U.S. Army Research, Development and Engineering Command

TECHNOLOGY DRIVEN. WARFIGHTER FOCUSED.

Insensitive Munitions and Energetic Materials Workshop

Institute for Multi-Scale Reactive Modeling

William H. Davis
Ernest L. Baker
David G. Pfau

11-14 May 09

Institute Formation

- ARDEC and ARL responded to HPCMO* call for HSAI** proposals
  - "An Institute to advance the computational toolset for the IM modeling community"
  - Reactive chemistry of explosives and propellants for use by the insensitive munitions modeling community (one of six technical areas)
- DA ASAALT (Dr. Parmentola) selected ARL-ARDEC proposal to go forward to DoD
- DoD HPCMO awarded IMSRM and two others on 6 Feb 08
- **Develop a user-friendly, agile toolkit for rapid design tradeoffs and assessments to predict the response of munitions to threats and hazards**

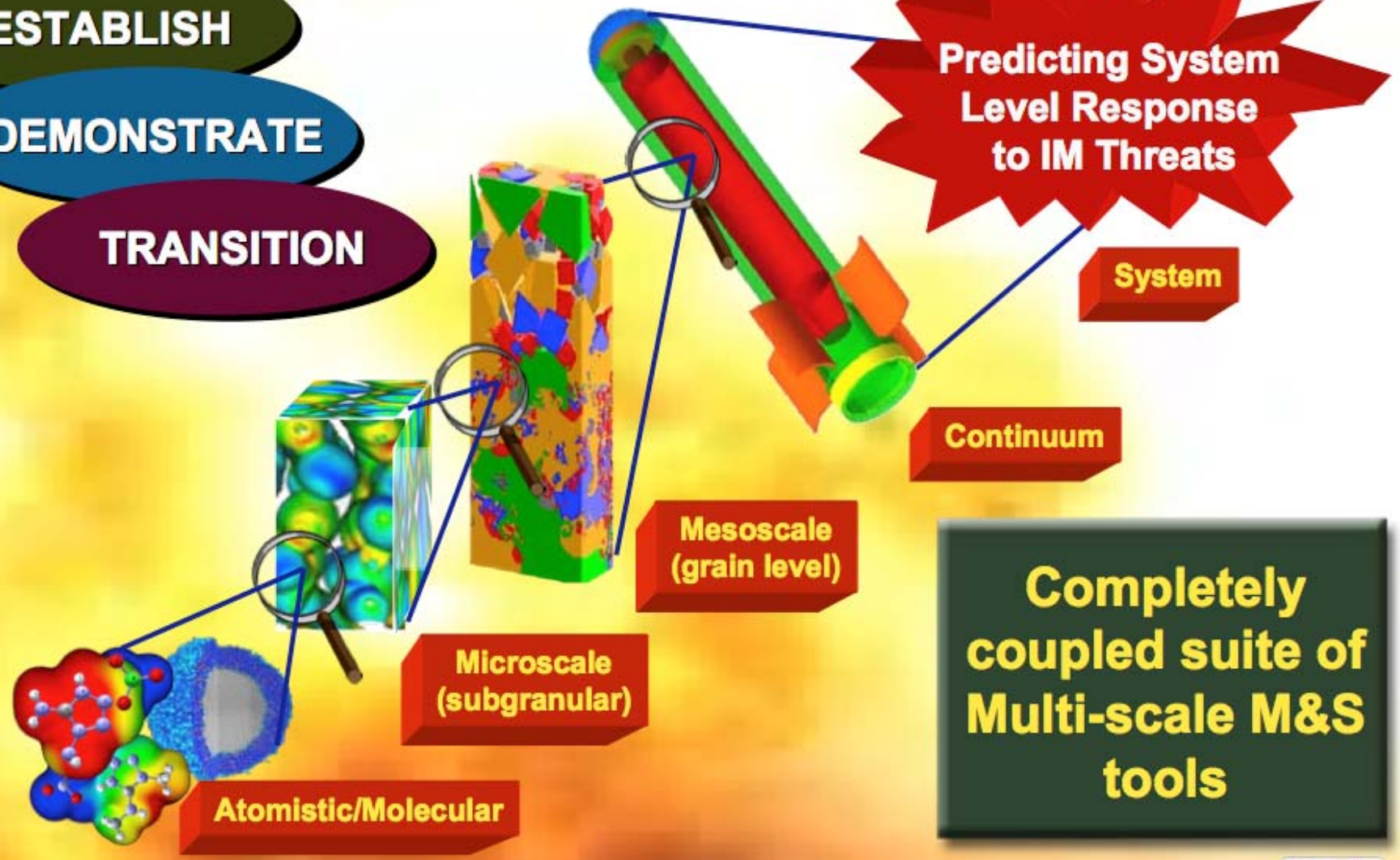
*** High Performance Computing Modernization Office**
**** High Performance Supercomputing Application Institute**

