Highly-Scalable Discrete-Particle Simulations with Novel Coarse-Graining: Accessing the Microscale

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2017 LAMMPS Workshop and Symposium
August 2, 2017 at UNM in Albuquerque, NM
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DoD Supercomputing Resource Centers (DSRCs):
Army Research Laboratory (ARL)
Air Force Research Laboratory (AFRL)
Army Engineer Research and Development Center (ERDC)

Los Alamos National Laboratory (LANL)
National Nuclear Security Administration (NNSA)
Texas Advanced Computing Center (TACC)

High Performance Computing Modernization Program (HPCMP)
This study was supported by the U.S. Dept. of Defense High Performance Computing Modernization Program (HPCMP)
User Productivity Enhancement, Technology Transfer, and Training (PETTT) activity (GSA Contract No. GS04T09DBC0017 through Engility Corporation)

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Motivation

Microstructure dependent shock response of Energetic Materials (EM)

- EM composites are highly microstructured
- Sensitivity and performance believed to be due to localized “hot spots”
**Microstructure Hot Spot Mechanisms**

**SINGLE IDEAL VOID:** 10 nm

- 10 nm void – 3 km/s shock
- Collapsing void causes initiation
- Reactions at void location proceed farther and faster

Product Gas Mixture

HCN, NO₂, NO, H₂O, N₂, H₂, CO, CO₂

RDX Concentration

\[ \text{C}_3\text{H}_6\text{N}_6\text{O}_6 \]
Goal: EM Composite Models

Approaching the scale of “dirty binder” regions

EM crystallite

polymer

inter-granular void

(yellow spheres, bonding not shown)


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## HPC Machines Used

<table>
<thead>
<tr>
<th>System</th>
<th>Trinity Phase 2 (KNL)</th>
<th>Stampede-2</th>
<th>Thunder</th>
</tr>
</thead>
<tbody>
<tr>
<td>Facility</td>
<td>Los Alamos National Laboratory (LANL)</td>
<td>Texas Advanced Computing Center (TACC)</td>
<td>US Airforce Research Laboratory (AFRL)</td>
</tr>
<tr>
<td>Peak Perf.</td>
<td>~27 PFLOP/s DP</td>
<td>~11 PFLOP/s DP</td>
<td>4.3 PFLOP/s DP</td>
</tr>
<tr>
<td>Approx. Size</td>
<td>~8,900 Nodes</td>
<td>~3,600 Nodes</td>
<td>3,216 Nodes</td>
</tr>
<tr>
<td></td>
<td>~605,200 Cores</td>
<td>~244,800 Cores</td>
<td>115,776 Cores</td>
</tr>
<tr>
<td>June 2017</td>
<td>est. #6 or #7 (like Cori)</td>
<td>#12 on Top500.org</td>
<td>#36 on Top500.org</td>
</tr>
<tr>
<td>Kind</td>
<td>Cray XC40</td>
<td>Dell PowerEdge C6320P</td>
<td>HPE/SGI ICE X</td>
</tr>
<tr>
<td>Processor</td>
<td>Intel Xeon Phi 7250 KNL</td>
<td>Intel Xeon E5-2699v3 HSW</td>
<td></td>
</tr>
<tr>
<td>Node &amp; Core Details</td>
<td>One 1.4 GHz CPU/node</td>
<td>Two 2.3 GHz CPUs/node</td>
<td></td>
</tr>
<tr>
<td></td>
<td>68 cores/CPU (in 34 tiles)</td>
<td>18 cores/CPU</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4 Hardware Threads/core</td>
<td>1 Hardware Thread/core</td>
<td></td>
</tr>
<tr>
<td>Threads</td>
<td>Up to 272 threads/node</td>
<td></td>
<td>36 threads/node</td>
</tr>
<tr>
<td>Memory Hierarchy</td>
<td>32kB L1/core + 512kB L2/tile</td>
<td>32kB L1/core + 256kB L2/core</td>
<td></td>
</tr>
<tr>
<td></td>
<td>16 GB MCDRAM/node</td>
<td>22.5 MB L3/CPU</td>
<td></td>
</tr>
<tr>
<td></td>
<td>96 GB DDR4/node</td>
<td>128 GB DDR4/node</td>
<td></td>
</tr>
</tbody>
</table>

