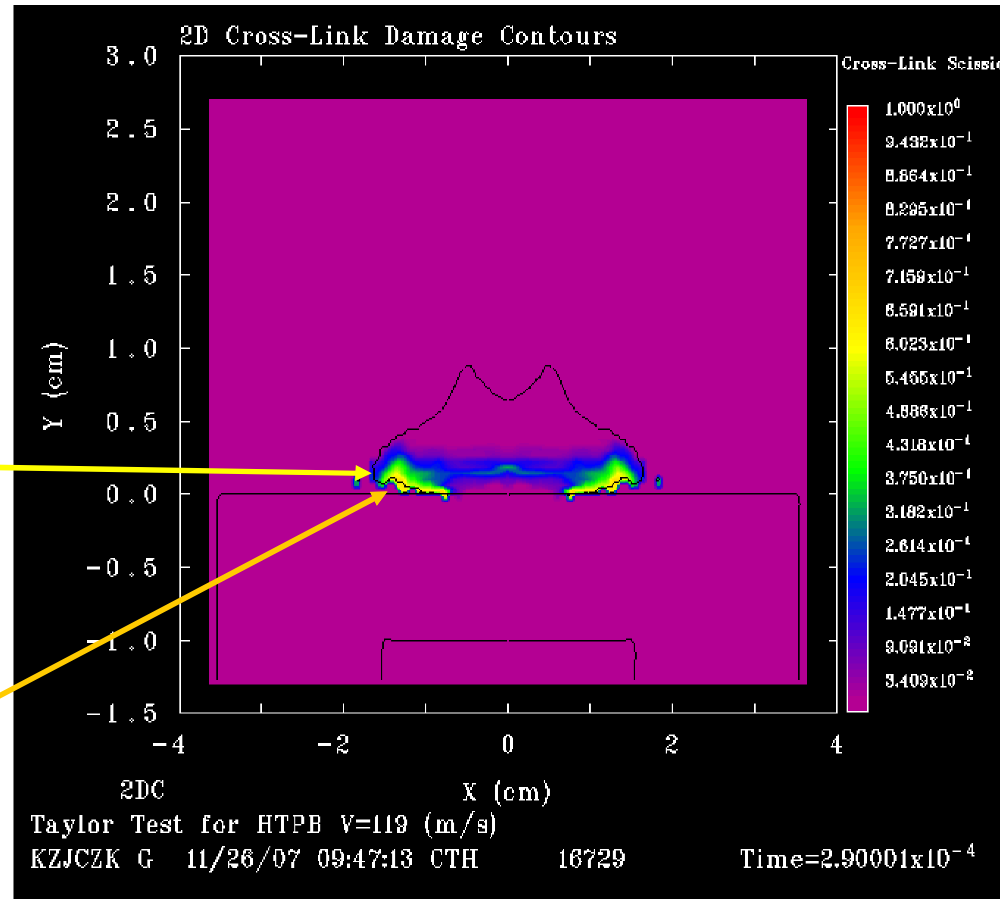
1D Wave Profile Test Simulation for HTPB 273 m/sec
KZJBMZ 11/26/07 09:16:56 CTH