Conclusion 2

ESTABLISH

DEMONSTRATE

TRANSITION



Completely coupled suite of Multi-scale M&S tools

Institute Highlights (from initial briefing to HPCMO)

Statutory Requirements: *IM compliant munitions*

DoD Directive 5000.1; Chairman, Joint Chiefs of Staff Instruction (CJCSI) 3170.01F; and CJSC Manual (CJSCM) 3170.01B

Institute will *revolutionize* M&S in munition design process

- Multiscale capability, incorporating fundamental physics/chemistry
- Reduction of empiricism
- Faster Design and Implementation
- Reduced risk, cost and time
- Extrapolation to novel, potentially more capable designs

Challenges

Overall: Coupling methods and codes for time/length scales

1. MD parameterization of EM
2. Mesoscale simulation of EM response
3. Homogenization methods

Impact if HSAI not chosen

- Perpetuation of M&S tools with high levels of empiricism/inaccuracies
- Inability ot extrapolate beyond existing IM threats
- Continued reliance on full-scale testing
- Increased development cost and time

Controlling the Energetic Materials Response to Threats Is KEY to IM Compliant Weapons

HPC

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Transitioning the software

ARL-ARDEC

DoD R&D

PEOs/ PMs

DoE R&D

Academia

Industry

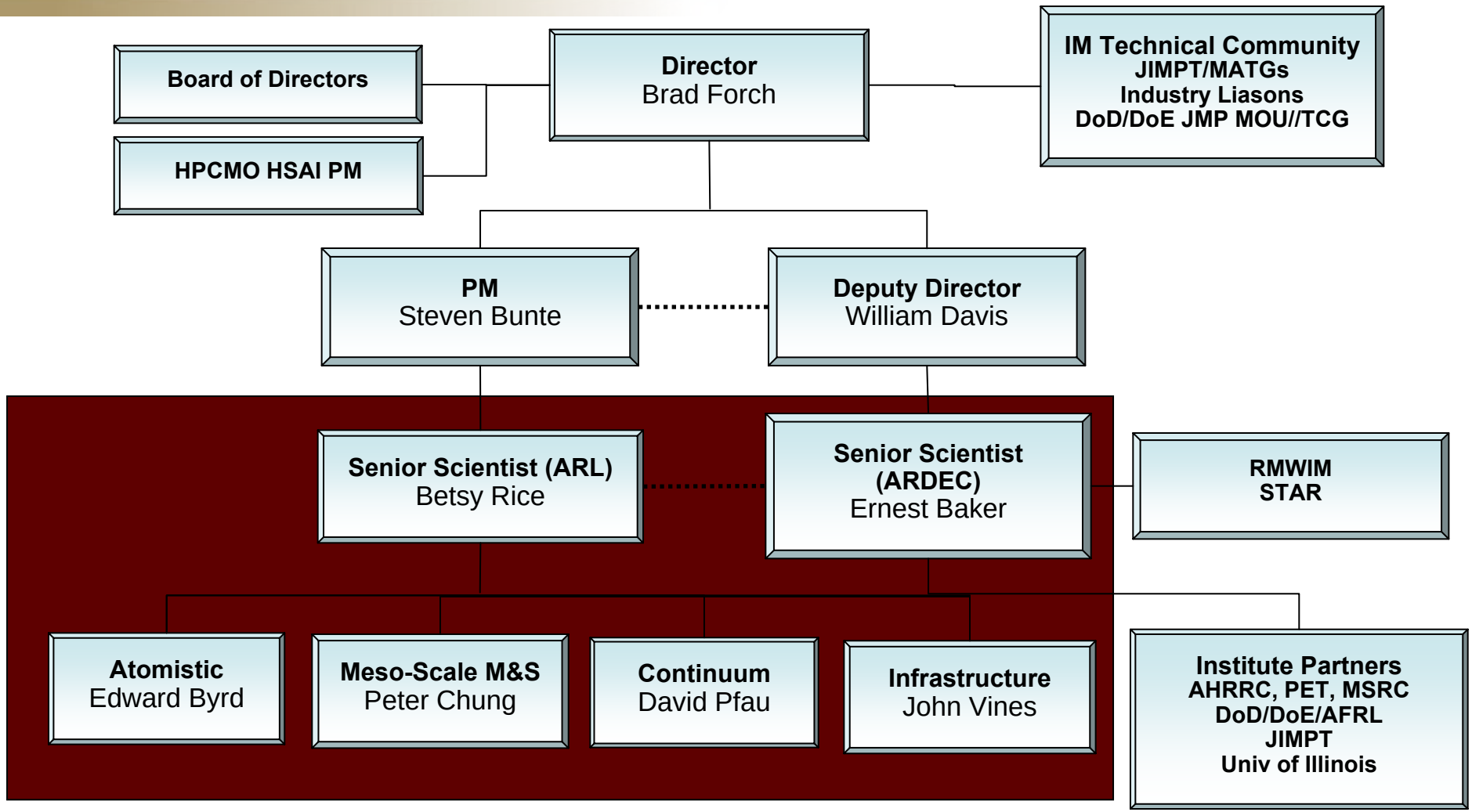
HSAI web site

- Installation
- User Guides
- Release Notes
- Error reports
- Training
- Examples
- Test Suite
- Benchmarks