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EM Shock Simulations at Scale: Inputs & Steps

Simulation Steps for a Shock applied to polycrystalline RDX:
1. Load initial positions of all particles
2. Equilibrate at 325 Kelvin for 150 ps
3. Apply (fix wall/lj93) and Propagate Shock Wave for 350 ps
Total of 500 ps simulated time

<table>
<thead>
<tr>
<th>Model Name</th>
<th>Sample Size (nm³)</th>
<th>Number of RDX Molecules</th>
<th>Number of Atoms</th>
<th>Grain Size Average (nm)</th>
<th>Number of Grains</th>
</tr>
</thead>
<tbody>
<tr>
<td>Small</td>
<td>40 x 40 x 2,500</td>
<td>20,452,820</td>
<td>429,509,220</td>
<td>30</td>
<td>243</td>
</tr>
<tr>
<td>Medium</td>
<td>100 x 100 x 2,500</td>
<td>126,259,367</td>
<td>2,651,446,707</td>
<td>75</td>
<td>90</td>
</tr>
<tr>
<td>Large</td>
<td>300 x 300 x 2,500</td>
<td>1,126,926,339</td>
<td>23,665,453,119</td>
<td>225</td>
<td>31</td>
</tr>
</tbody>
</table>
EM Shock Simulations at Scale: Atomistic Estimate

Estimating* Time-to-Solution with USER-REAXC in LAMMPS:

1. Real runs have typical Computational Intensity of 500 to 2000 atoms/core
2. At 600 atoms per KNL core, achieve approximately 1.5 time steps/second
3. A 0.1 fs time step for a 500 ps simulation gives $5 \times 10^6$ time steps
4. On 8,820 nodes of Trinity Phase 2 (using 564,480 KNL cores):

<table>
<thead>
<tr>
<th>Model Name</th>
<th>Sample Size (nm$^3$)</th>
<th>Number of RDX Molecules</th>
<th>Number of Atoms</th>
<th>Atoms/KNL Core</th>
<th>Wall Time (estimated*)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Small</td>
<td>40 x 40 x 2,500</td>
<td>20,452,820</td>
<td>429,509,220</td>
<td>761</td>
<td>7 weeks</td>
</tr>
<tr>
<td>Medium</td>
<td>100 x 100 x 2,500</td>
<td>126,259,367</td>
<td>2,651,446,707</td>
<td>4,697</td>
<td>10 months</td>
</tr>
<tr>
<td>Large</td>
<td>300 x 300 x 2,500</td>
<td>1,126,926,339</td>
<td>23,665,453,119</td>
<td>41,924</td>
<td>7.4 years</td>
</tr>
</tbody>
</table>

*Estimates are ideal scaling extrapolations by Aidan Thompson & Stan Moore (SNL) based on smaller EM simulation runs on Trinity with the USER-REAXC package in LAMMPS.

There has to be a better way!
A Better Faster Way: Use Coarse-Graining (CG)

Why Coarse-Grain Simulation?

- Highly heterogeneous materials
- Dynamic responses over wide range of spatial and temporal scales
- All-atom simulation is too slow

- sacrifice atomistic detail
- gain computational speed
1-site CG Model of RDX

**Force-Matching**

Minimize

\[ \chi^2 = \left< | F_{\text{Atomistic}} - F_{\text{CG}} |^2 \right> \]

CG potential fit by *force matching*

CG and atomistic model

**Pros:**
- Good standard state properties and Hugoniot
- Good mechanical properties vs pressure

**Cons:**
- Does not capture shear band formation
- Melting point is too high at high pressures

CG Method: Dissipative Particle Dynamics (DPD)

