INSTITUTE FOR MULTI SCALE REACTIVE MODELING

US ARMY RDECOM®

MSRM

Multi Scale Reactive Modeling Advances

TECHNOLOGY DRIVEN. WARFIGHTER FOCUSED.

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2012 Insensitive Munitions and Energetic Materials Technology Symposium

Overview

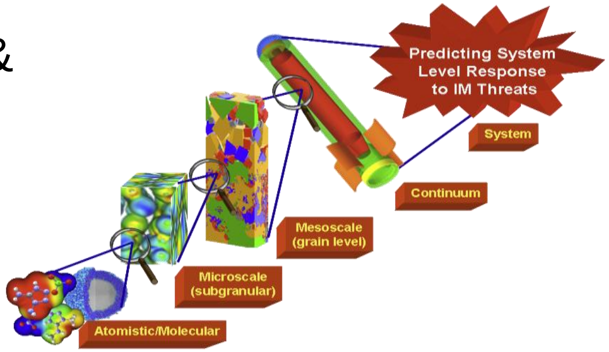
- The MSRM Institute

- Recent Developments
  - Detonation Shock Dynamics
  - ParticalPack
  - Homogenization Framework
  - Structure-based Continuum Parameters

- Summary

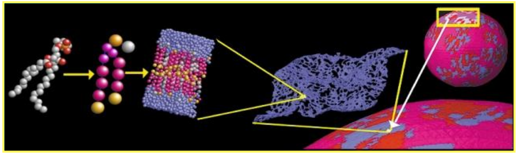
The MSRM Institute

- The MSRM is a collaborative effort between ARDEC & ARL; 6 year funded program 2009-2014



- Sponsor: Army High Performance Computing Modernization Office (HPCMO)

- Mission: Advance the computational supercomputing toolset for the Insensitive Munitions design community from atomistic to continuum scales; transition results; education and outreach to users