SW V&V

- SW V&V Plan
- Requirements
- Design
- Integration
- Testing
- Installation
- Maintenance

IMSRM Organization



Board of Directors

1st IMSRM BoD meeting took place 8 Jan 09 at ARL/Aberdeen
BoD Approved Strategic and 09 Annual

Board of Directors

Cray Henry, HPCMO

John Parmentola, ASA(ALT)

Tony Melita, OSD

Seham Salazar, PEO Ammunition

Jill Smith, ARL

Pat Baker, ARL

Barbara Machak, ARDEC

Steve Cornelius, AMRDEC

Robert Sierakowski, AFRL

Judah Goldwasser, ONR/DARPA

IMSRM Team Breakout

Mesoscale

Peter Chung

Embedding Methods
Constitutive Methods
Mesoscale Methods
Averaging or statistical sampling methods

Atomistic

Edward Byrd

SW Assessment
Perform simulations at all scales
V&V of all results

Continuum

David Pfau

Continuum codes (hydrocodes)
Non-ideal IM explosives
Thermal kinetics & ignition
Coupled reaction fracture/damage

Infrastructure

John Vines

Testing/optimizing SW
Benchmarking
Establishing standards
Establish/maintain web site

Continuum Team

Reaction Coupling Lead
David Pfau

Mesoscale
Ernie Baker
Luis Costa
Anthony Dawson

Financial Manager
Christine Frankovic

ALE3D Analysis
David Pfau
Dan Suarez
Luis Costa
Anthony Dawson
Jack Pincay

Knowledge Manager
Luis Costa

Thermochemistry
Ernie Baker
Christos Capellos
Leonard Stiel
Eric Bixon

Reactive Materials
Paul Redner
Ruslan Mudryy

DSD Univ of Illinois
Scott Stewart
John Bdzil

DSD LLNL/LANL
Rose McCallen
Mark Short
John Walter

HPC
Chuck Chin
Dan Murphy

EWMTD
- *Combined Effects Warheads Branch*
- *Explosives Research Branch*
- *Explosives Dev Branch*

QESA

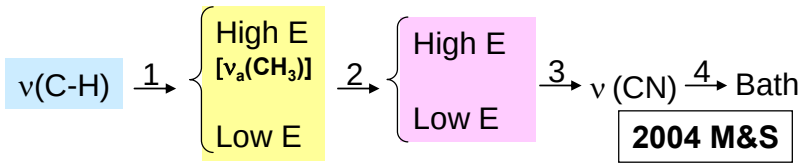
Molecular/Explosives
Frank Owens

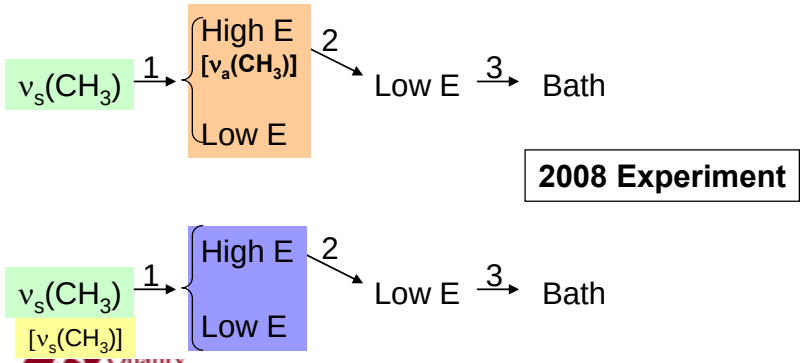
RMWIN Coordination
Stan DeFisher

Atomistic Team

Establish methodologies to characterize energy transfer mechanisms.

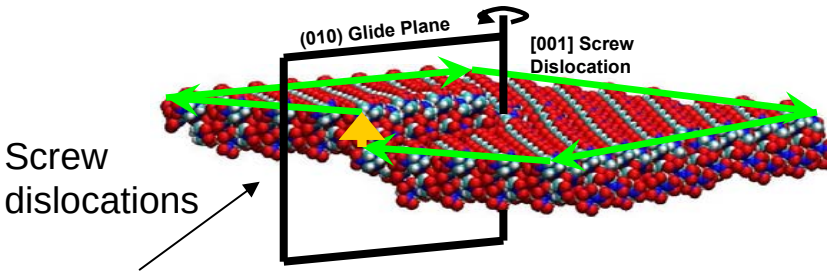
MSA: Develop methods to monitor, characterize condensed phase energy evolution for two systems (liquid NM and crystalline RDX).

