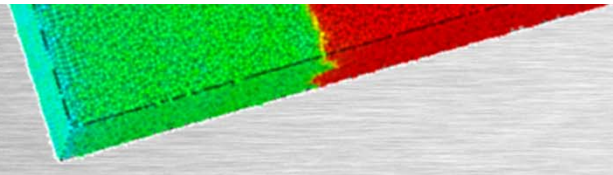
Recent Extensions of Dissipative Particle Dynamics Methods and Application to Hierarchical Multiscale Simulation



James P. Larentzos[1], Brian C. Barnes[2], John K. Brennan[2], Michael S. Sellers[2], Timothy I. Mattox[1], and Martin Lísal[3,4]

[1]Engility Corporation at the U.S. Army Research Laboratory

[2]U.S. Army Research Laboratory, Rodman Materials Research Laboratory, Aberdeen Proving Ground, MD, USA 21005

[3]Laboratory of Chemistry and Physics of Aerosols, Institute of Chemical Process Fundamentals of the ASCR, v. v. i., Rozvojová 135/1, 165 02 Prague 6-Suchdol, Czech Republic

[4]Department of Physics, Faculty of Science, J.E. Purkinje University, České Mládeže 8, 400 96 Ústí n. Lab., Czech Republic

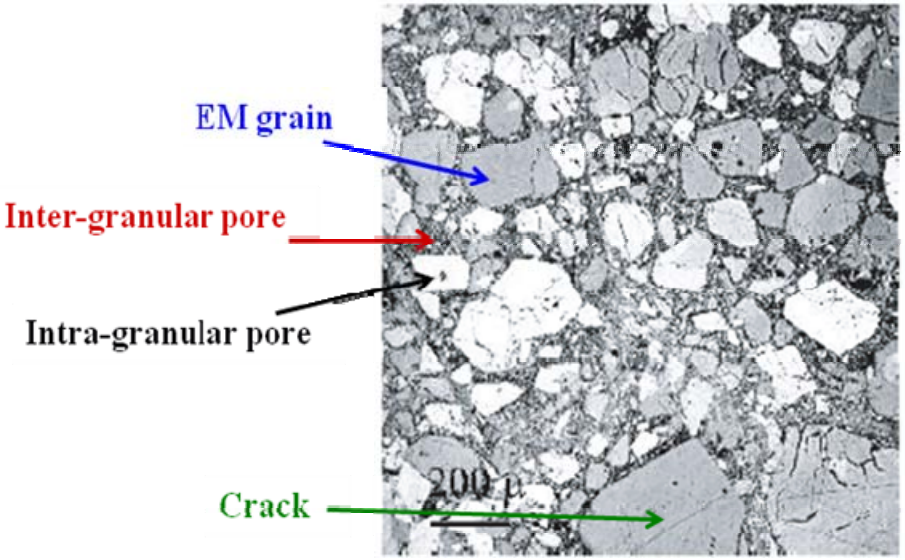
Modeling Energetic Materials

- **Understand → Predict / Tailor**

- an explosive formulation exhibits **phenomena at many length scales**

- **various simulation types** are suited for particular scales

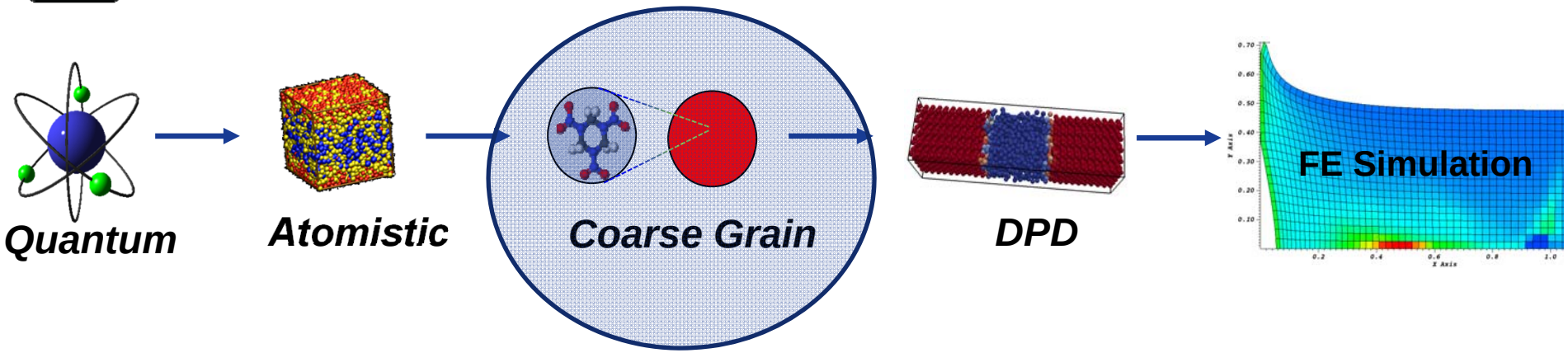
- Multi-scale Response of Energetic Materials (**MREM**)

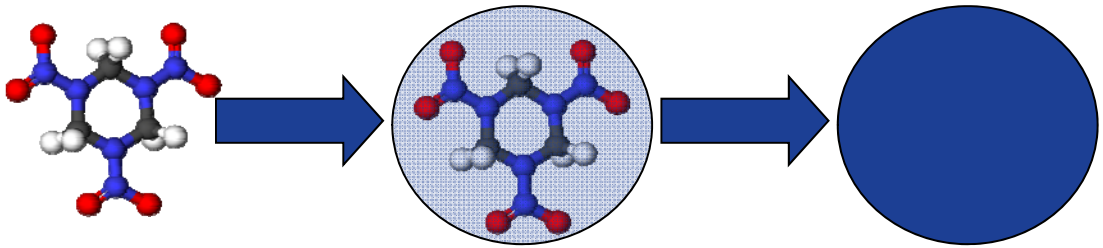


Valuable information at every scale

Skidmore, C.B., Phillips, D.S., Howe, P.M., Mang, J.T., and J.A. Romero, 1998, 11th International Detonation Symposium, Snowmass Village, Colorado, pp. 268.

Coarse Grain Modeling





- Gain Computational Speed By Removing Atomistic Detail
- **Challenge:** Retaining Atomistic Physics With CG Model

Coarse-Grain Method Development

Need to capture known thermo-mechanical responses:

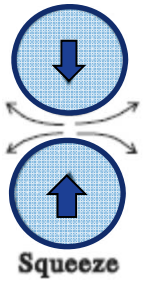
- ✓ Phase transitions
- ✓ Structural rearrangements
- ✓ Mechanical deformation
- ✓ Chemical reactivity

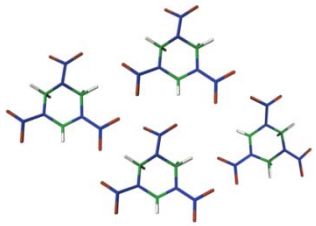
Dissipative Particle Dynamics (DPD) method

Dissipative Particle Dynamics (DPD)

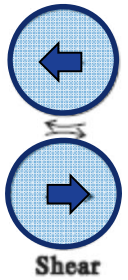
$$m_i \frac{dv_i}{dt} = \sum_{i \neq j} \left(F_{ij}^{CG} + F_{ij}^{D} + F_{ij}^{R} \right)$$

F^D parallel $\gamma^{||}$





F^D perpendicular $\gamma^{\perp}$



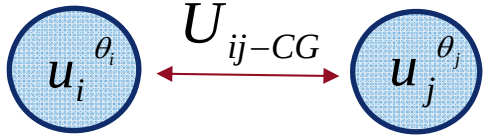
Additional forces on particle can recapture lost degrees of freedom

Hoogerbrugge and Koelman, *Europhys. Lett.*, **19** (1992)

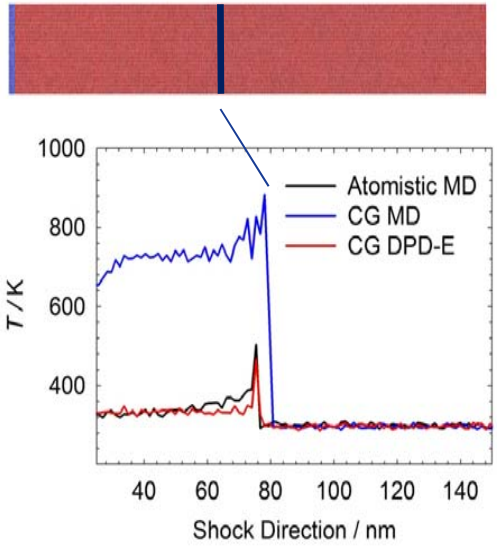
Constant Energy Dissipative Particle Dynamics (DPD-E)

$$E = \sum_i KE_i + \sum_i U_{i-CG} + \sum_i u_i$$

Explicit | *Implicit*



internal energy and temperature of cg particle



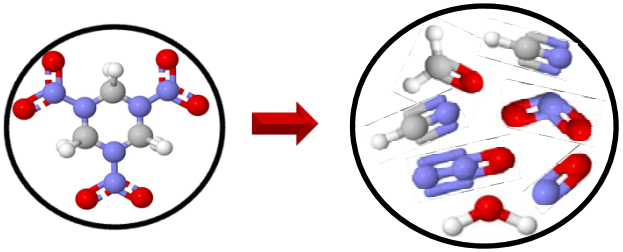
Lisal, M., Moore, J.D., Izvekov, S., Schweigert, I.V., Larentzos, J.P., Brennan, J.K., *in preparation*