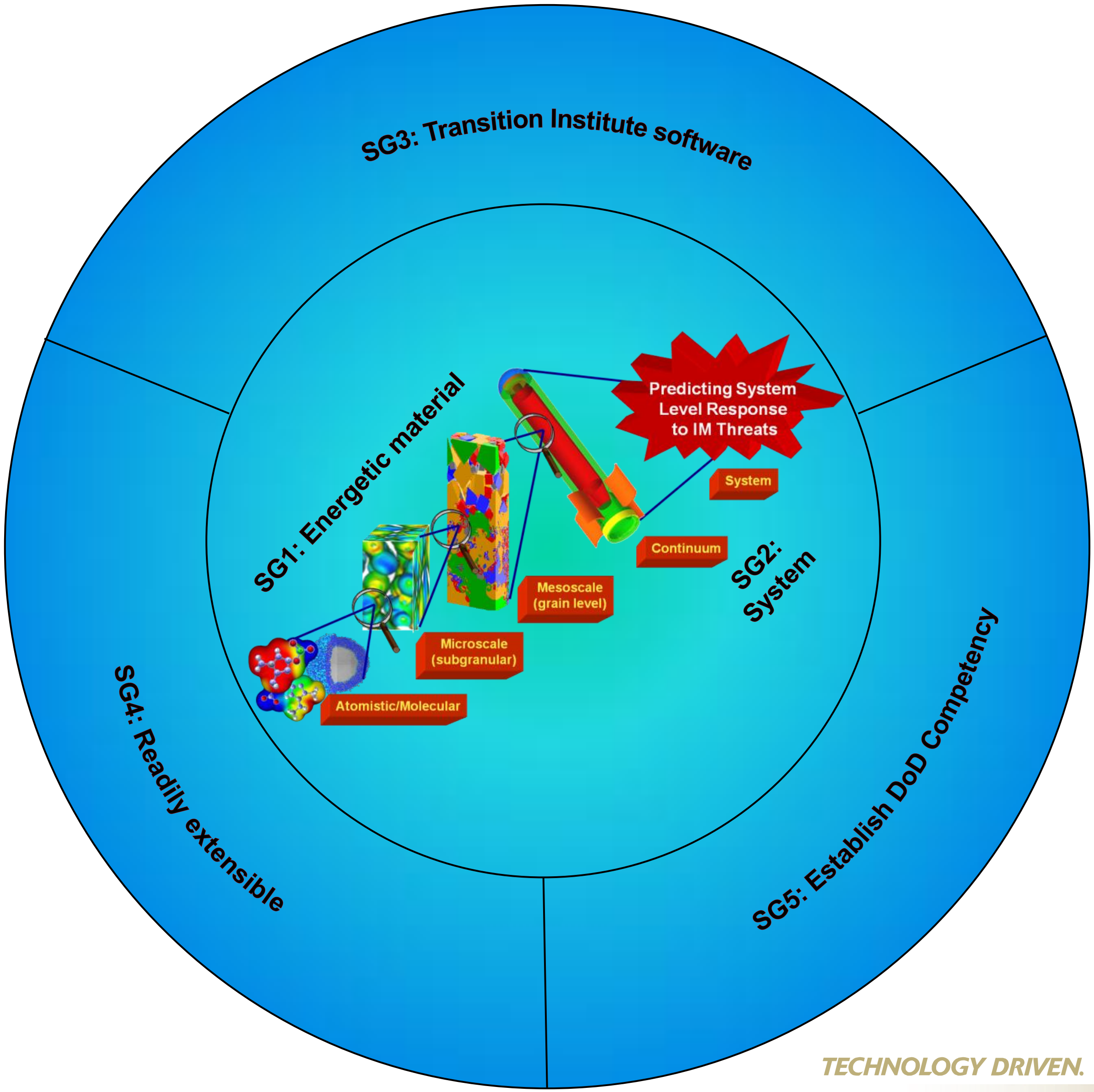
Limitations of current M&S

- High levels of empiricism/inaccuracies
- Inability to extrapolate beyond existing IM threats
- Continued reliance on full-scale testing
- Large development cost and time

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

MSRM: Strategic Goals



Recent Developments

- Recent Institute developments have supported advancements in supercomputing toolsets/software and methods for HPC assets
- Enhanced Detonation Shock Dynamics (DSD)
  - Enhance and extend the LLNL DSD code implementation
  - Completed unconfined DSD characterization tests of IMX-104
  - Currently testing confined DSD characterization of IMX-104
- ParticalPack software - creates representative volume elements of explosives with distribution of particle sizes and varying binder thickness
- Homogenization Framework that introduce scale-dependent and stochastic effects
- Grain scale structure-based studies of thermal properties for Improved cook-off performance

Detonation Shock Dynamics

- Detonation Shock Dynamics (DSD) is a computational approach that will allow highly accurate modeling of the HE reaction, without the high burden of computational expense that traditional reactive flow simulations (such as with an Ignition and Growth model)

- With a DSD computational tool, weapons designers can predict HE behavior in complex geometries and ensure their warheads will function as intended, both for safety as well as effectiveness

- DSD is the geometric theory and implementation of the representation of a curved shock front in a detonation, implemented as a pre-processor step & currently being developed for dynamic lighting times

Our goal was to develop predictive DSD capability to compute lighting times of ideal and non-ideal HE

DSD Theory

- The first assumption behind DSD is that the velocity of the detonation wave normal to the shock wave is only a function of the curvature. Combined with an appropriate boundary condition describing the HE/confinement interface, DSD provides a complete description of detonation propagation.