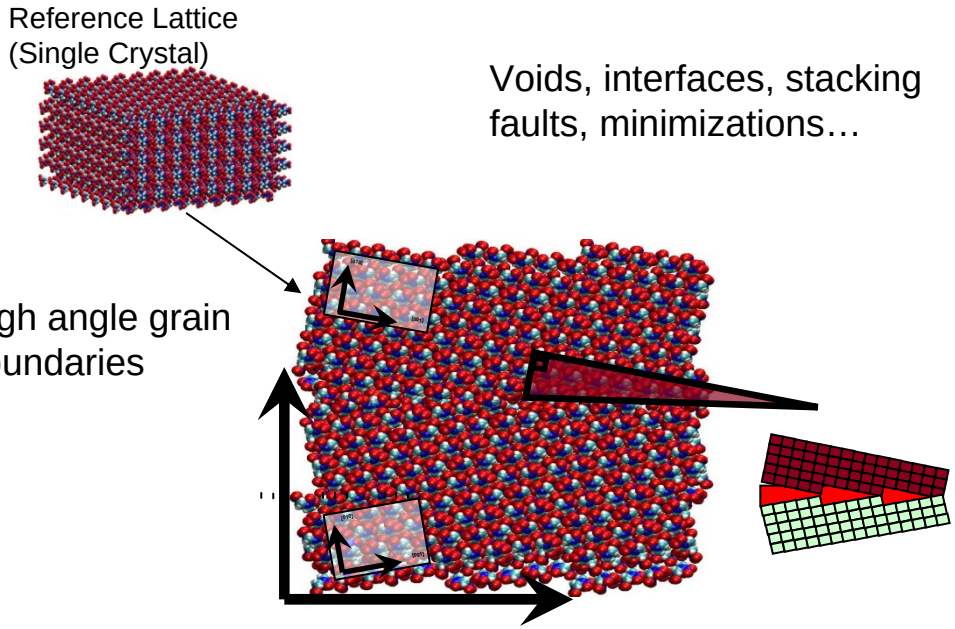




Develop a catalog of defected large/complex molecular crystals of RDX

MSA: Generate models of stacking faults, twins, stepped grain boundaries, voids in RDX