Taylor Rod Impact



damage

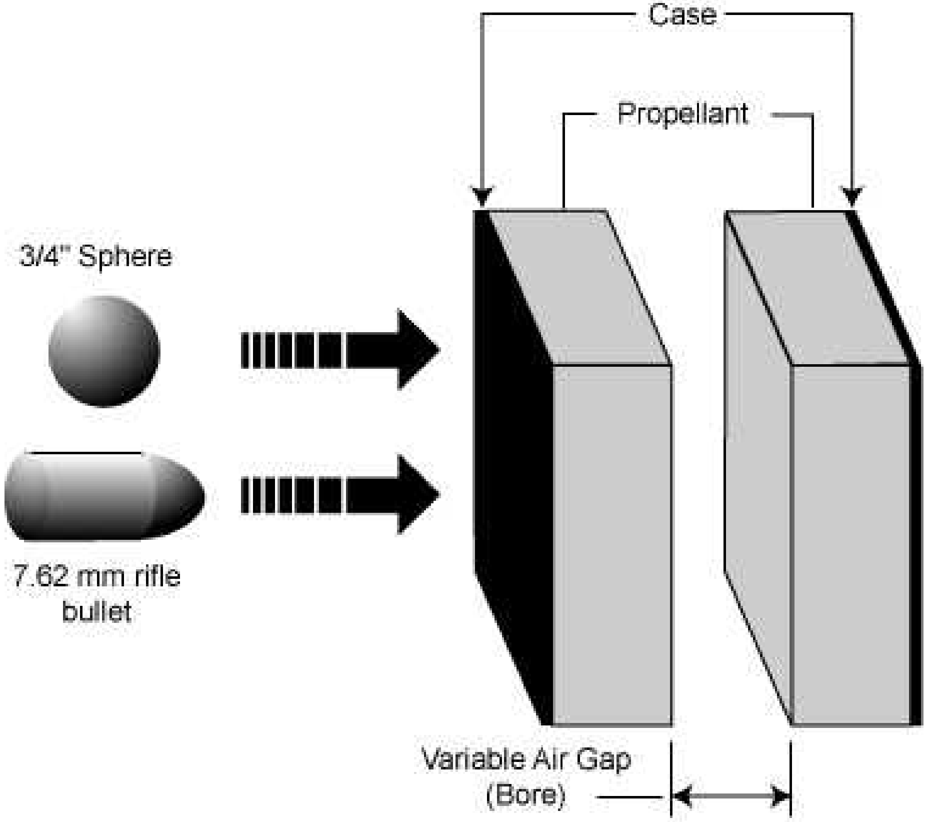
partial lift-off

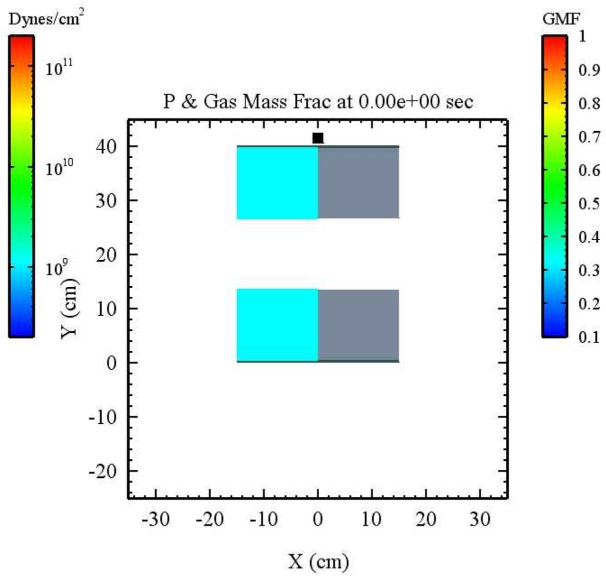


Reaction Model

- Initiation mechanisms (pyrolysis phase)
  - SDT: Shock compression (density change)
  - DDT: Compaction of scission porosity
  - XDT: Compaction of decohesion porosity
  - Shear initiation (future effort)
  - Except for DDT, reaction products fill decohesion sites
- Transition to detonation
  - Grain regression at decohesion pore surfaces (all mechanisms except DDT)
  - Grain regression at crack/fragment surfaces for DDT