Conservation of energy/momentum – Particles exchange momentum/heat

J. Bonet Avalos and A. Mackie, *Europhys. Lett.*, **40** (1997)
P. Espanol, *Europhys. Lett.*, **40** (1997)

Constant Energy Dissipative Particle Dynamics (DPD-E) with Reactions

coarse-grain reactor



CG-RDX → decomposed RDX

Generalization and extension of pioneering work by Maillet, Soulard, Stoltz

J. B. Maillet, L. Soulard, and G. Stoltz *A reduced model for shock and detonation waves. II. The reactive case* Europhys. Lett. **78**, 68001 (2007)

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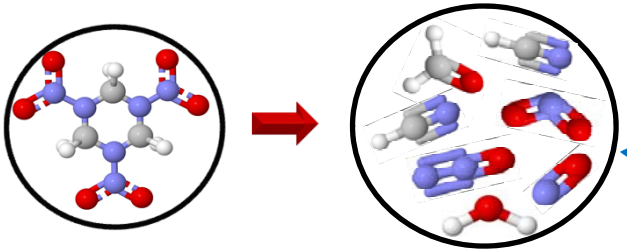

CG-RDX → decomposed RDX

behaves as perfectly-stirred batch reactor at every time step

- consider additional progress variable for each particle
  - **extent of reaction:** λ_i
- reactions occur within CG particle and NOT through bond breaking between particles
- requires input of reaction mechanisms and kinetics
- chemical energy released/gained is translated to internal and kinetic energy

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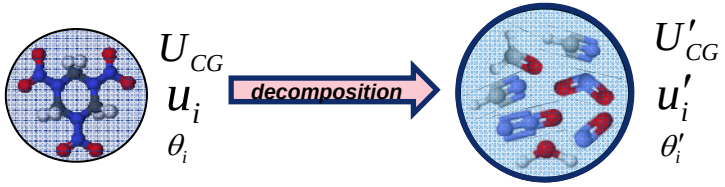
RDX Decomposition



RDX

Product Gas Mixture
($HCN, NO_2, NO, H_20, N_2, H_2, CO, CO_2$)

CG Particle Reactor

Reduced Reaction Model

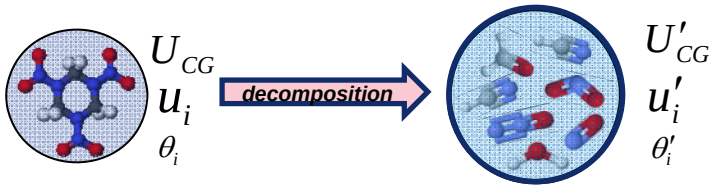
RDX→ 3HCN + 3/2(NO2 + NO + H2O) **endothermic**

HCN + NO2 → NO + ½(N2 + H2) + CO **exothermic**
HCN + NO → CO + N2 + ½H2
NO + CO → ½N2 + CO2

Arrhenius Form $k_{Rx}(\theta_i) = A_{Rx} e^{-E_{a-Rx}/k_B\theta_i}$

Brennan, J.K., Lísal, M., Moore, J.D., Izvekov, S., Schweigert, I.V., Larentzos, J.P. **Coarse-Grain Model Simulations of Nonequilibrium Dynamics in Heterogeneous Materials** *The Journal of Physical Chemistry Letters* **2014** *5* (12)

RDX Decomposition



RDX

Product Gas Mixture
($HCN, NO_2, NO, H_20, N_2, H_2, CO, CO_2$)

In General

- **Not an explicit "reactive" potential**
- **No bond breaking**
- **Number of particles is constant**
- **Requires input of chemical reactions and kinetics**
- ***Chemical character* is represented by change in inter-particle potential**

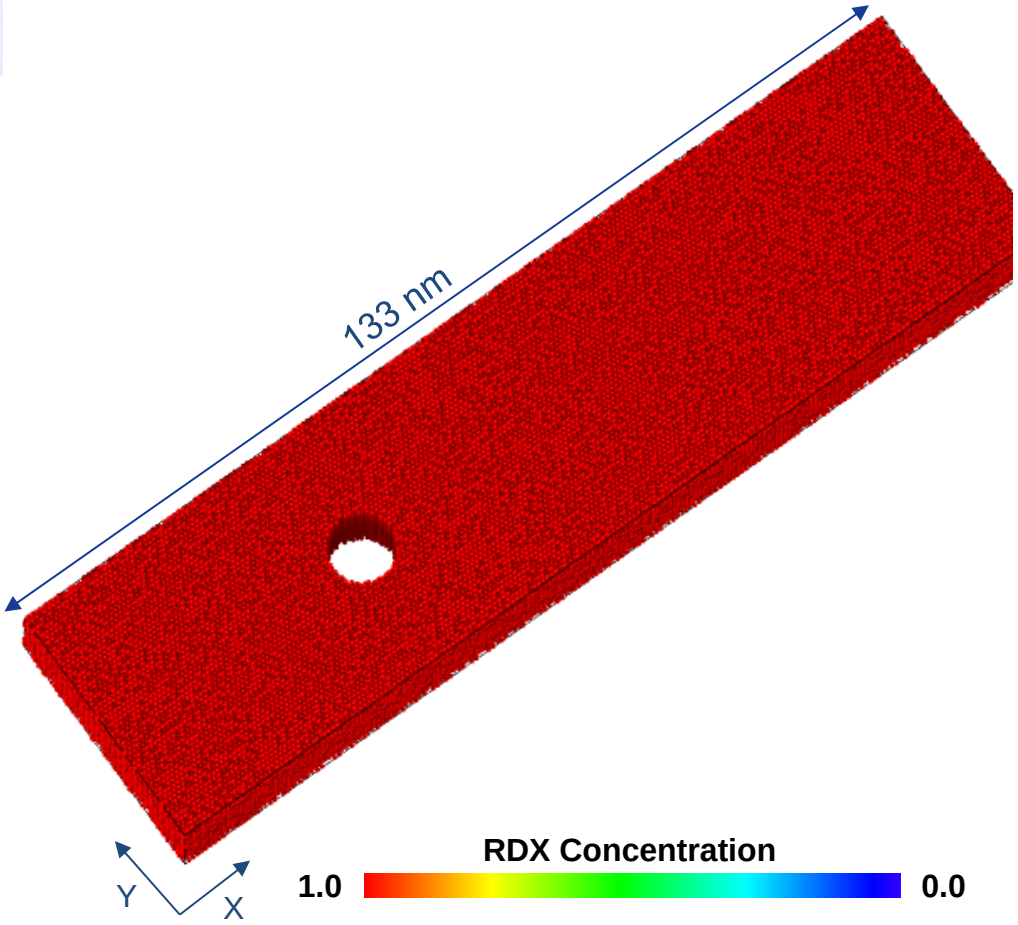
Simulate chemistry through a change in particle energy - internal/external

Brennan, J.K., Lísal, M., Moore, J.D., Izvekov, S., Schweigert, I.V., Larentzos, J.P. **Coarse-Grain Model Simulations of Nonequilibrium Dynamics in Heterogeneous Materials** *The Journal of Physical Chemistry Letters* **2014** *5* (12)

Shock Initiation of RDX

10nm Void – 3km/s Shock

- Shock initiation in perfect crystal
- Collapsing void causes initiation at downstream face
- Reactions at void location proceed to greater extent, faster



DPD with Velocity-Verlet Integration

- **DPD typically integrated using standard numerical integrators (e.g., velocity-Verlet)**

Deterministic Integration

- Velocity-Verlet Integration #1: For i = 1, …, N

$$\mathbf{p}_i \leftarrow \mathbf{p}_i + \frac{\Delta t}{2}\mathbf{F}_i$$

$$\mathbf{r}_i \leftarrow \mathbf{r}_i + \Delta t \frac{\mathbf{p}_i}{m_i}$$

- Force Calculation:

$$\mathbf{F}_i = \sum_{j \neq i} (\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R)$$

- Velocity-Verlet Integration #2: For i = 1, …, N

$$\mathbf{p}_i \leftarrow \mathbf{p}_i + \frac{\Delta t}{2}\mathbf{F}_i$$

Lisal, Brennan, Bonet Avalos, *J. Chem. Phys.*, 135 (2011)