2007 Award Recipient

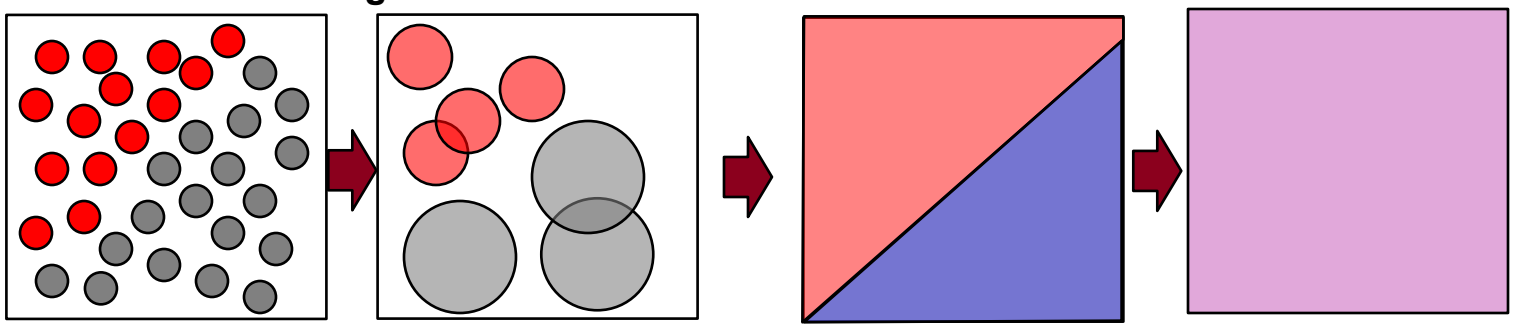
Mesoscale Team

Paving the Way for FY10 critical elements

Atomistic | **Meso** | **Continuum**

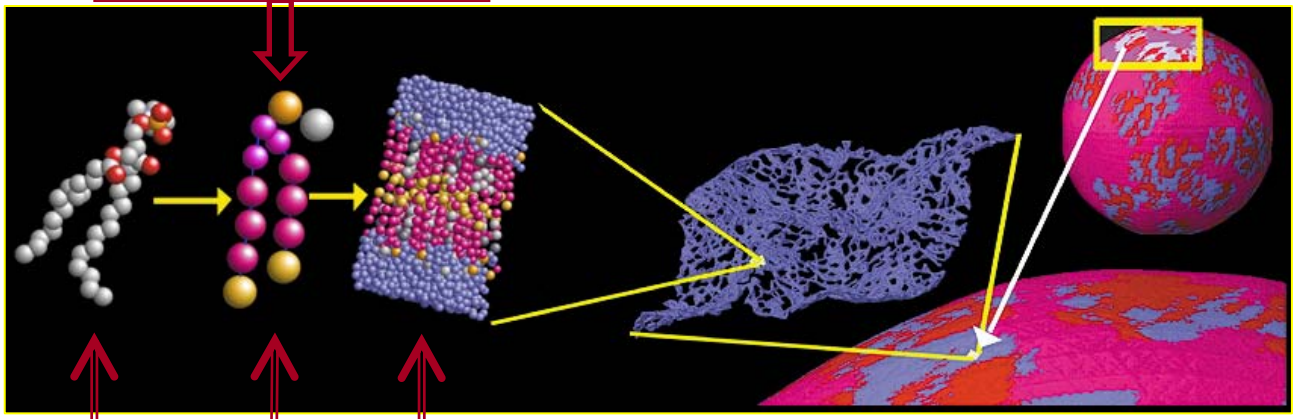
ARL (Izvekov)
Generalized Coarse Graining Procedures

AFRL/UIUC (Horie, Stewart)
Ignition and Burn Mechanisms



Smeared continuum

Particle Based Coarse-Graining



All-atom simulations.
Scale: **Ang/ns**

nm/μs

~10^4 times faster than all-atom simulation

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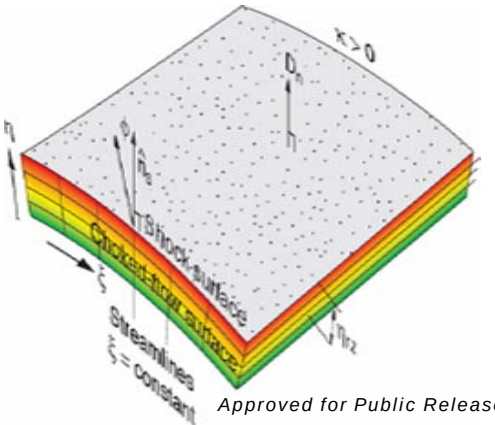
Non-ideal IM explosives - DSD

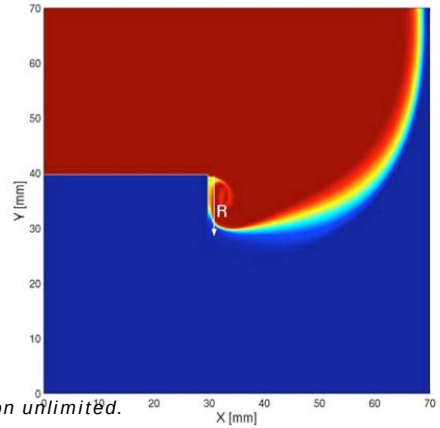
Non-ideal IM explosives

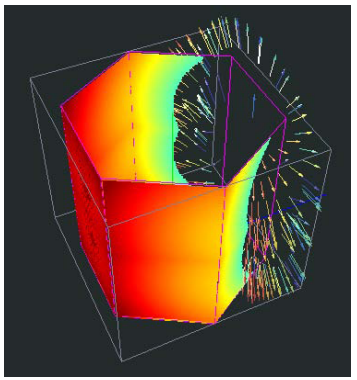
- Measure: Accurate prediction of behavior/performance of new and emerging non-ideal IM formulations such as IMX-101 and IMX-102.
- Metric: Incorporate advanced reactive chemistry with modeling of non-ideal detonation into large critical diameter item hydrocode analysis. Use advanced reactive chemistry to demonstrate improved accuracy among several and various large critical diameter items.

Annual Goals

- Institute personnel will collaborate with detonation shock dynamics (DSD) and high rate continuum hydrocode computer program developers in order to couple a new DSD computer program to a high rate continuum modeling computer program, providing a new detonation velocity modeling capability for non-ideal IM explosive formulations.
  - MSA: : Selection of Institute partners based on DSD development and high rate continuum model implementation expertise. Cooperative interfacing of DSD capability to selected high rate continuum computer program.
  - MOS: Initial DSD/hydrocode burn time capability and algorithms that represent detonation fronts of non-ideal explosives in accordance with DSD theory. Demonstrated 10% improved burn times for diverging detonation of IM explosive in FY10