BVR-Like and IM Bullet Fragment Setup

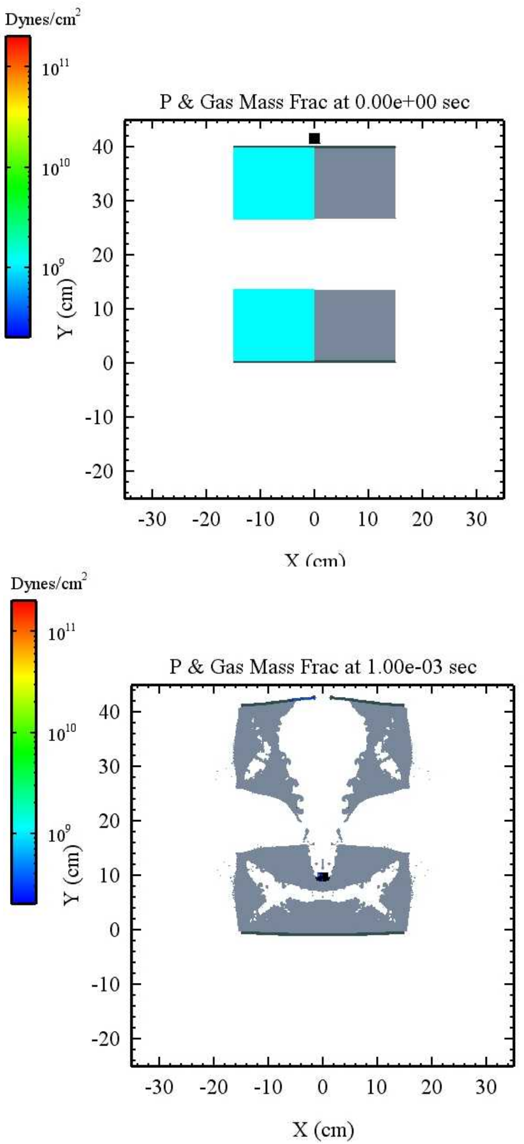




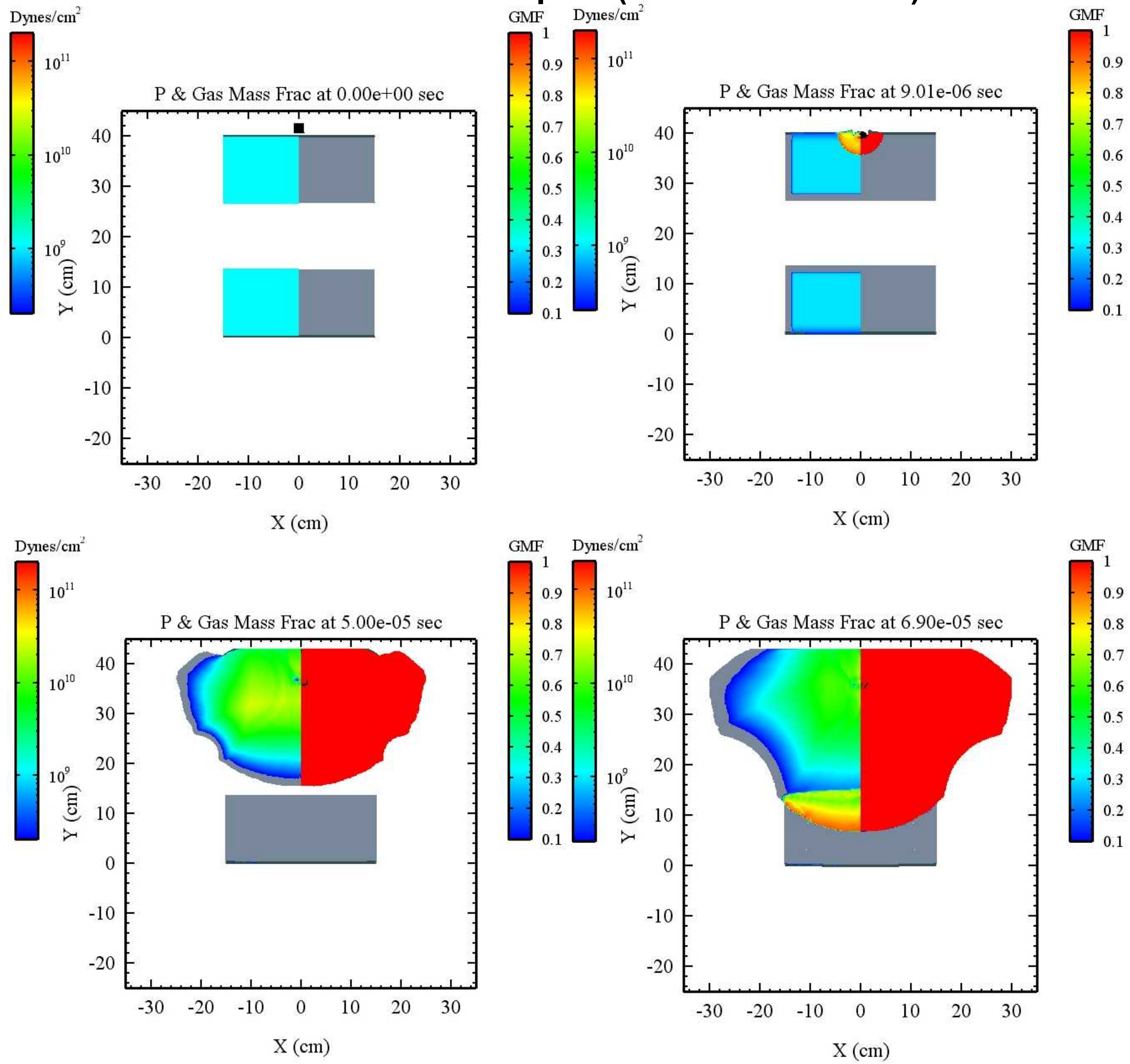
- 2D Computational Parametric Study
- Full CDAR-K Implementation
- Simulation of the response of HTPB/AP/Al/RDX propellant in the super large scale gap test (SLSGT)

2D CTH BVR Simulations

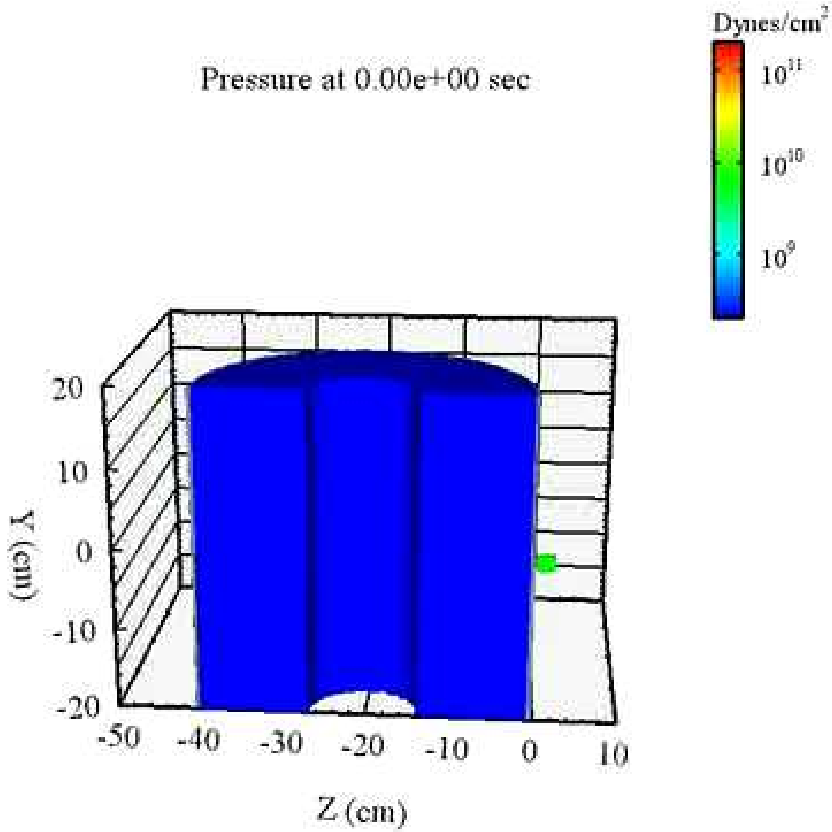
1.0 km/sec Impact (No Reaction)