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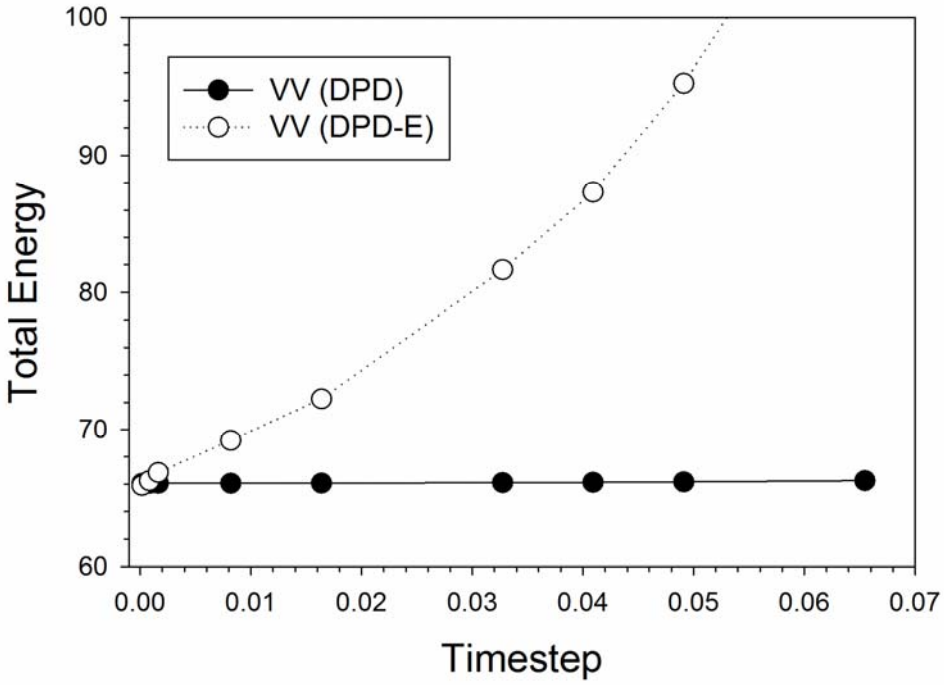
DPD Fluid (Reduced Units)



Lisal, Brennan, Bonet Avalos, *J. Chem. Phys.*, 135 (2011)

DPD with Velocity-Verlet Integration

- **DPD typically integrated using standard numerical integrators (e.g., velocity-Verlet)**
- **Velocity-Verlet algorithm works well for DPD, but DPD-E limited to small timesteps**
- **Stochastic nature of the algorithm requires special consideration**

Deterministic Integration

- Velocity-Verlet Integration #1: For i = 1, …, N

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- Velocity-Verlet Integration #2: For i = 1, …, N

$$\mathbf{p}_i \leftarrow \mathbf{p}_i + \frac{\Delta t}{2}\mathbf{F}_i$$

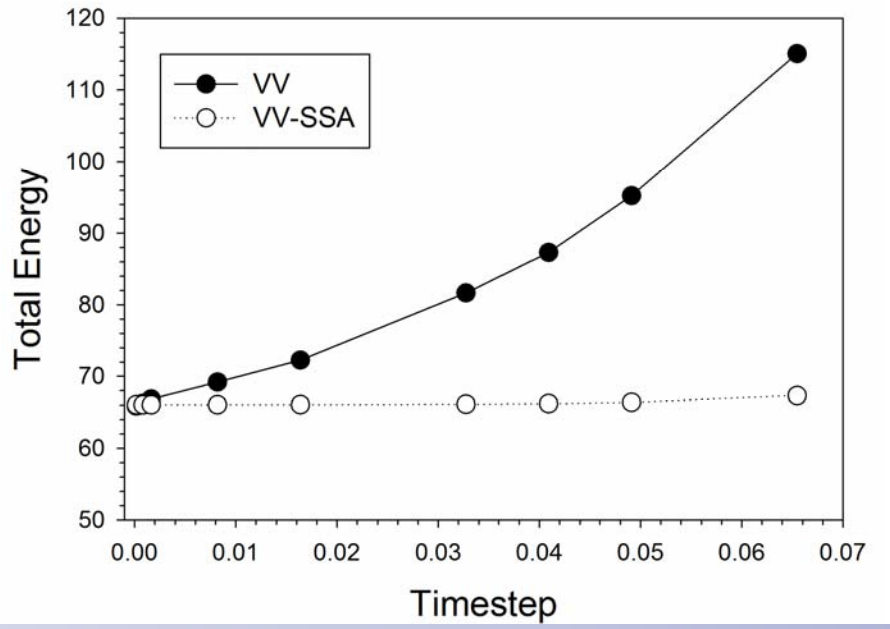
Split stochastic components of the force into separate integration steps through the Shardlow splitting technique

Lisal, Brennan, Bonet Avalos, *J. Chem. Phys.*, 135 (2011)

Shardlow Splitting Algorithm

- Split momenta integration into deterministic dynamics and stochastic dynamics
- Both can then be integrated using standard numerical integrators (e.g., velocity-Verlet)
- Readily extended to other DPD variants (not true for other integrators)
- Larger time steps allowable (~10-100x larger, with comparable energy conservation)

DPD-E (Reduced Units) (Serial Processor)

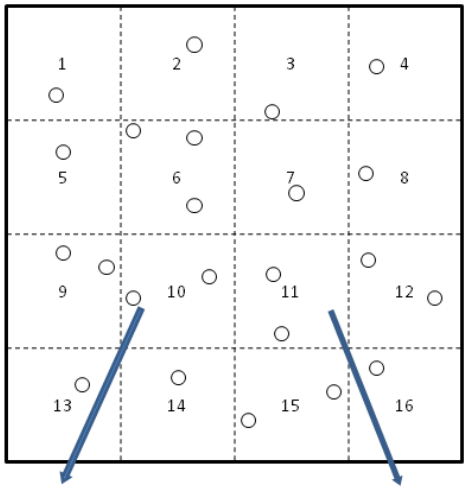


Recursive nature of the stochastic integration makes SSA difficult to parallelize!

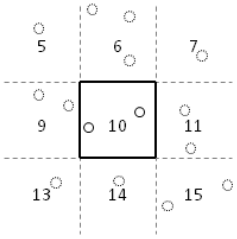
Lisal, Brennan, Bonet Avalos, *J. Chem. Phys.*, 135 (2011)

SSA Parallelization in a Domain Decomposition Framework

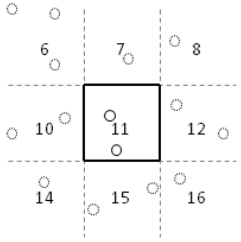
Domain Decomposition



Processor 10



Processor 11

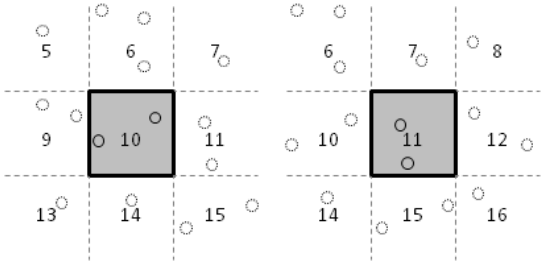


Larentzos, Brennan, Moore, Lísal and Mattson, *Comp. Phys. Commun., 185, 1987-1998* (2013).

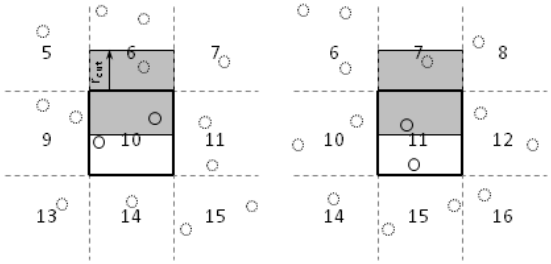
Staged Communication

- Split stochastic integration into multiple stages
  - Particles interact on exactly one processor per stage
- Define a directional communication scheme
  - Active Interaction Regions (AIR) turn particle interactions on/off in a consistent direction
  - Account for all particle interactions

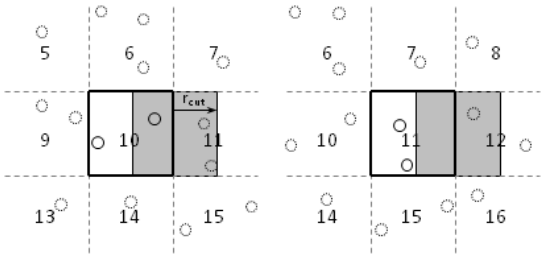
Stage 1



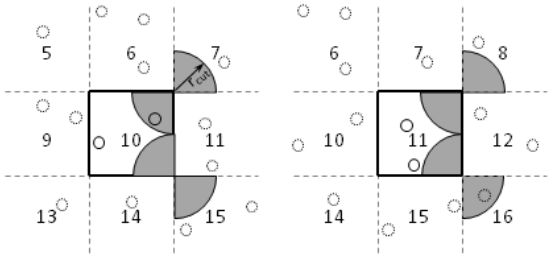
Stage 2



Stage 3



Stage 4



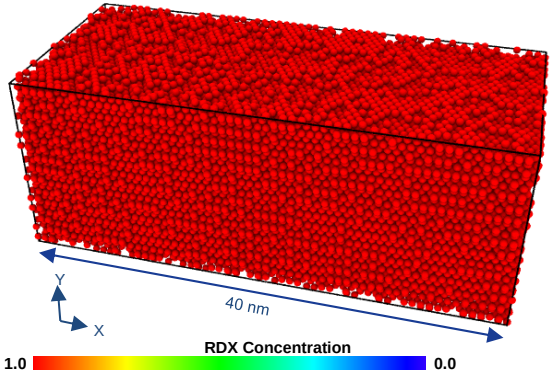
Summary

Constant Energy DPD (DPD-E) in LAMMPS

- Shardlow Splitting Algorithm (SSA) Integration Scheme
- Allows for larger time steps w/ better energy conservation