More specifically, DPD with Reactions (DPD-RX)

- Constant-E (or H) DPD helps recapture lost degrees-of-freedom from CG-ing
- Thermal behavior can be recovered

Each CG Particle Modeled as a Batch Reactor

RDX Decomposition

RDX → 3HCN + 3/2(NO₂ + NO + H₂O)  \[ \text{endothermic} \]

HCN + NO₂ → NO + ½(N₂ + H₂) + CO \[ \text{exothermic} \]
HCN + NO → CO + N₂ + ½H₂
NO + CO → ½N₂ + CO₂

A simple matter of coding...

Several years to implement previous slides in an ARL customized LAMMPS:

- Constant Energy Dissipative Particle Dynamics (DPD-E) Method
- Serial and Parallel Stochastic Integration Scheme: Shardlow Splitting Algorithm (SSA)
  †Note: The SSA allows ~2 orders of magnitude larger time-step size than Velocity-Verlet for DPD-E.
- Reaction Kinetics Solver for “Batch Reactors” (DPD-RX)

Dr. Larentzos (with Dr. Barnes) presented above at LAMMPS Workshop August 7, 2015:

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

Last two years (~17,000 changed/added lines of code since Jan 2017):

- Merged USER-DPD into mainline LAMMPS
- Made the neighbor list code more modular to support SSA, etc.
- Optimized the code for performance on modern architectures
- Improved scalability and portability via a Kokkos implementation
A few problems on the way...

• Stochastic... means Random
  • Changes in particle force evaluation order, *will* change the end trajectories!
  • Had to develop sophisticated validation scripts and methods
• Simulating a billion particles will overflow 32-bit integers... someplace...
• Creating input files of a billion particles is hard.
• Reading those input files has to scale too...
• Don’t talk to me (yet) about saving/storing full trajectories of a billion particles!
• Many parallel computations can’t be easily described as a one-dimensional loop over independent coordinates or units of work.
  • To expose parallelism within the SSA required a new “coloring” scheme, expressed as a new neighbor “list” in LAMMPS
  • Developed a way to compactly represent a work plan for the parallel evaluation of non-interfering particle pairs in the SSA
• Automatic Vectorization flags for compilers are not magical
• The KNL based supercomputers were in “Early Access/Pioneer” periods
  • Our code caused physical failure of KNL nodes in odd ways... not seen by others
We did some runs...

Tested the code using tiny versions of the shock simulations on:

- ARL KNL testbed system
- TACC KNL testbed system
- Haswell production systems at the various DoD DSRCs

Made MPI geometry selections for three Computational Intensities

- High, ~5000 particles per KNL core
- Moderate, ~2000 particles per KNL core
- Low, ~570 particles per KNL core

Ran the simulations for a Gordon Bell Prize submission on:

Trinity/KNL

Stampede-2

Thunder
**USER-DPD Time-to-solution on Trinity Phase 2**

**Energetic Material Simulation Milestones:**
- Scaled to over 0.5 million cores
- Ran 1.1 billion DPD-RX particles for 0.5 ns of simulated time