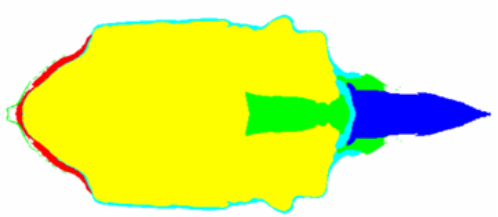


Non-ideal IM explosives - DSD

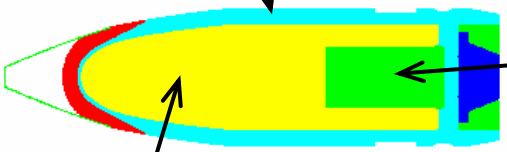
ARDEC Applications

IM Advanced Smaller Munitions

Less sensitive explosives with larger critical diameters

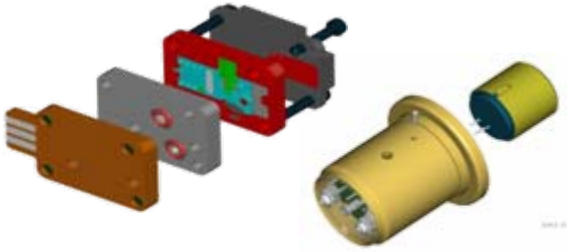


Hardened Steel Case



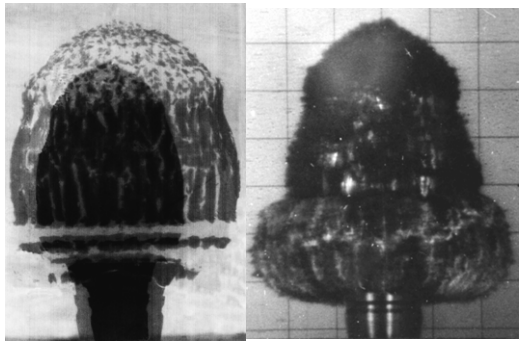
Hardened Fuze Technology

Base/Nose Mounted Fuze



Increased Lethality Fragmentation

Combined Effects High Explosive



ALACV

Hardened Projectile for increase warhead survivability against Urban Structures

Urban Wall Bash-through (Brick-Over-Block, Tile &/or Adobe)

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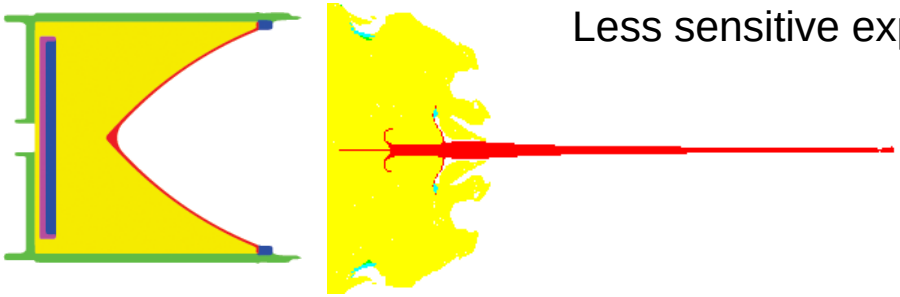
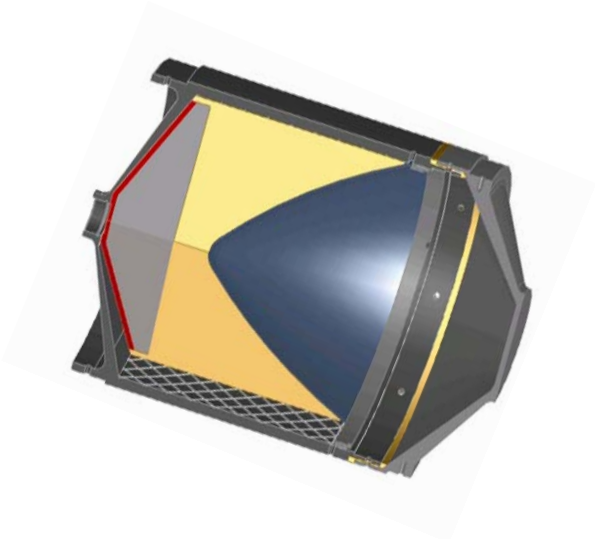
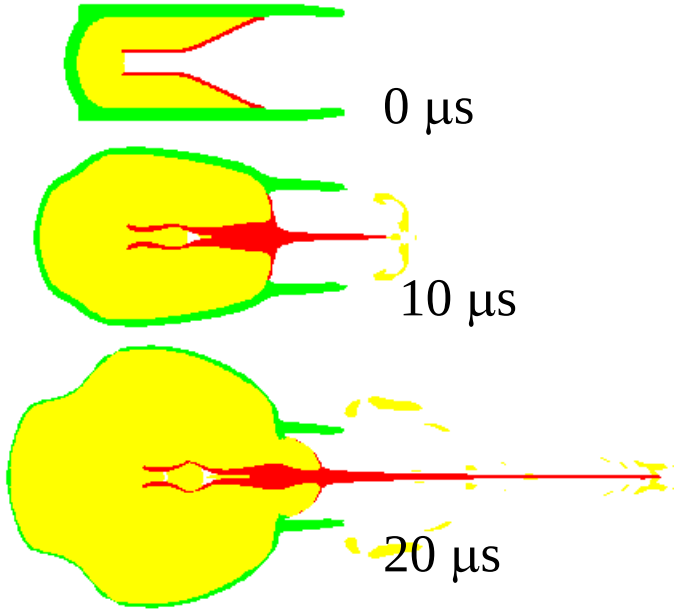
IM Shaped Charges