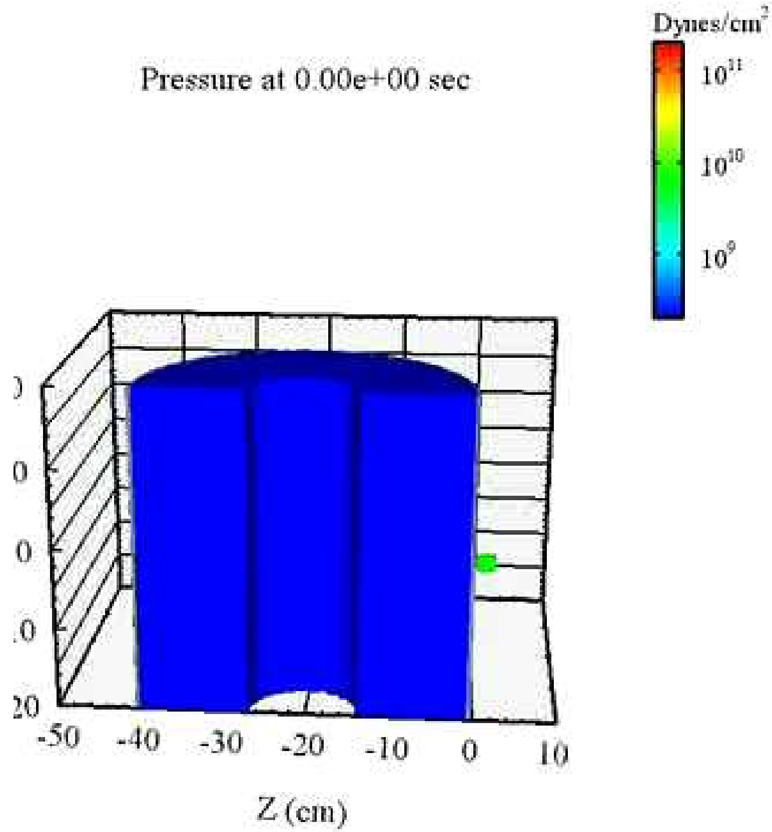
2.6 km/sec Impact (Reaction in Both)



3D CTH BVR Simulations



1.0 km/s dying reaction



2.6 km/s sustained reaction

LLNL Propellant Modeling Program

LLNL JMP and Core DOE Efforts for the US-UK PA

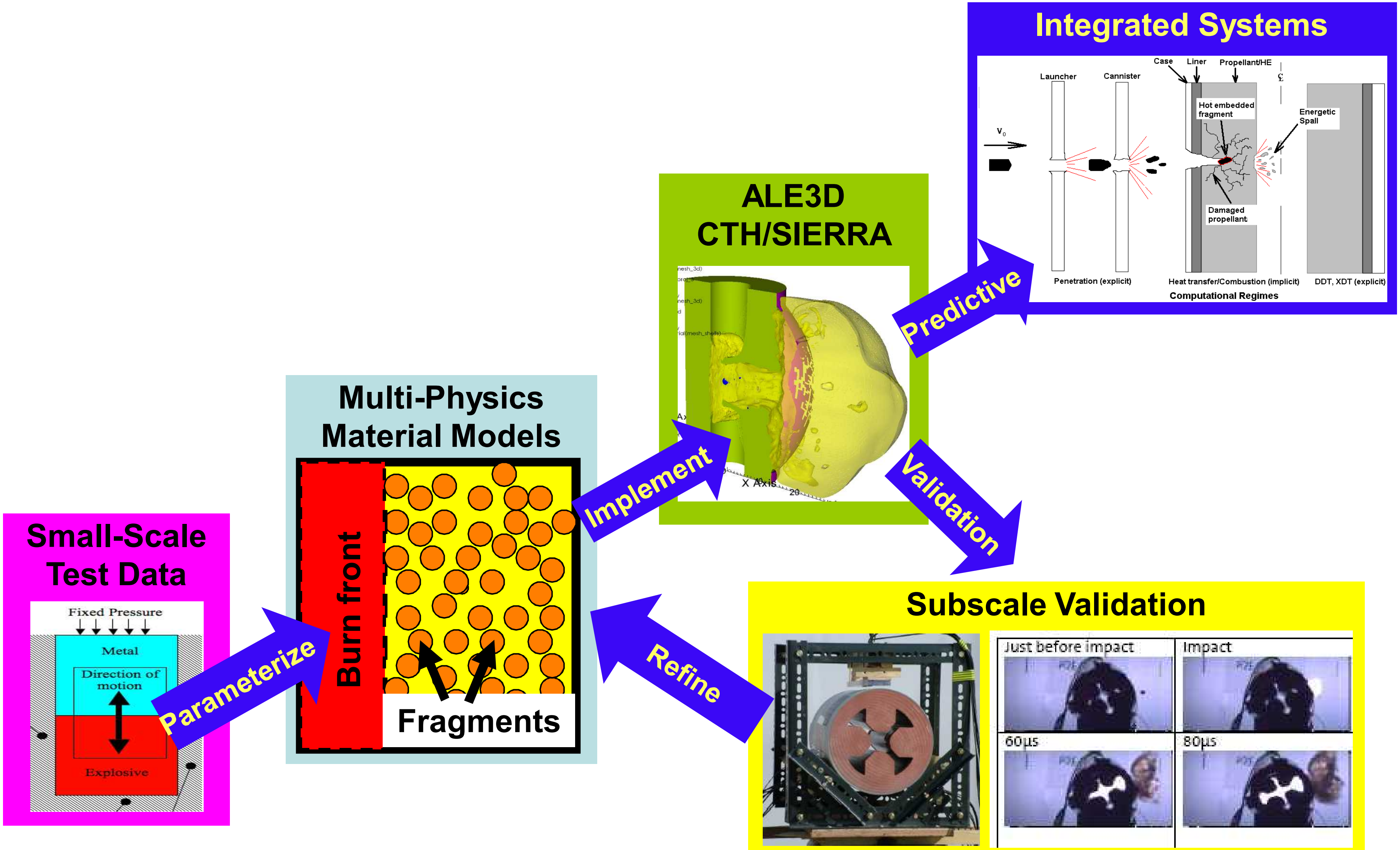
Materials Modeling Timeline

LLNL 9-Jul-08 **By:** Watkins (LLNL)