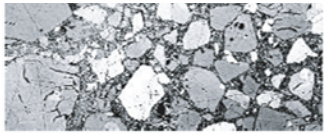
Reaction DPD (DPD-RX) in LAMMPS

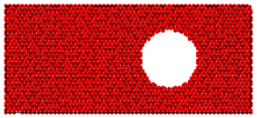
- Extension of DPD-E
- Works seamlessly with SSA stochastic integration scheme
- Concentration-dependent potentials
  - Exponential-6 and table potentials
- Concentration-dependent equation of state (EOS)
- Reaction kinetics solvers for non-stiff and stiff ODEs
  - 4th Order Runge-Kutta
  - GNU Scientific Library (GSL) suite of ODE solvers
  - CVODE
  - CUDA implementations for RK4 and CVODE solvers

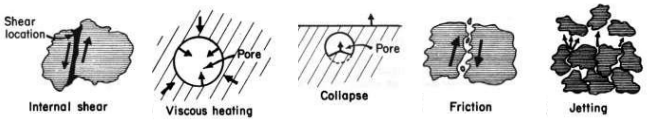


Future Work

- Continued model refinements – potentials, reaction set
- Investigate effects of microstructure

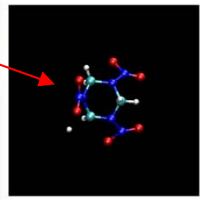






Introduction

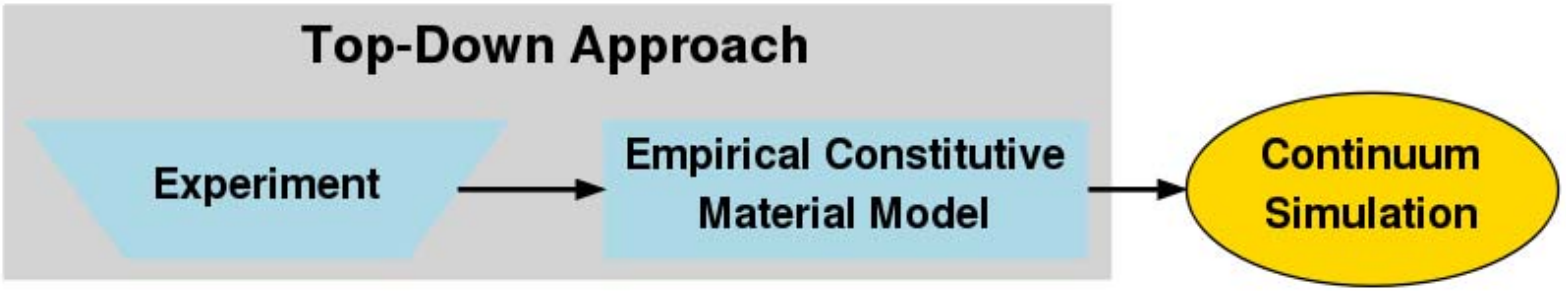
GOAL: Development of *Physics Based* Multiscale Modeling and Simulation Capability



Microstructural Heterogeneity

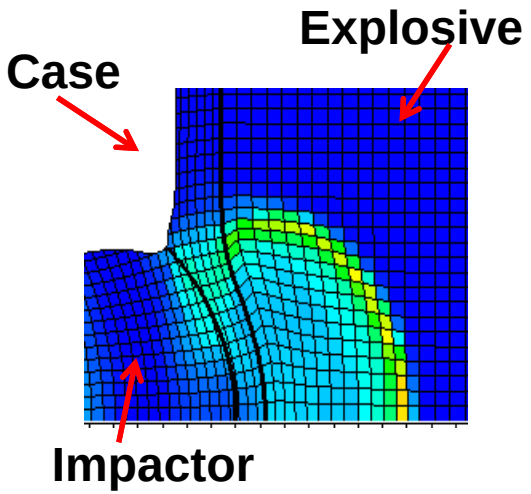
Skidmore, C.B., Phillips, D.S., Howe, P.M., Mang, J.T. and Romero, J.A., *11th International Detonation Symposium*, Snowmass Village, Colorado, pp. 268

Continuum State-of-the-art



Top-Down Approach:

- Heavily reliant on testing
- Expensive, time consuming
- Non-transferable
- Limited in scope



Progression to Payoff

Top-Down Approach:

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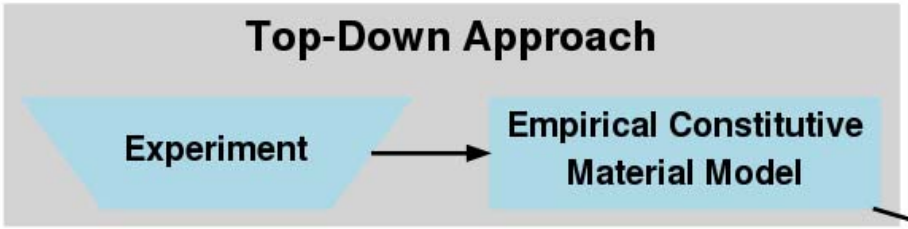
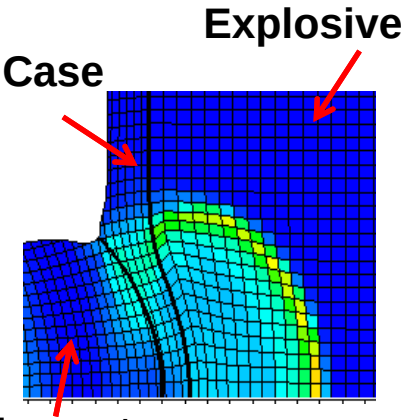
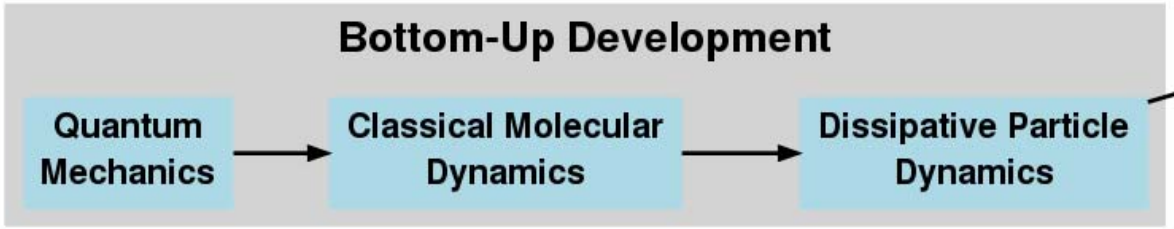
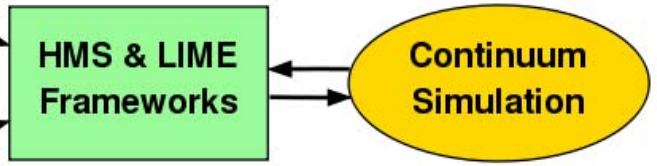
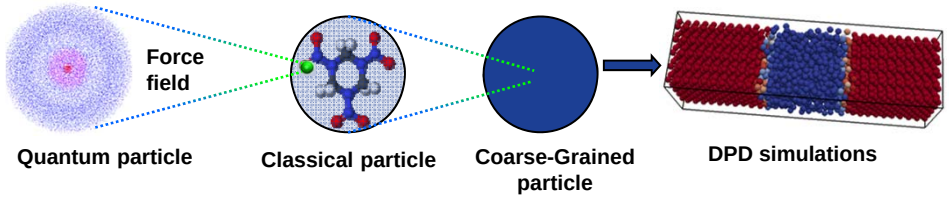