Less sensitive explosives with larger critical diameters





Continuum Team

Non-ideal IM explosives

Collaboration with detonation shock dynamics DSD and high rate continuum hydrocode computer program developers in order to couple a new DSD computer program to a high rate continuum modeling computer program, providing a new detonation velocity modeling capability for non-ideal IM explosive formulations.

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Kinetics & ignition

Research in and application of thermal ignition, reaction kinetics and equation of state for aluminum. Initial work is represented in a thermochemical equilibrium code. We will work to implement a new explicit partial reaction equation of state into a hydrocode in order to develop a reaction coupling approach, giving it a more robust predictive capability for metalized IM explosives.

Coupled reaction fracture/damage

Incorporate and demonstrate the capability to perform large scale chemical reactions coupled to energetics fracture damage based on mesoscale predictive models. New energetics fracture and failure modeling capabilities are beginning to emerge based on meso/macro approaches (namely the Visco-Scram and Visco-DCA codes). We will perform either code linkage or in-code coupling of these new and emerging energetics fracture and failure models to energetics reactive flow calculations.

Thermal Chemistry & Ignition

ARDEC Development

- Development of thermochemical equilibrium model (JAGUAR)
- Formal optimization of EXP-6 potentials for H-C-N-O detonation products to available experimental data
- Implementation of analytic cylinder model and JWL/JWLB equation of state parameterization using formal non-linear optimization
- Aluminum and aluminum reaction products equation of state development and implementation
- Partial reaction equation of state development and implementation into high rate continuum modeling (CALE)

Planned ARDEC IMSRM Development

- Development of atomistic based EXP-6 potentials for H-C-N-O products for which no data exists
- Development of equations of state for non-ideal IM explosives
- Implementation of partial reaction equation of state into ALE-3D

Kinetics and Ignition

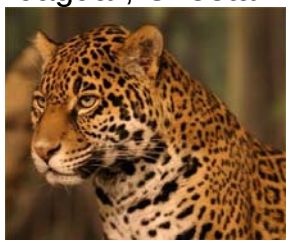
- Measure: Accurate prediction of behavior/performance of new and emerging non-ideal IM formulations such as IMX-101 and IMX-102.
- Metric: Incorporate advanced reactive chemistry with modeling of non-ideal detonation into large critical diameter item hydrocode analysis. Use advanced reactive chemistry to demonstrate improved accuracy among several and various large critical diameter items.

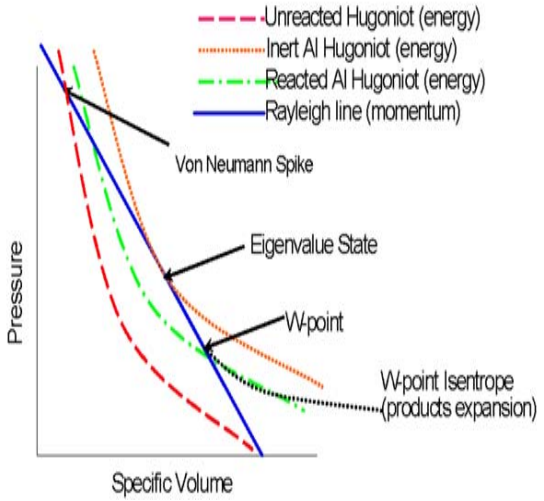
Annual Goals

Research in and application of equation of state for aluminum. Initial work is represented in a thermochemical equilibrium code. We will work to implement a new explicit partial reaction equation of state into a hydrocode in order to develop a reaction coupling approach, giving it a more robust predictive capability for metalized IM explosives