Project: US/UK Project Arrangement No. D-06-UK-0014
Insensitive Munitions Hazards: Modeling & Simulation

Organization	Date Due	Status	Description	PI/PL
LLNL	Oct. 2010	On Track	Simulate single BFI into HPP rocket motor in launch tube	Springer
LLNL	Sept. 2010	On Track	Integrated simulations with fragmentation and venting	Springer
LLNL	Sept. 2010	On Track	Impact-induced damage and ignition model	Springer
LLNL	Apr. 2010	On Track	Mesoscale (multiphase) sub-detonics decks	Stevens
LLNL	Sept. 2010	On Track	Damage dependant burn models for HMX	Springer
LLNL	Nov. 2009	On Track	BVR spall tests complete	Springer
LLNL	Oct. 2008	On Track	Complete N-9 characterization	Springer
LLNL	Sept. 2010	At Risk	Pressure/Damage-dependant kinetic HPP model	Springer
LLNL	Aug. 2009	At Risk	Complete HPP characterization	Springer
Redstone	Aug. 2008	At Risk	HPP samples received	Neidert
LLNL	Oct. 2009	On Track	Simulate single BFI into HPP rocket motor	Springer
LLNL	Sept. 2009	On Track	Porosity-Permeability models	Springer
LLNL	Sept. 2009	On Track	Second tier fracture model (9/10)	Faux
LLNL	Sept. 2009	On Track	First tier fracture and fragmentation	Faux
LLNL	Aug. 2009	On Track	Finish comparison of current UK models	Springer
UK	Sept. 2008	On Track	Receive UK models	Milne
LLNL	Apr. 2009	On Track	Spiral 2 sub-SDT impact models	Reaugh
LLNL	Apr. 2009	On Track	Cheetah for afterburn	Springer
LLNL	Apr. 2009	On Track	Pressure-dependant kinetic HMX model	Springer
LLNL	Apr. 2009	On Track	Damaged PBXN-9 burn rate	Springer
LLNL	Sept. 2008	On Track	Simulate single BFI into analog HPP rocket motor	Springer
LLNL	Aug. 2008	On Track	Initial fragmentation and venting capability	Springer

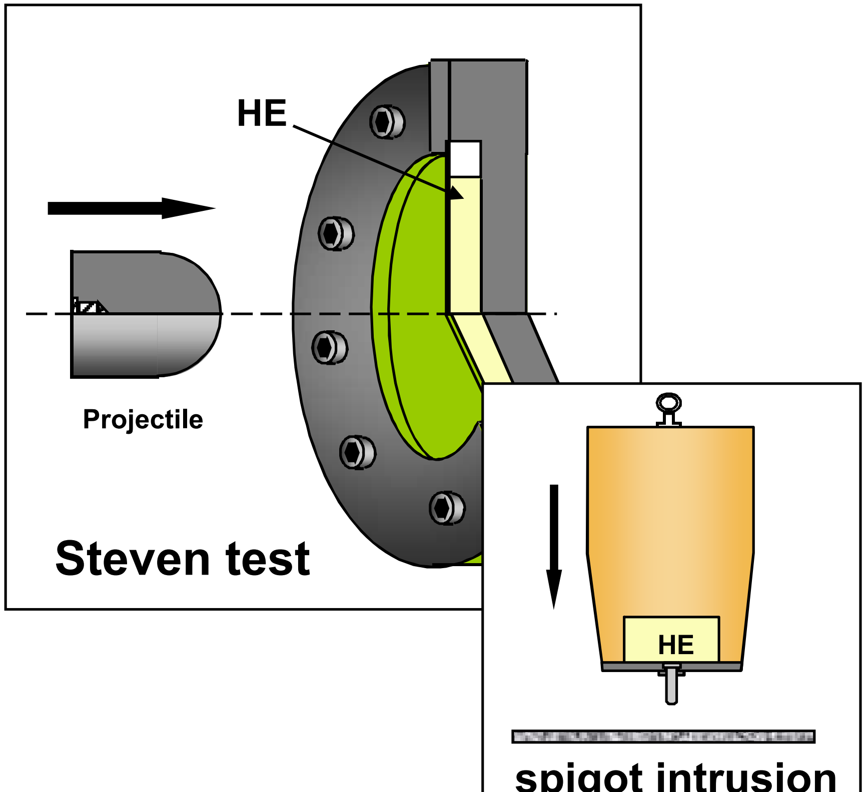
Integrated Modeling and Experimental Approach Leads to a Predictive Capability



Non-Shock Ignition Models

Ignition

Impact tests provide the necessary data for ignition model development



Non-shock ignition models are being implemented in codes

$$D_I = \int_0^t \left(\frac{\sigma_n}{\sigma_0}\right)^{\gamma} \left(2 - \frac{3|s_2|}{Y}\right)^{\delta} \frac{d\varepsilon_p}{dt} dt$$