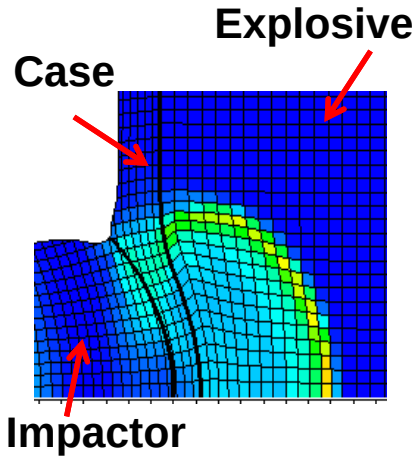


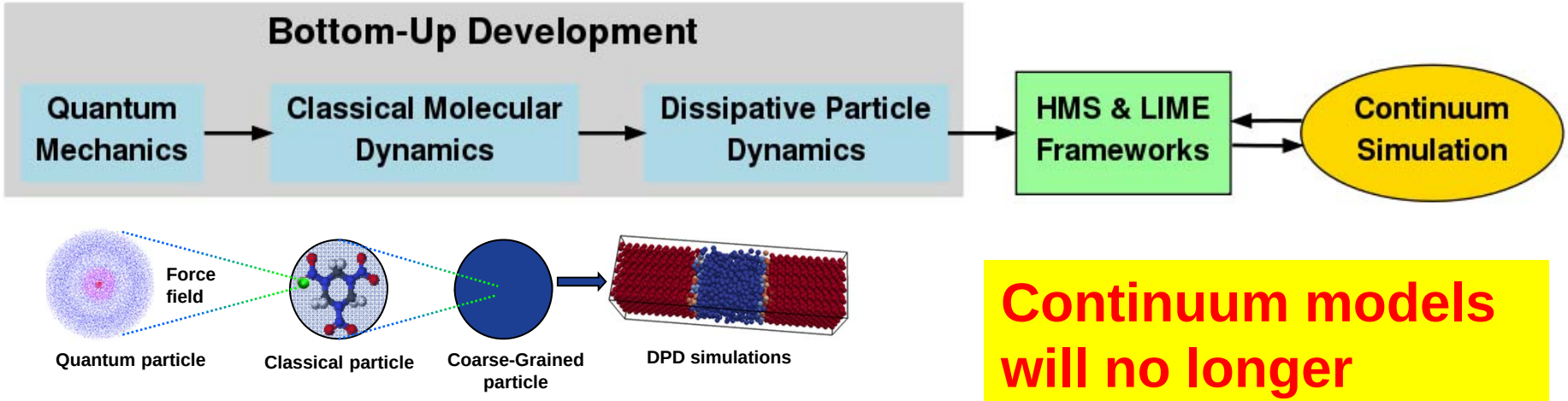
Bottom-Up Development

- Physics based
- Transferable
- Materials by Design
- Began with EOS

In Progress: Incremental Plan

Future Vision: Top-Down Removed





Bottom-Up Development

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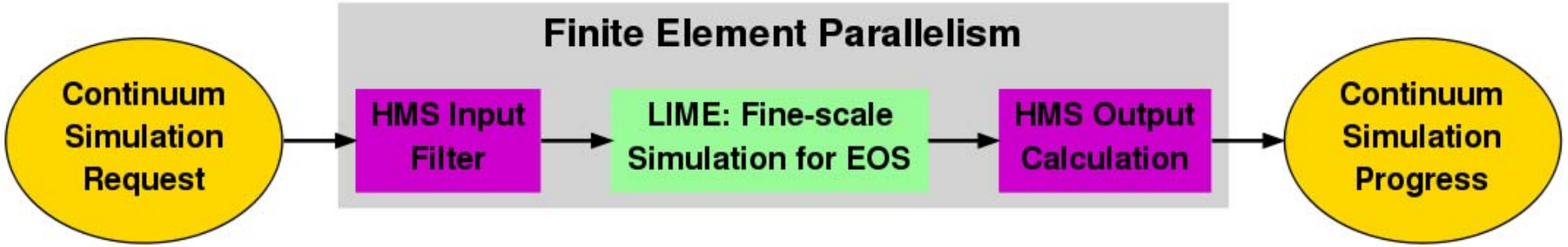
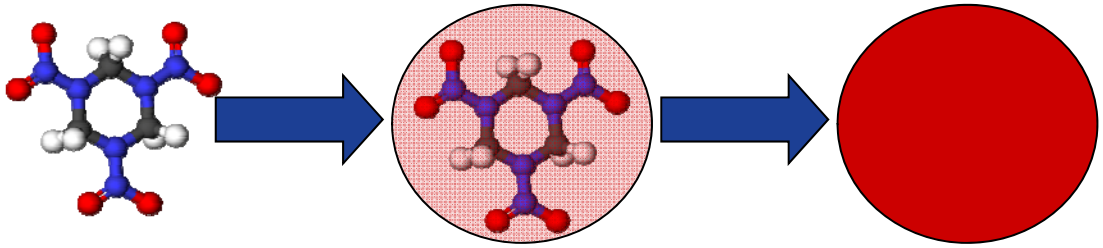
Continuum models will no longer require data from experiment.

Solution Structure

Solution Execution at Runtime



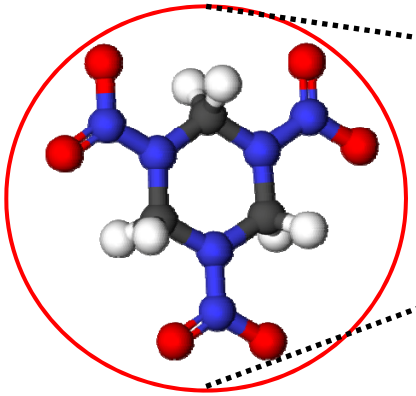
Fine-scale Model



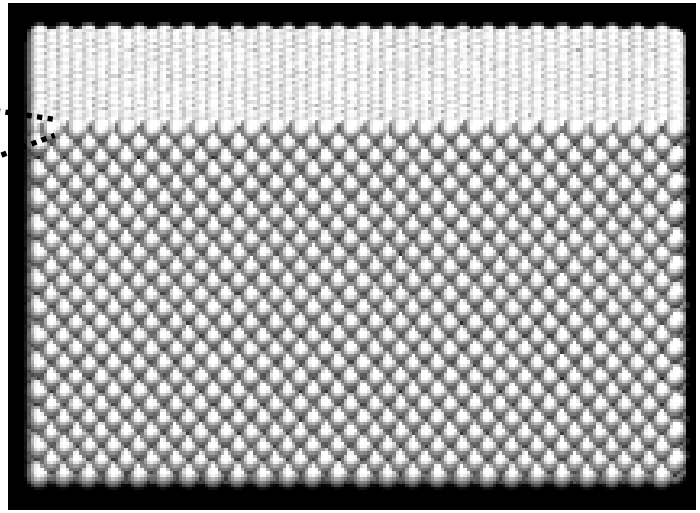
All intramolecular degrees-of-freedom coarse-grained

RDX

$C_3H_6N_6O_6$



21 atoms



- ***Sacrifice atomistic detail***
- ***Gain computational speed***

S. Izvekov, P.W. Chung, and B.M. Rice, *J. Chem. Phys.*, **135**, 044112 (2011)

Fine-scale Method

Dissipative Particle Dynamics (DPD-E) Equation of Motion

- Both momentum and energy conserved
- Internal energy variable assigned to each particle, u_i

$$\frac{d\mathrm{r}_i}{dt} = \mathrm{v}_i(t)$$ ***position***

dissipative forces

random forces

$$m_i \frac{d\mathrm{v}_i}{dt} = \mathrm{f}_i(t) = \sum_{i \neq j} \left(\mathrm{F}_{ij}^C + \mathrm{F}_{ij}^D + \mathrm{F}_{ij}^R \right)$$ ***velocity***

$$\frac{du_i}{dt} = -\frac{1}{2m_i}\left(p_i - p_j\right) \bullet \left(F_{ij}^D + F_{ij}^R\right) + \dot{q}_{ij}^D + \dot{q}_{ij}^R$$ ***internal energy***

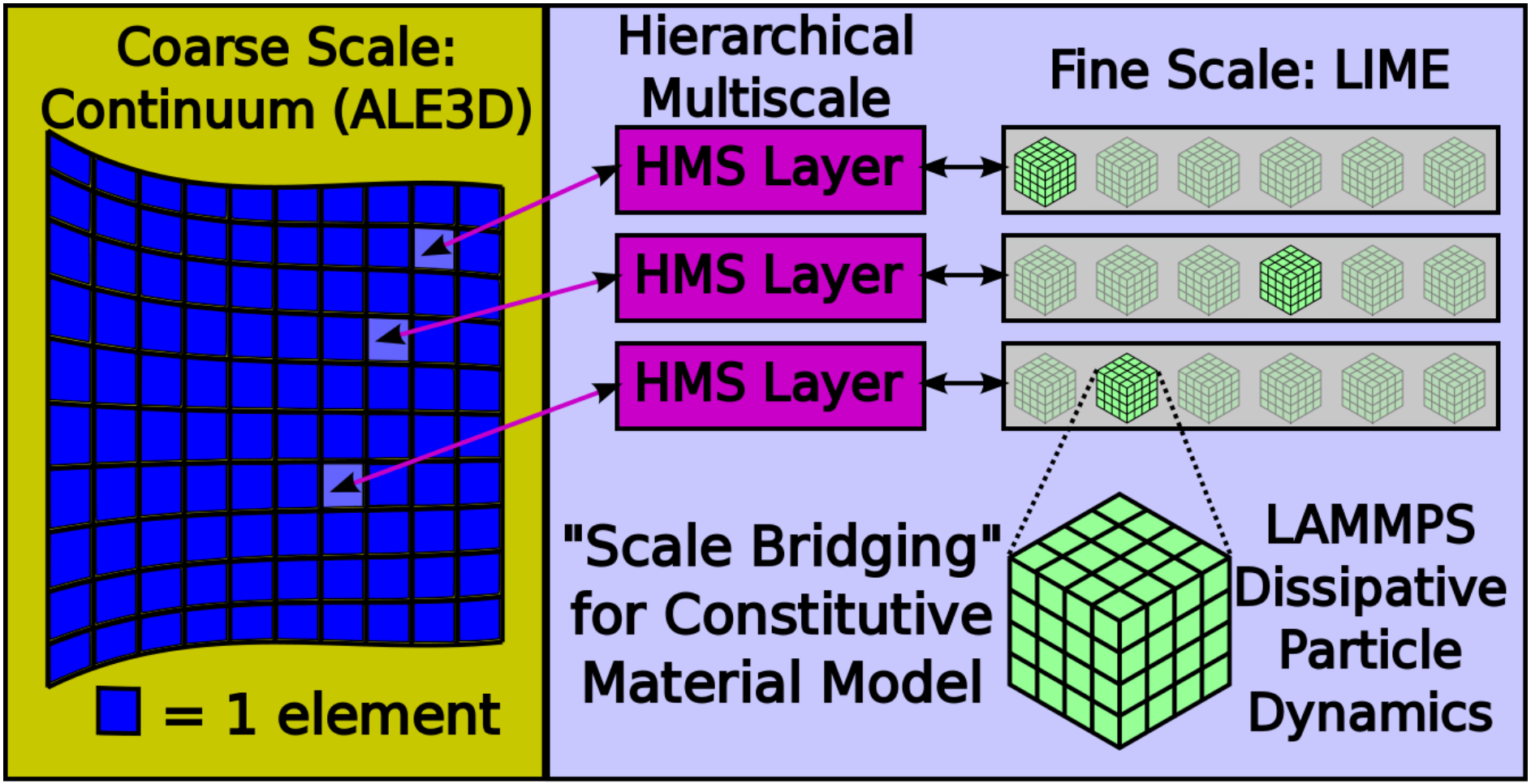
particles exchange *momentum* and *thermal energy*