*Science results in hours, not years!* 

<table>
<thead>
<tr>
<th>Computational Intensity</th>
<th>Model Name</th>
<th>Trinity KNL Nodes</th>
<th>KNL Cores Used</th>
<th>Particles per Core</th>
<th>Atoms per Core</th>
<th>ReaxFF Estimated Wall Time</th>
<th>USER-DPD Measured Wall Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>High</td>
<td>Small</td>
<td>63</td>
<td>4,032</td>
<td>5,073</td>
<td>106,525</td>
<td>18.8 years</td>
<td>8.93 hours</td>
</tr>
<tr>
<td></td>
<td>Medium</td>
<td>390</td>
<td>24,960</td>
<td>5,058</td>
<td>106,228</td>
<td>18.7 years</td>
<td>9.50 hours</td>
</tr>
<tr>
<td></td>
<td>Large</td>
<td>3,465</td>
<td>221,760</td>
<td>5,082</td>
<td>106,717</td>
<td>18.8 years</td>
<td>11.02 hours</td>
</tr>
<tr>
<td>Moderate</td>
<td>Small</td>
<td>162</td>
<td>10,368</td>
<td>1,973</td>
<td>41,426</td>
<td>7.3 years</td>
<td>3.75 hours</td>
</tr>
<tr>
<td></td>
<td>Medium</td>
<td>988</td>
<td>63,232</td>
<td>1,997</td>
<td>41,932</td>
<td>7.4 years</td>
<td>4.34 hours</td>
</tr>
<tr>
<td></td>
<td>Large</td>
<td>8,820</td>
<td>564,480</td>
<td>1,996</td>
<td>41,924</td>
<td>7.4 years</td>
<td><strong>5.59 hours</strong></td>
</tr>
<tr>
<td>Low</td>
<td>Small</td>
<td>561</td>
<td>35904</td>
<td>570</td>
<td>11,963</td>
<td>2.1 years</td>
<td>1.67 hours</td>
</tr>
<tr>
<td></td>
<td>Medium</td>
<td>3,465</td>
<td>221,760</td>
<td>569</td>
<td>11,956</td>
<td>2.1 years</td>
<td>1.64 hours</td>
</tr>
</tbody>
</table>
USER-DPD Scaling on Trinity/KNL & Stampede 2

Weak and Strong Scaling: Trinity/KNL

- Ideal Strong
- Large Problem
- Medium Problem
- Small Problem
- High Intensity
- Moderate Int.
- Low Intensity
- Stampede-2

Total Wall Time (hours)

KNL Cores (thousands)
USER-DPD Scaling on Trinity/KNL & Stampede 2

Weak and Strong Scaling: Trinity/KNL

- Ideal Strong
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Total Wall Time (hours)

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USER-DPD Scaling on Trinity/KNL & Stampede 2

Weak and Strong Scaling: Trinity/KNL

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KNL Cores (thousands)

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- Large Problem
- Medium Problem
- Small Problem
- High Intensity
- Moderate Int.
- Low Intensity
- Stampede-2

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USER-DPD Scaling on Trinity/KNL & Stampede 2

Weak and Strong Scaling: Trinity/KNL

- Ideal Strong
- Large Problem
- Medium Problem
- Small Problem
- High Intensity
- Moderate Int.
- Low Intensity
- Stampede-2

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A 1.1 Billion Particle Polycrystal Shock Simulation

~225 nm grains

2500x300x300 nm³

• snapshots after 100 ps

RDX Decomposition

particles at grain interface(s)

\[ u_p = 2.25 \text{ km/s} \]

• Particles highlighted if at least 10% of RDX has decomposed

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A 1.1 Billion Particle Polycrystal Shock Simulation

~225 nm grains

2500x300x300 nm³

• snapshots after 200 ps

RDX Decomposition

$u_p = 2.25 \text{ km/s}$

• Particles highlighted if at least 10% of RDX has decomposed
A 1.1 Billion Particle Polycrystal Shock Simulation

~225 nm grains

2500x300x300 nm³

• snapshots after 300 ps

RDX Decomposition

\[ u_p = 2.25 \text{ km/s} \]

• Particles highlighted if at least 10% of RDX has decomposed

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A 1.1 Billion Particle Polycrystal Shock Simulation

~225 nm grains

2500x300x300 nm$^3$

• snapshots after 400 ps

RDX Decomposition

$u_p = 2.25$ km/s

• Particles highlighted if at least 10% of RDX has decomposed

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A 1.1 Billion Particle Polycrystal Shock Simulation

~225 nm grains

2500x300x300 nm³

• snapshots after 500 ps

RDX Decomposition

• Particles highlighted if at least 10% of RDX has decomposed

\[ u_p = 2.25 \text{ km/s} \]
A 1.1 Billion Particle Polycrystal Shock Simulation