Stress-strain dependence

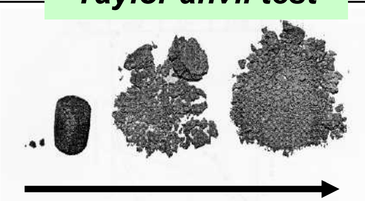
We will improve predictive capability of models by incorporating composition, grain structure, and thermomechanical properties

Models are Needed for Key Mechanisms

Damage

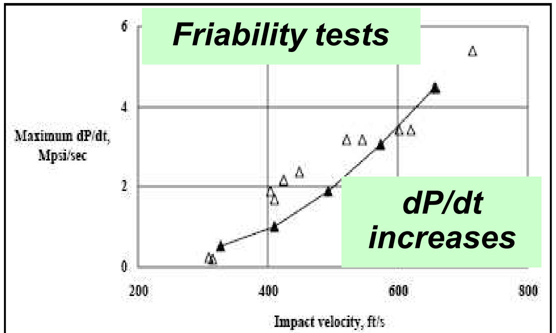
Influence of impact fragmentation

Taylor anvil test



Increasing impact velocity

Friability tests



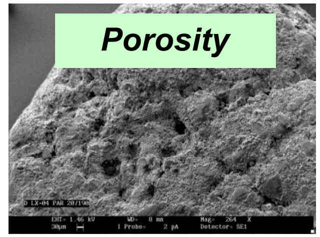
dP/dt increases

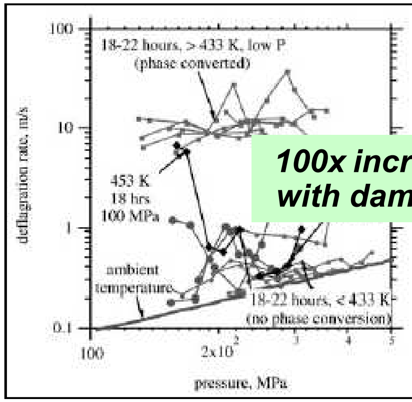
$$d = \left(\frac{\sqrt{20}K_{Ic}}{\rho c \dot{\varepsilon}}\right)^{2/3}$$

Grady-Kipp & similar models in code

Influence of porosity

Porosity



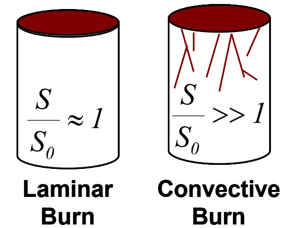


100x increase with damage!

Porosity from kinetic models

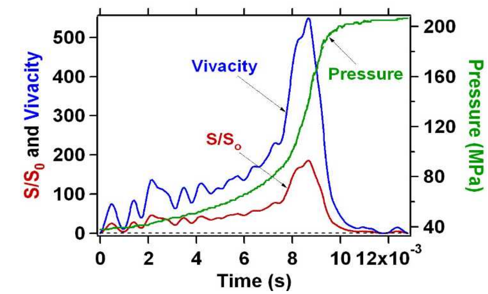
$$\phi_2 = 1 - \left\{ \left[\frac{(V_2)_{HOT}}{V_1}\right] \frac{1}{(1+\xi)} \left[\sum_{i\in s} \left(\frac{v_{i2,HOT}}{1+\alpha_i \Delta T} \frac{\rho_{i,0}}{\rho_{\beta,0}} \right) \right] \right\}$$

Influence of burn-front cracking



Increased surface area with burn progression

LX-10 exhibits convective burning w/out initial damage



Need models in code that predicts the 100x increase in surface area with pressure

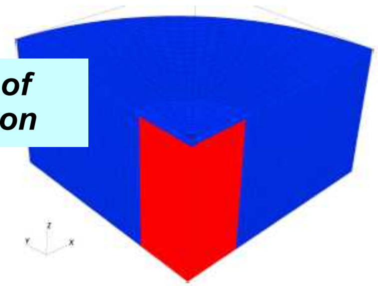
We will improve predictive capability of models by incorporating intrinsic fracture resistance of grains & binder, and interface strength