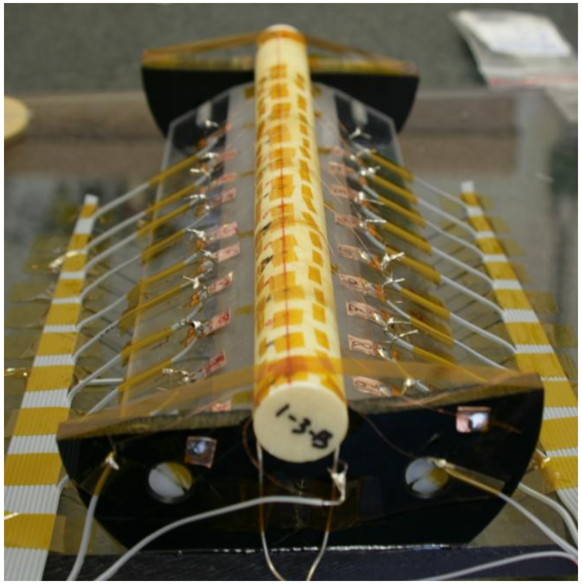
- This mathematical approach serves to keep track of sub-scale physics in the reaction zone without needing to march element-by-element through the reaction zone with a reactive flow approach (Doesn't take as much time)

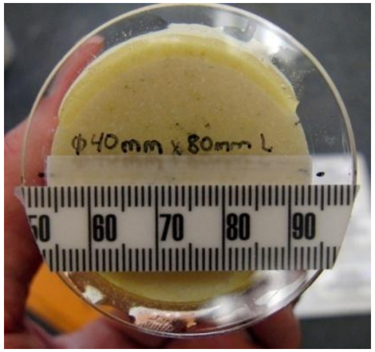
- Work by Bdzil extended the theory to include high-order terms to better capture expansion, as well as state-sensitive reaction rates

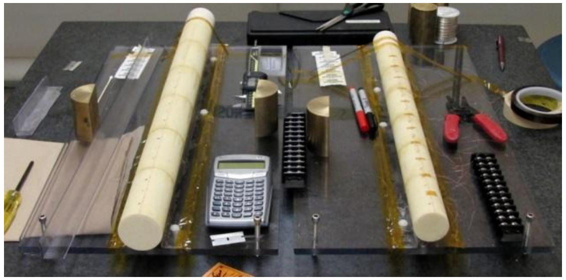
- Parameterized DSD models exist for traditional IM explosives (such as PBX9502), and non-ideal materials (such as Ammonium Nitrate-Fuel Oil), and work is currently ongoing to parameterize IMX-104

DSD: Experiments IMX-104

- Completed unconfined rate stick performance tests for 50, 40, & 30mm diameter
  - Detonation velocities and shock front curvature shapes were measured



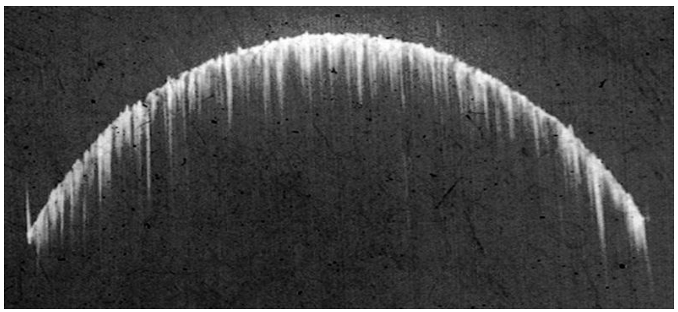


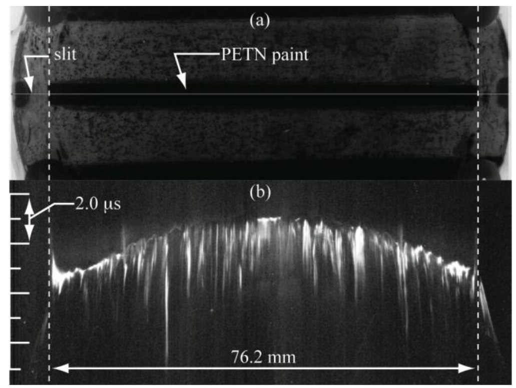


- The rate-stick detonation wave break-out shape and timing data was analyzed to obtain an IMX-I04 DSD calibration consisting of a detonation front curvature vs. normal detonation velocity relationship

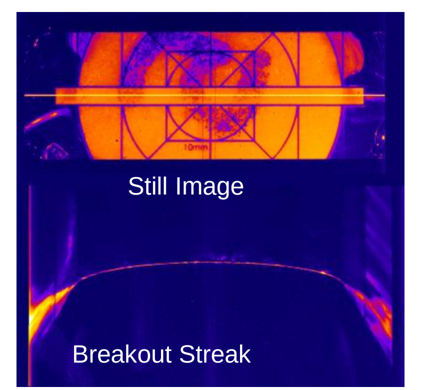
DSD: Experiments IMX-104

- This data yielded the relationship between the normal detonation velocity Dn and the shock front curvature for each test.