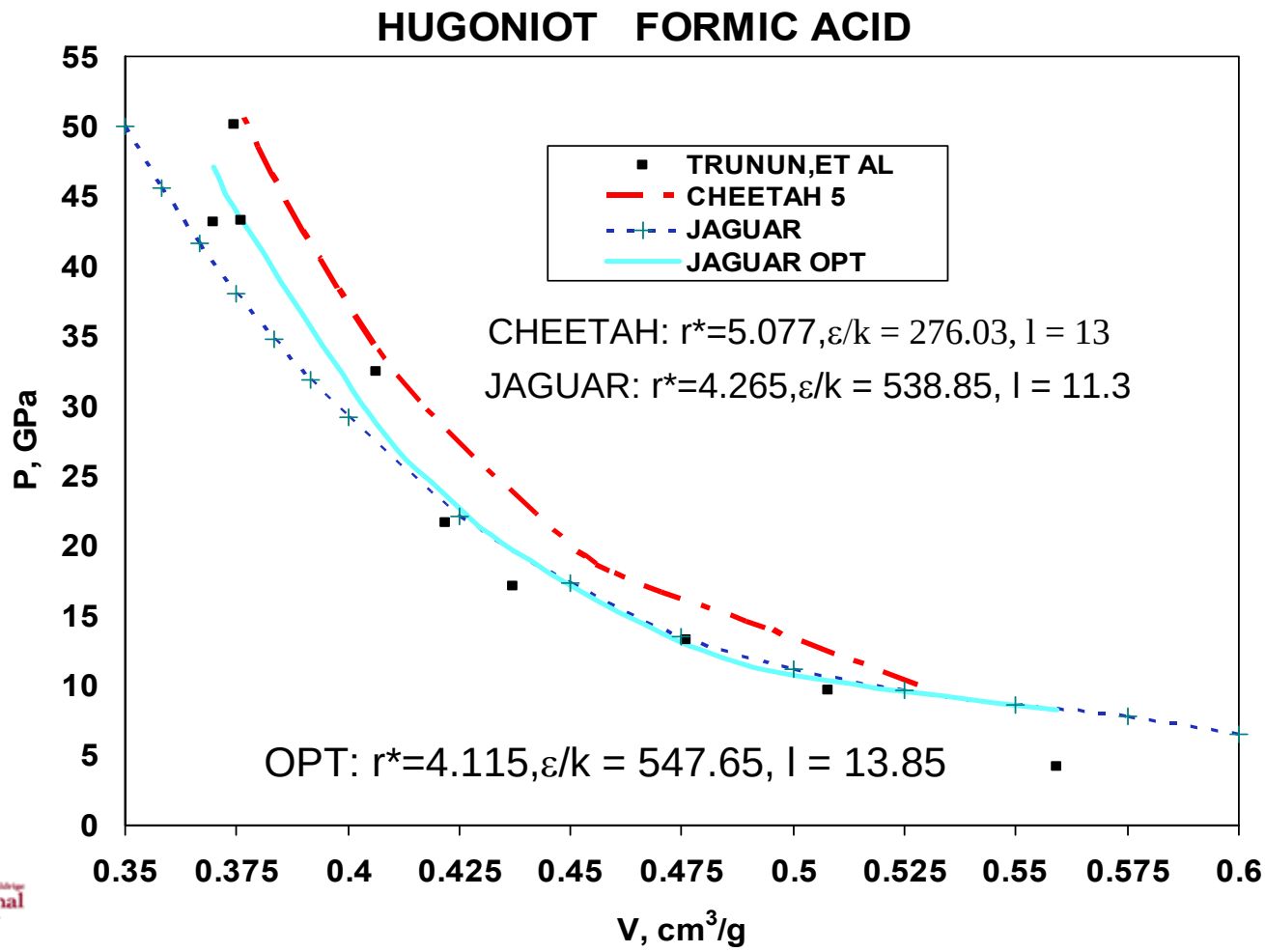
- MSA: Development of new partial reaction equation of state parameterization routine algorithms in thermochemical equilibrium code representing aluminum, boron or silicon reactions in an IM formulation realistically. Inclusion of new partial reaction equation of state capability with metalized explosive in a hydrocode.
- MOS: Implementation of new capability and algorithms in thermochemical equilibrium code that represent partial reactions in accordance with eigenvalue detonation theory and/or other means of calculating and parameterizing partially reacted equations of state. Implementation of a new partial reaction equation of state into a hydrocode. Demonstrated agreement to cylinder test data for metalized IM explosive within 5% in FY10.

Jaguar, Cheetah





Experimental Hugoniot values for formic acid compared with current Cheetah and Jaguar EXP-6 parameters. New optimized parameters.



Conclusion

- Nominal 6 year funded program with planned POM 5 year extension
- Important collaborative effort between ARL and ARDEC in EM/IM computation
- Potential to radically alter IM development methodology
- Coordination/collaboration DoE Labs
- Well-funded synergy of size spectrum approaches to Insensitive Munition / Energetic Material develolpment, analysis and prediction

FIN