Convective Burn Models Based on Multiphase Model Framework

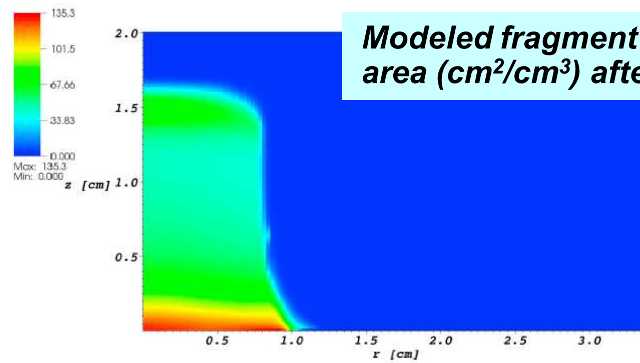
Flame/Burn

Multi-phase / variable particle velocity

Computational configuration of Comp-B Taylor Anvil simulation

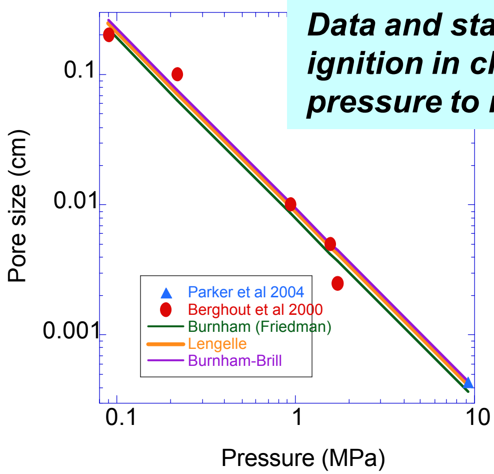


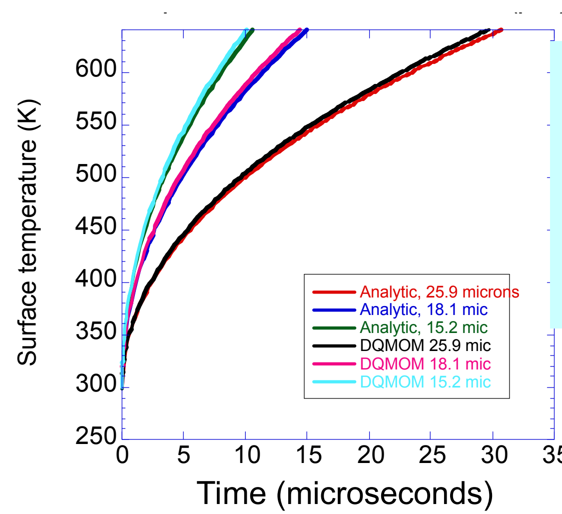
Modeled fragment surface area (cm^2/cm^3) after 20 μs



Convective burn model

Data and stability model suggest ignition in closed pores requires pressure to reach critical value





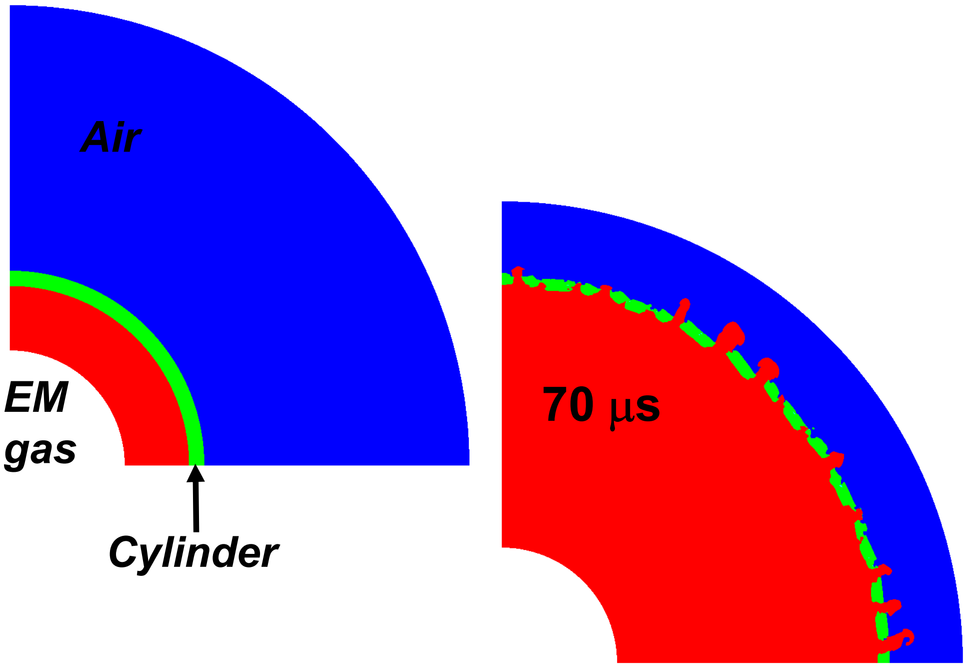
Sub-grid model calculates surface heating of pores. Ignition requires particle surface to reach critical temperature.

Convective burn models are important for capturing explosive violence

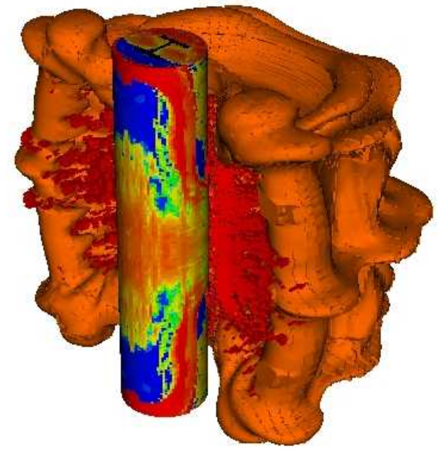
Fragmentation and Venting

Confinement

Numerical framework incorporated in code to predict fragmentation and product gas venting



Loss of confinement affects overall blast impulse



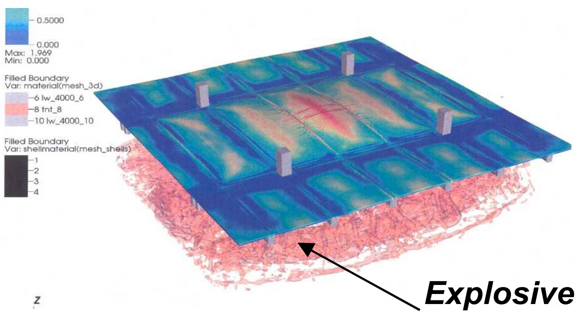
Loss of confinement can also affect the fragmentation process