30mm Charge



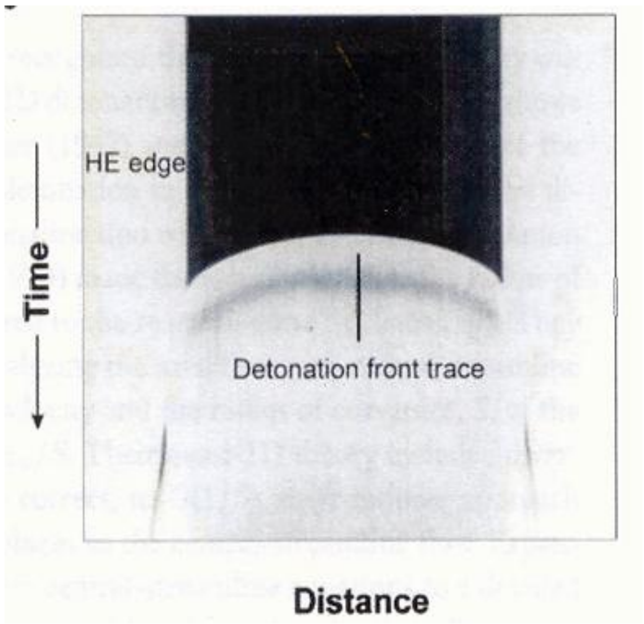
- We have and are currently performing test characterization for DSD at Los Alamos. We have completed test series to develop the Dn-K relation for IMX-104 and we are in process with tests to characterize the ABC for IMX-104.

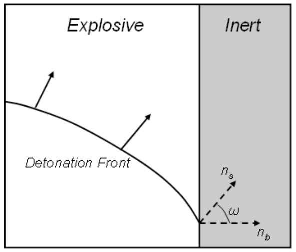
Los Alamos NATIONAL LABORATORY

DSD: Angle Boundary Condition

- Angle boundary condition (ABC) refers to the angle the curved shock front makes with confinement, which is a characteristic of the energetic and confinement materials

- Scheduled for multiple material confinement rate stick performance tests
  - Steel-confined and aluminum-confined tests



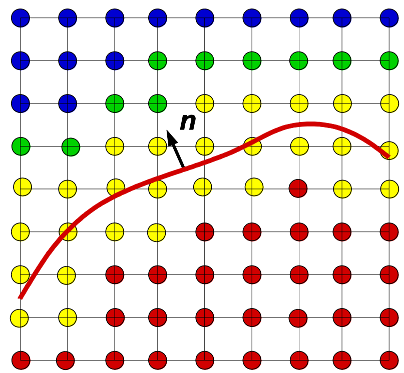


DSD: Implementation

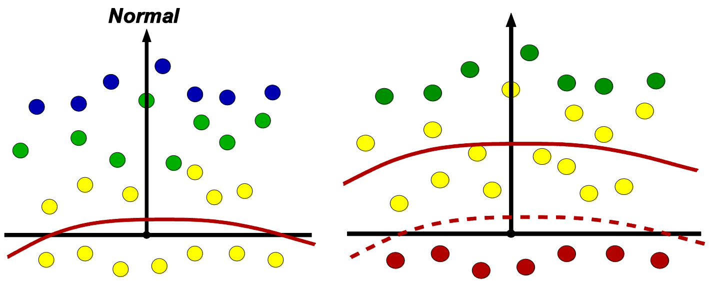
- The DSD model implemented in ALE3D is based on the asymptotic analysis of the reactive Euler (inviscid flow) equations.