2500x300x300 nm$^3$ RDX Polycrystal, ~225 nm grains

RDX Decomposition

$u_p = 2.25$ km/s

• Particles highlighted if at least 10% of RDX has decomposed
Conclusions

Material Science:
• O(billion) particle DPD-RX simulations are now feasible
• Science results in hours, not years!
• Studies of microstructure effects on EM sensitivity are ongoing

Computational Science:
• Scaling Simulations to >500,000 cores takes a village
• Even with help of Kokkos, intra-node parallelism is tough
• Scaling the simulation itself isn’t enough
  • How to generate the input sets at scale?
  • How to save the results without overloading the IO system?
  • How to do the analysis of the now much larger results?
  • How to archive the results?
Future & Collaborative Work

- Hierarchical modeling techniques to reach larger scales
- Studying alternatives/improvements to Kokkos
- DPD method improvements

Questions?  
timothy.mattox@engilitycorp.com

Again, “Thank you!” to all the many people, agencies, and understanding spouses that made this work possible!
Backup Slides
## USER-DPD Time-to-solution: Three Machines Data

<table>
<thead>
<tr>
<th>Machine</th>
<th>Model Name</th>
<th>Nodes</th>
<th>Cores Used</th>
<th>Particles per Core</th>
<th>Atoms per Core</th>
<th>ReaxFF Estimated Wall Time</th>
<th>USER-DPD Measured Wall Time</th>
<th>Estimated Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thunder (HSW)</td>
<td>Small</td>
<td>51</td>
<td>1,836</td>
<td>11,140</td>
<td>233,937</td>
<td>18.5 years</td>
<td>8.64 hrs</td>
<td>1.9 x 10^4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>114</td>
<td>4,104</td>
<td>4,984</td>
<td>104,656</td>
<td>8.3 years</td>
<td>3.87 hrs</td>
<td>1.9 x 10^4</td>
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<tr>
<td></td>
<td></td>
<td>452</td>
<td>16,272</td>
<td>1,257</td>
<td>26,396</td>
<td>2.1 years</td>
<td>1.54 hrs</td>
<td>1.2 x 10^4</td>
</tr>
<tr>
<td></td>
<td>Medium</td>
<td>312</td>
<td>11,232</td>
<td>11,241</td>
<td>236,062</td>
<td>18.7 years</td>
<td>9.71 hrs</td>
<td>1.7 x 10^4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>702</td>
<td>25,272</td>
<td>4,996</td>
<td>104,916</td>
<td>8.3 years</td>
<td>4.87 hrs</td>
<td>1.5 x 10^4</td>
</tr>
<tr>
<td>Stampede2 (KNL)</td>
<td>Small</td>
<td>63</td>
<td>4,032</td>
<td>5,073</td>
<td>106,525</td>
<td>18.8 years</td>
<td>8.81 hrs</td>
<td>1.9 x 10^4</td>
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<td>1.61 hrs</td>
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</tr>
<tr>
<td></td>
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<td>24,960</td>
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<td>4.60 hrs</td>
<td>1.4 x 10^4</td>
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Comparison of Microstructure Types

- ~1/10th of sample is shown after 50 ps
- Particles shown if at least 30% of RDX has decomposed

Particle Internal Temperature

$u_p = 2.25 \text{ km/s}$

$2500 \times 40 \times 40 \text{ nm}^3$
Comparison of Microstructure Types

• ~1/10<sup>th</sup> of sample is shown after 50 ps
• Particles shown if at least 30% of RDX has decomposed

Particle Internal Temperature

$u_p = 2.25$ km/s
$2500 \times 40 \times 40$ nm$^3$

**Random 10-nm voids in a single crystal**
- 37,866 particles
- 27,445 particles
- 39,410 particles

**Random 5-nm voids in a single crystal**
- 2,260 particles
- 1,556 particles
- 1650, 1528 particles

**Polycrystals**
- 1,119 particles

**Temp. distributions**
USER-DPD Scaling on Thunder

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