Energy dissipated by frictional forces stored in particle internal energy

J. Bonet Avalos and A. Mackie, *Europhys. Lett.*, **40** (1997)

P. Espanol, *Europhys. Lett.*, **40** (1997)

HMS Conceptual View



W. E, B. Engquist, X. Li, W. Ren, and E. Vanden-Eijnden, *Commun. Comp. Phys.*, **2**, 367-450 (2007)

J. Knap, C.E. Spear, K.W. Leiter, R. Becker and D.A. Powell *Int. J. Num. Meth. Eng.*, *submitted*

Automating LAMMPS

- Simulation & Analysis
- Swapping Ensembles
- Start to Finish

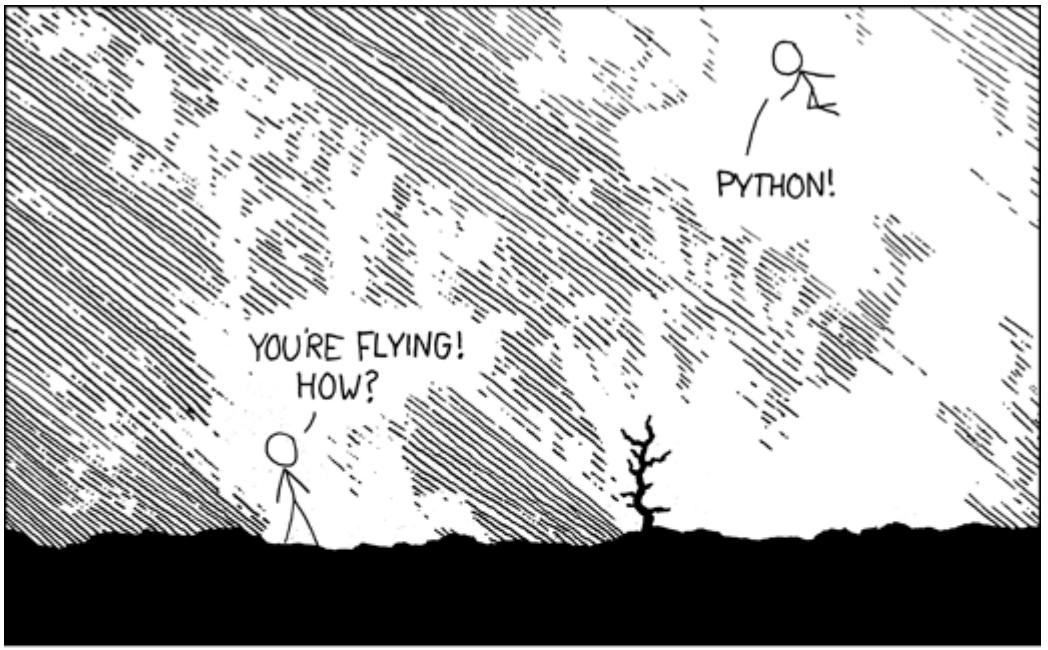
How??

The Python Interface

don't go alone:

numpy, mpi4py

"Program yourself out of a job"



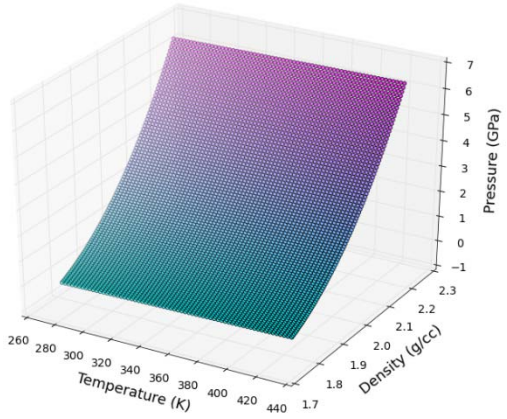
xkcd.com/353

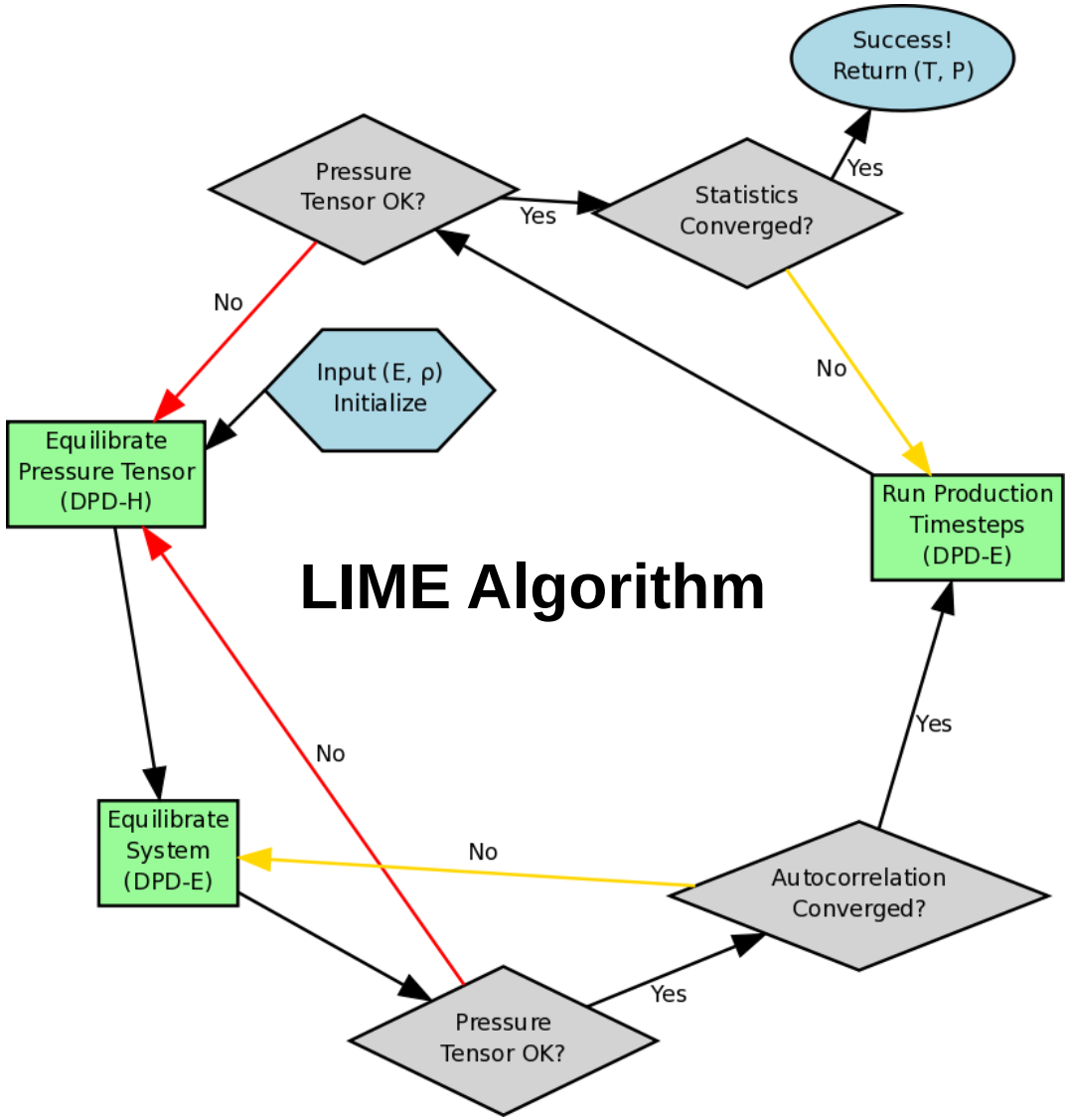
Fine-scale Implementation

LIME: LAMMPS Integrated Materials Engine

New Tool for Automating Classical MD/DPD

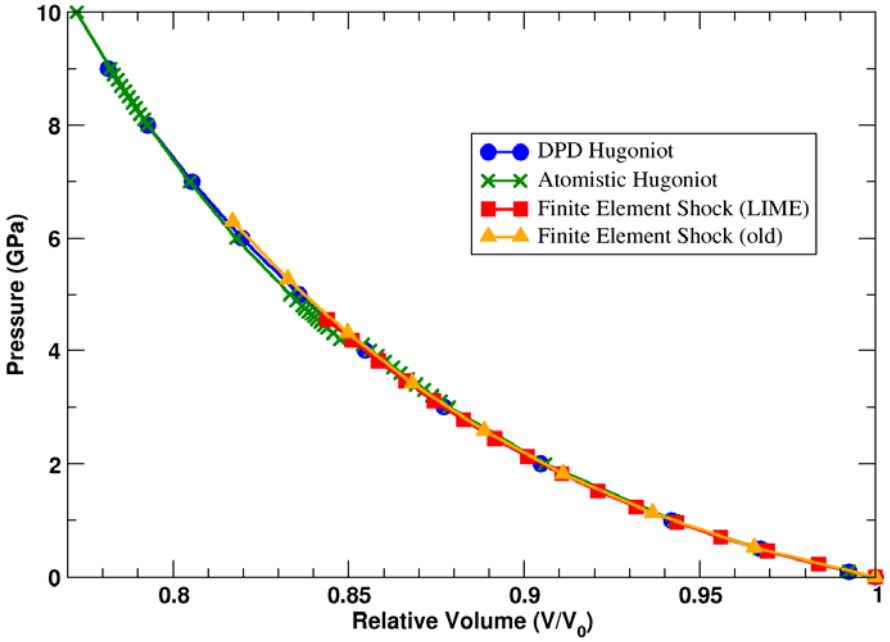
- **Adaptable, Extensible**
- **"On-the-fly" HMS Fine-scale**
- **Implemented Coarse-Grain Model of RDX**
- **Generated EOS Tables for HMS Validation (below)**