- The DSD capability are implemented as an external library in the multiphysics code, ALE3D. Released DSD v1.1.1 as part of ALE3D version 4.16

- Computational mesh are set to one of four statuses:
  - **Inactive**, corresponding to nodes that have a default distance
  - **Feasible**, representing nodes whose distance to the burn front is to be computed
  - **Trusted** where the nodes whose distance is defined , nodes of half-lit cells
  - **Retired** where the node is lit and is deleted from the search list



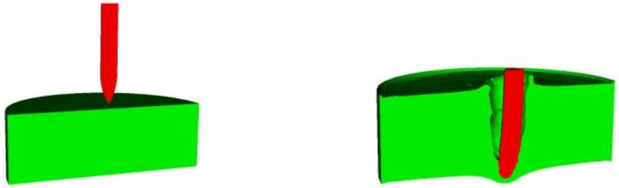
- Integrated in times using a 3rd-order Runge-Kutta scheme



DSD: Software Improvements

- An initial parallel algorithm has been developed for 2-D and 3-D computational space for arbitrarily connected quadrilateral or hexahedral meshes

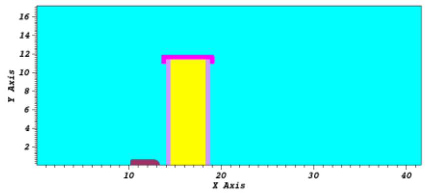
- Dynamic DSD allows for deformation of the geometry during the ALE3D run

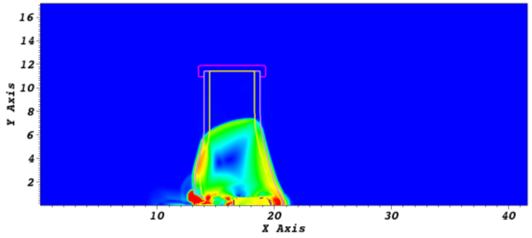


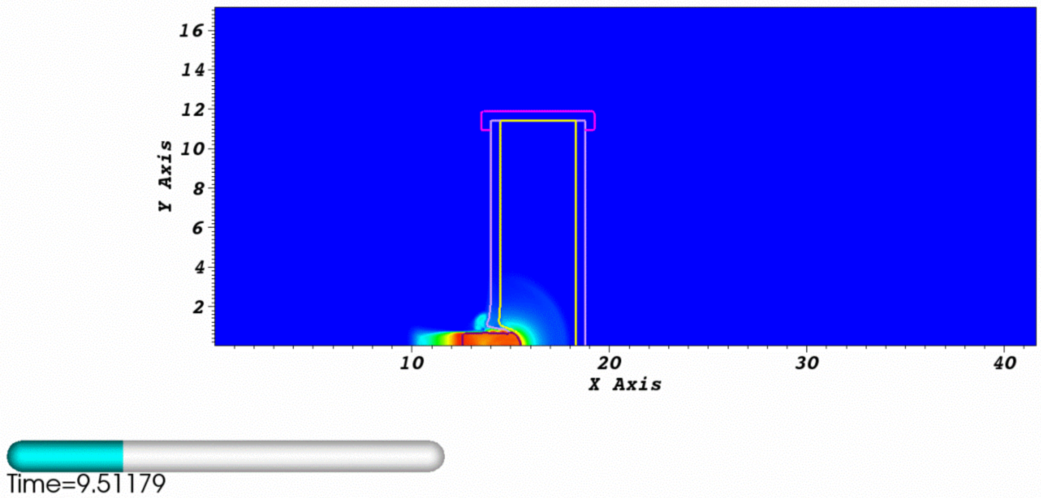
- Enhanced with more accurate tracking of the shock using Angle Boundary Condition code treatment; ABC refers to the angle the curved shock front makes with confinement, which is a characteristic of the energetic and confinement materials.   (parameterizing from confined test)