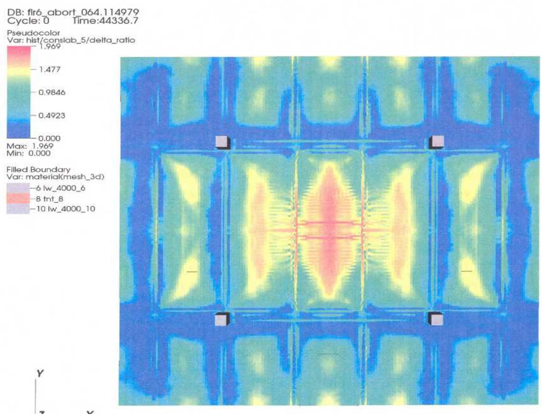
We will incorporate stochastic fracture models to improve capability for predicting blast impulse and fragmentation- key IM signatures

Fragment and Blast Impulse Enable Assessment of Weapon Effects

Violence

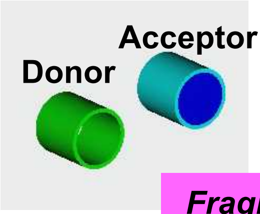
Blast-structure interactions



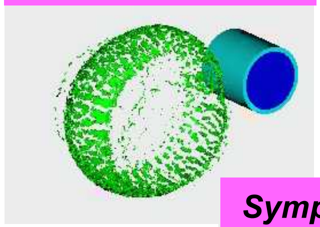


Concrete floor damage shown in yellow-red colors

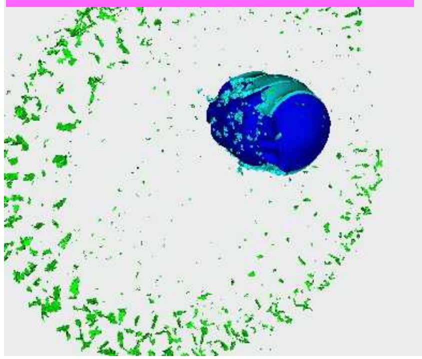
Sympathetic detonation modeling



Fragmentation of donor munition



Sympathetic detonation of acceptor munition

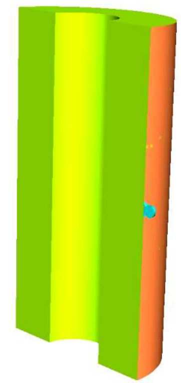


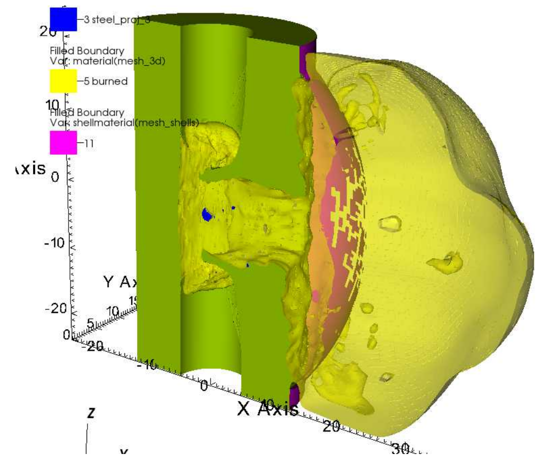
Modeling tools can be used to develop effective strategies for the prevention and mitigation of structural damage or sympathetic detonation (e.g., barrier design)

LLNL Milestone: Simulate Single Bullet/Fragment Impact

Sub-scale rocket motor ALE3D simulations:

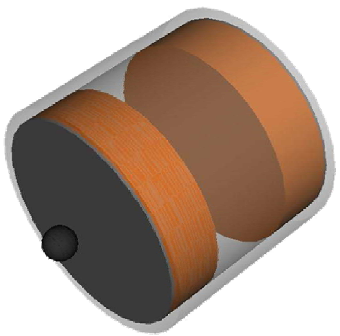
- ***25 cm diameter x 50 cm long metal-encased rocket motor with 10 cm bore***
- ***20 gm spherical projectile at 2.5 km/s***
- ***Propellant Energetic Response to Mechanical Stimuli (PERMS) model***
- ***Initial capability to vent reacted propellant products from fractured case***

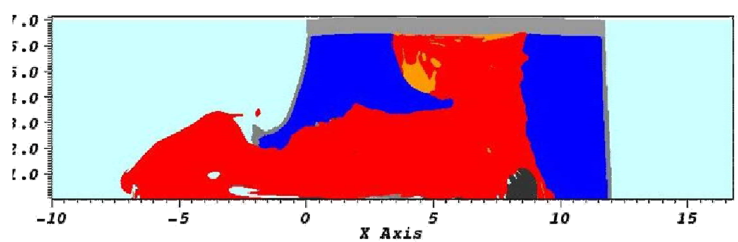




ALE2D simulations of China Lake BVR tests:

- ***5” x 5” x 0.0625” steel plates, 5” x 5” x 1.25” propellant slabs, 2” air gaps (bores)***
- ***2” PMMA side plates at periphery***
- ***0.75” steel spherical projectile at 1.2 km/s***
- ***Propellant Energetic Response to Mechanical Stimuli (PERMS) model***





Conclusions

- Both LLNL and SNL have mature efforts under the Joint Munitions Program in non-ideal reactive wave behavior that applies to propellants
- LLNL current approach is based on PERMS with extensions from multiphase flow
    - LLNL plans to extend their convective burn model for explosives based on their multiphase framework to propellants
- SNL approach is based on CDAR
    - CDAR has both Continuum Mixture Theory and multiphase flow concepts integrated into the framework

- We believe that the technical relationships and exchanges fostered under the PA will be a valuable outcome

- We can't assume that simple models or single physics codes can be "glued" together and capture key physical processes