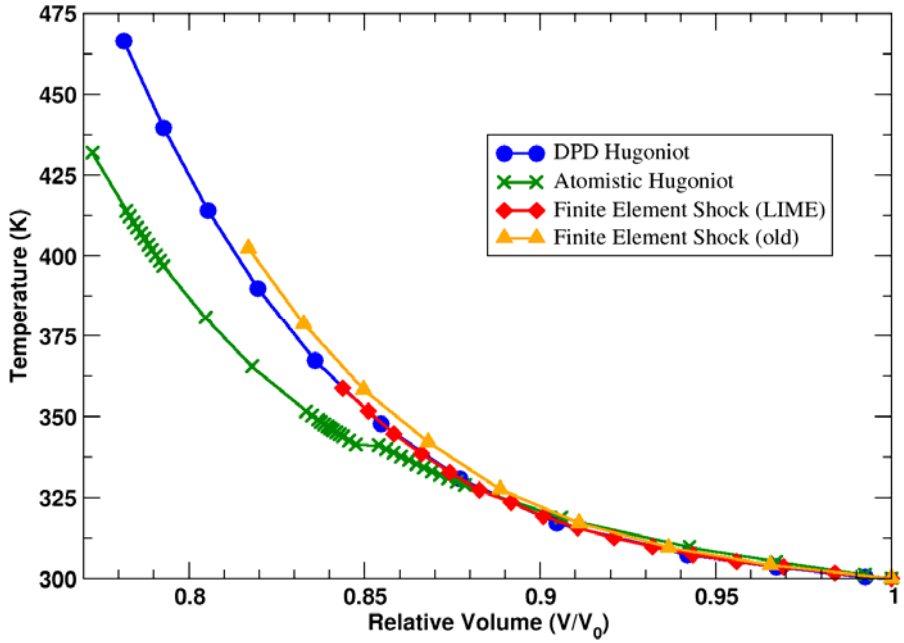




Initial Validation

ALE3D Equation of State (EOS) Replaced by LIME EOS



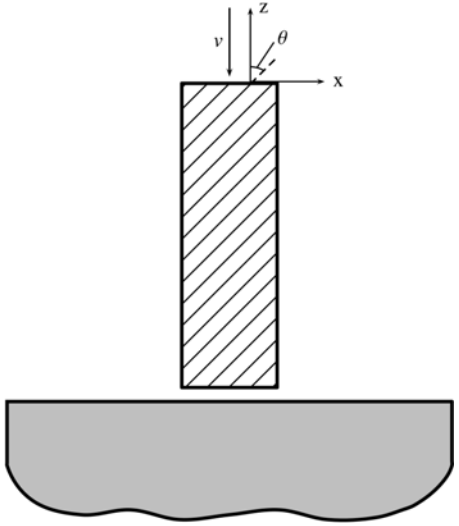


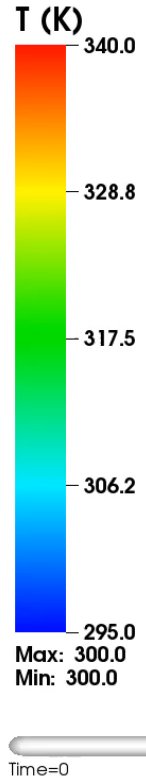
- **Finite Element Shock: LIME EOS Tables Improve Agreement Between Continuum and DPD Simulations Compared to Old EOS Tables**
- **DPD Speedup with LIME Variant & Adaptive Erpenbeck Method: ~20x Prior Method**

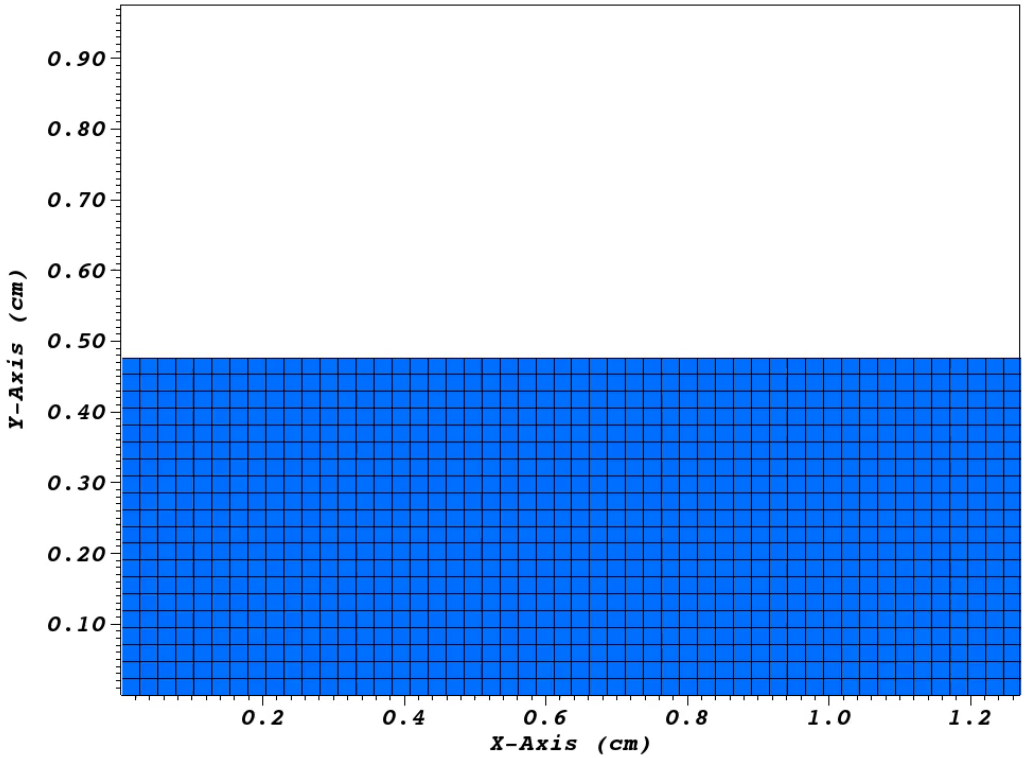
Established baseline for assessing accuracy and performance of subsequent embedded models.