Dynamic DSD

- Bullet/fragment impact problem to evaluate Dynamic DSD
  - Dynamic DSD supports lighting times “on-the-fly” as HE is being deformed
  - Dynamic DSD will be available in ALE3D v4.18







Valuable for fragment/bullet impact IM test predictions

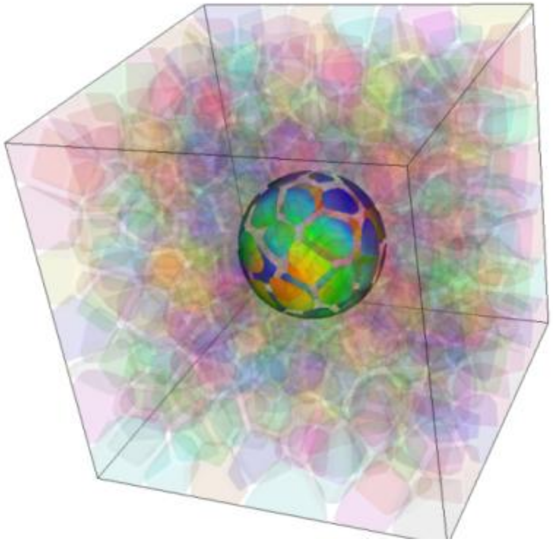
ParticlePack

ParticlePack is a MSRM software product developed in partnership with Lawrence Livermore National Laboratory and is currently deployed on DoD HPC resources.

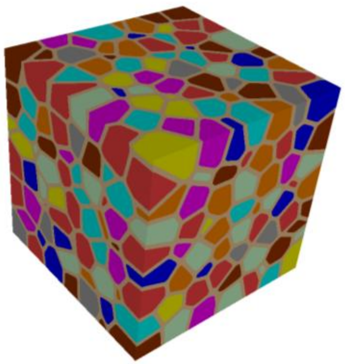
- Realistic packing is essential for accurate numerical representation of crystalline energetic composites in numerical models

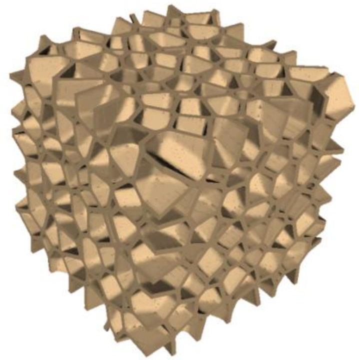
- ParticlePack is a standalone program that generates meso- or grain-scale realizations in ALE3D format, which are used for defining the geometry of defected, large complex molecular crystals in explosives, and complex geometry of packed shapes

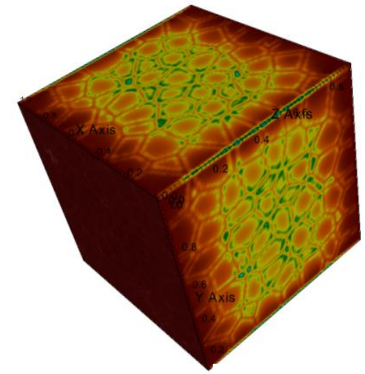
- ParticlePack generates numerical realization of actual energetic microstructure

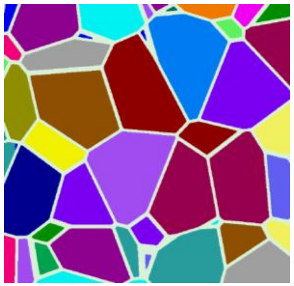


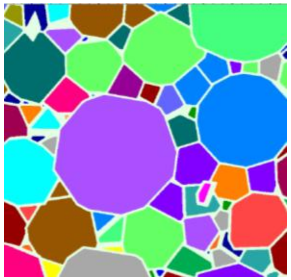
ParticlePack Examples

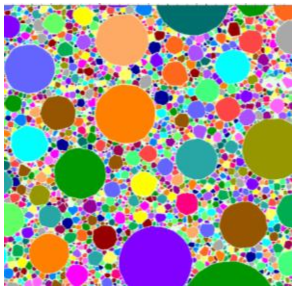




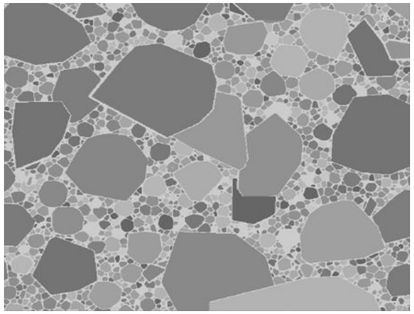




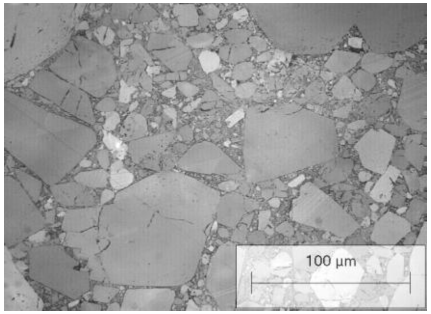




Current ParticlePack/ALE3D model



Energetic Microstructure

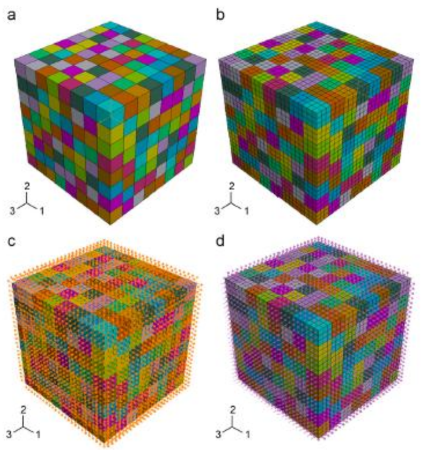


MSRM-ParticlePack improvements have lead to realistic grain scale microgeometries of EMs

Homogenization Framework

- Finite mesoscales heterogeneous random materials exhibit scale dependent and non-unique material response.

- The use of macrohomogeneity (or Hill) conditions ensure scaling of the material response to the infinite or macroscopic limit, where there exists a unique material response



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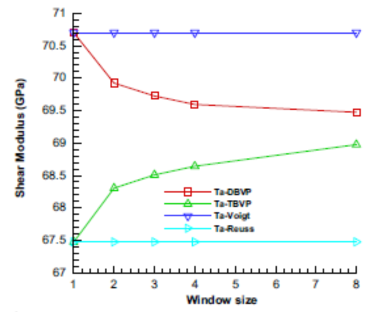
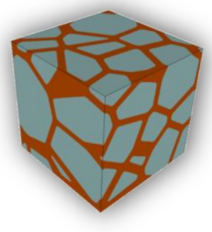


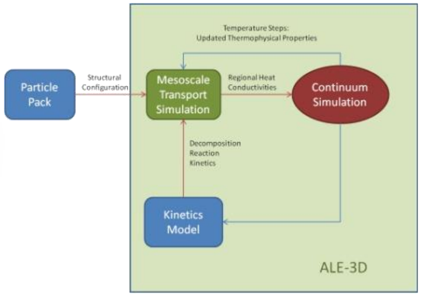
- This approach can be used to computationally investigate the scale-dependent properties of random materials for input into micromechanically based stochastic finite element schemes or constitutive models that introduce scale dependent and stochastic effects

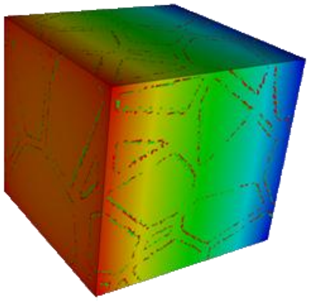
Grain-to-Continuum Parameters

- Structure-based Continuum Transport Parameters of Explosive Compositions by grain scale studies to improve predictive capability of thermal properties of continuum cook-off M&S

- By utilizing ParticlePack and hill condition to yield realistic transport properties of the composite materials at the gain scale, bulk material properties can be predicted for continuum transport parameters