Taylor Impact Test #1

Continuum Simulation of Taylor Test: LIME EOS Driven







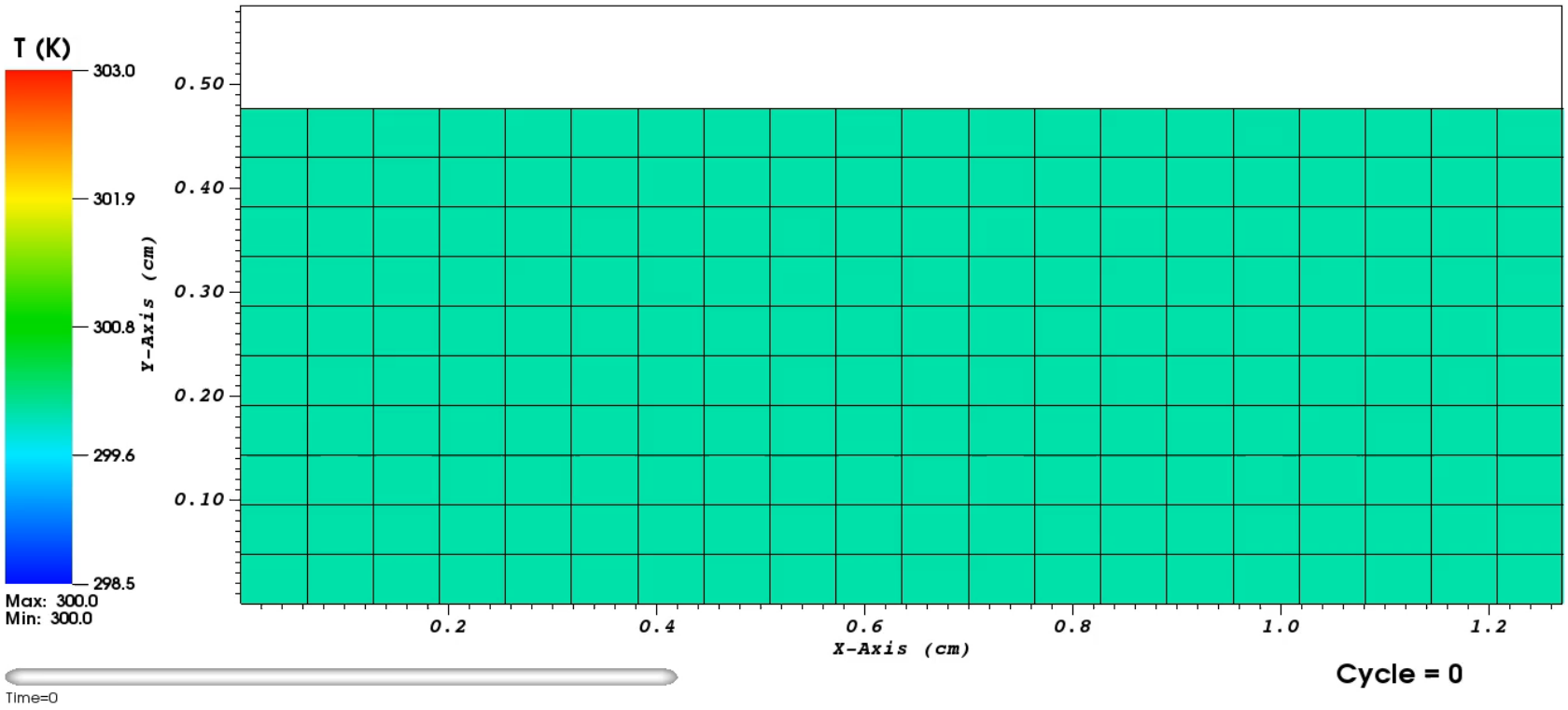
Simulation Details

- A Cylinder of Solid RDX Impacting a Rigid Anvil
- Impact Speed 200 m/s
- cm Lengths, Axial Symm.
- Colored by Temperature
- ALE3D & LIME EOS Tables
- Proof-of-Concept Before "On-the-fly" HMS

RDX Deformation and Hot Elements Observed

Table-driven precursor of “on the fly”

- Impact speed 55 m/s
- 200 elements
- Different timesteps due to larger elements
- Avoided pressures, densities where real material may fracture
- Reference simulation



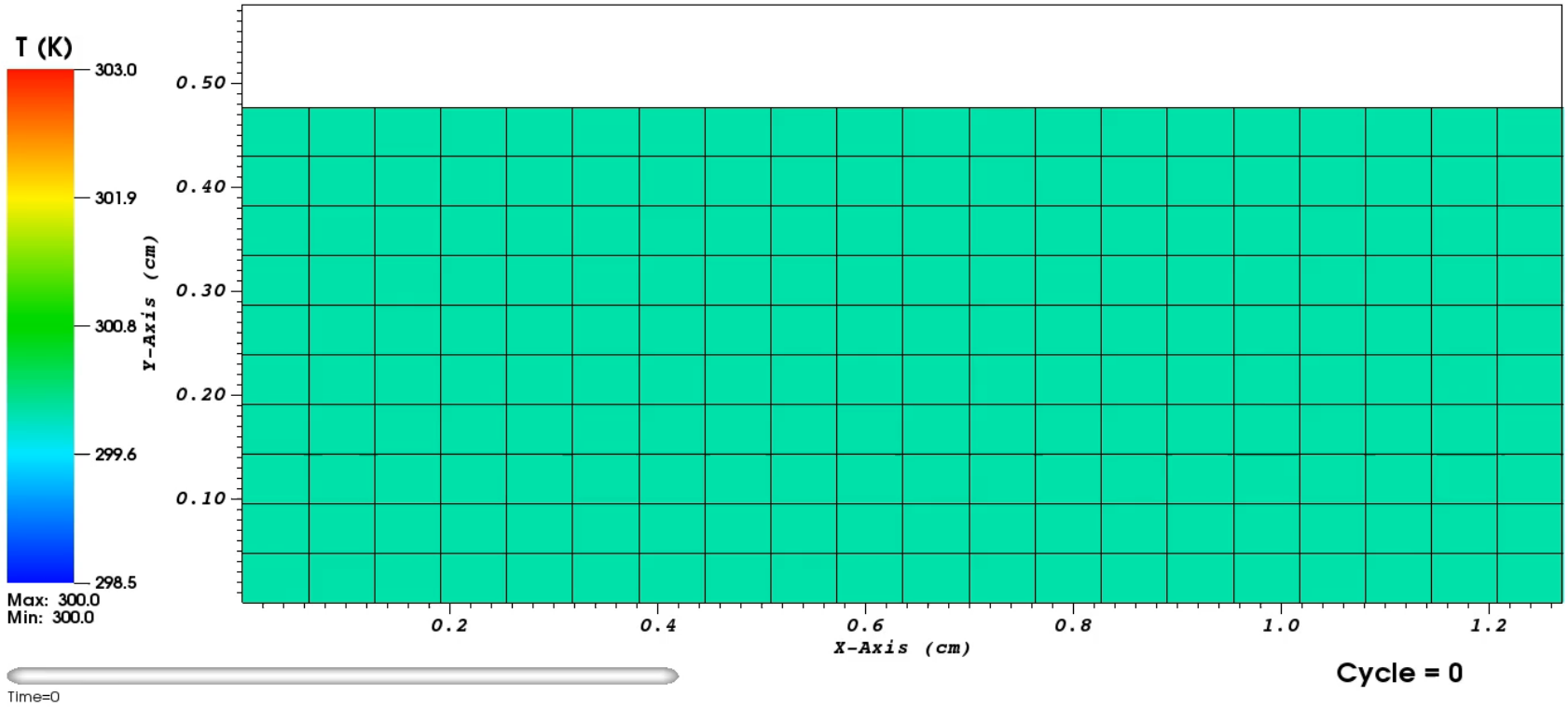
"On the fly" Hierarchical Multiscale

HMS has a heartbeat!

- ~200,000 total core hours
- Randomness due to statistical nature of simulations
- 34,800 fully automated results

HPC Challenges

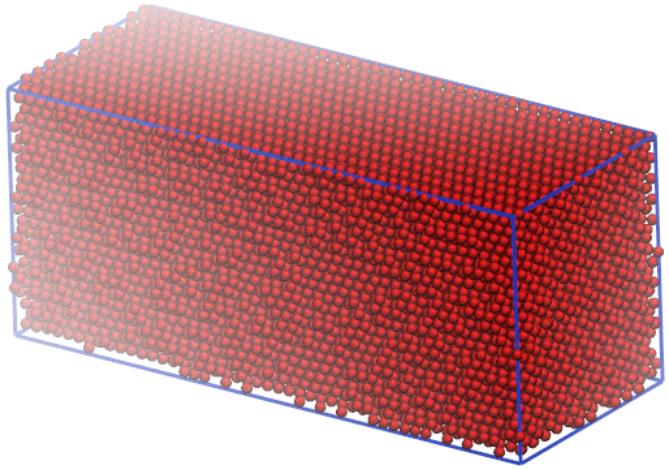
- Random failures (Lustre, Cray CCM ssh) stop jobs in progress; error handling
- Cray does not implement MPI_SPAWN
- 64 cores/elem needed for good throughput



Bottom-Up Development: a Multi-Year Effort to Improve Material Models for Hierarchical Multiscale Simulation

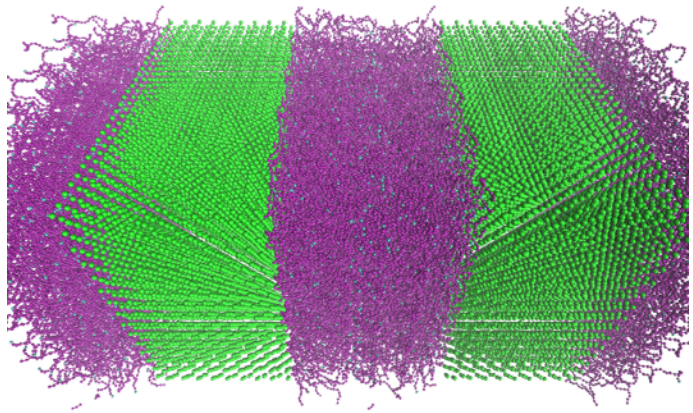
Material Model Functionality

- **Reactive equation of state (DPD-RX implementation for LIME)**
- **Defect and Initiation Statistics**
- **Deviatoric Stress & Plasticity**
- **Porosity**
- **Multi-Component Starting Systems (such as Binders or Solvent)**
- **More Complex Fine-Scale Models**



Development By All Collaborators

- **HMS: Adaptive Sampling (Speed!)**
- **HMS: Scaling to 100k CPU Cores**
- **ALE3D: Failure, Plasticity Models**
- **DPD: New, Improved CG Models**
- **DPD: Heterogeneous Computing**
- **LIME: Additional Material Properties**
- **LIME/HMS: Timescale Propagation**



Credits

Energetics & DPD
John Brennan
Martin Lísal (Czech Acad. Sci.)
Sergey Izvekov
Brian Barnes
Michael Sellers
Betsy Rice
William Mattson

Continuum & ALE3D
Rich Becker

Hierarchical Multiscale
Jaroslaw Knap
Carrie Spear (TAPE)
Ken Leiter

DoD HPC Modernization Program (HPCMP)
Productivity Enhancement, Tech Transfer & Training (PETTT)
James P. Larentzos (Engility)
Timothy I. Mattox (Engility)
Sean Ziegeler (Engility)
Christopher Stone (Computational Science & Engineering, LLC)

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Oak Ridge Associated Universities
Postdoctoral Fellowship

Computing Resources
DoD HPCMP
Defense Supercomputing Resource Centers (DSRCs)