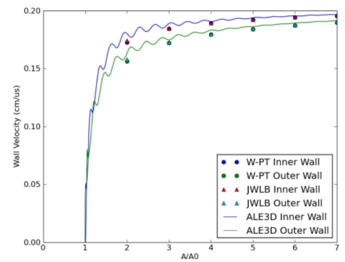


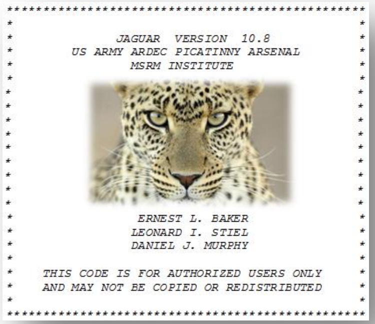




- Develop dynamic Hill condition to homogenize the case of thermal conductivity

Other Current Projects

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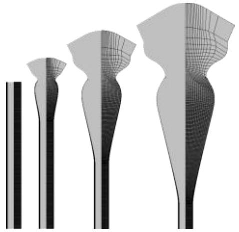
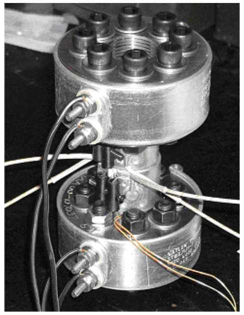


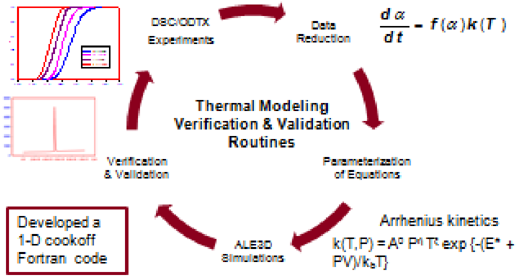
Coupled Thermochemistry/ Extended Libraries
Application to ALE3D-Cheetah-Jaguar with enhanced metals, semimetals, additional compounds analysis capability.

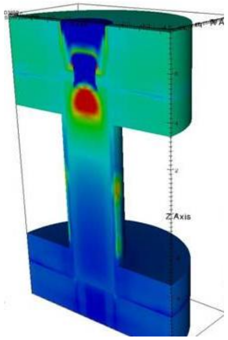
Condensed Matter Field Theory
Create a computationally tractable bridge from the molecular level through the meso-level to the macro-level using the tools and architecture of Condensed Matter Field Theory (CMFT). ATK/ARDEC partnership.

MSRM Use Cases
Munition-based problems or test cases for new developments and MSRM tools.

Reaction Kinetics/Thermal V&V
Methodologies and equations for isoconversional kinetic evaluation of Differential Scanning Calorimetry data, leading to DSC virtual capability in ALE3D.







Summary

- Recent MSRM institute developments have supported the IM modelling community and energetic/warhead analysts
- DSD characterization has been competed for IMX-104 and DSD algorithm/routine has been developed into production hydrodynamics code ALE3D, this framework will provide analysts a better tool in predicting detonation times of complex geometries and HE fills with non-ideal behavior.
- ParticalPack allows for creates representative volume elements of explosives with distribution of particle sizes and varying binder thickness. Recent improvements provide a void seeding capability for insertion of non-spherical random void or background material
- Homogenization Framework that introduce scale-dependent and stochastic effects to investigate the scale-dependent properties of random materials

Acknowledgments

- **ARDEC Team:**

  E. Baker, E. Bixon, L. Costa, W. Davis, G. Fast, J. Jablonski, D. Mackin, R. Mudryy, D. Murphy, D. Pfau, V. Stepanov, & Interns

- **Partners (academic, national labs, industry)**
  - Air Force Research Laboratory
  - Naval Research Laboratory
  - Lawrence Livermore National Laboratory
  - Los Alamos National Laboratory
  - University of Alabama at Birmingham
  - University of Illinois Urbana-Champaign
  - Brooklyn Polytechnic Institute of NYU
  - Navel Research Laboratory
  - ATK

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Questions