CCC7-119 Reactive Molecular Dynamics Simulations of Hot Spot Growth in Shocked Energetic Materials

Sandia National Laboratories ASC™

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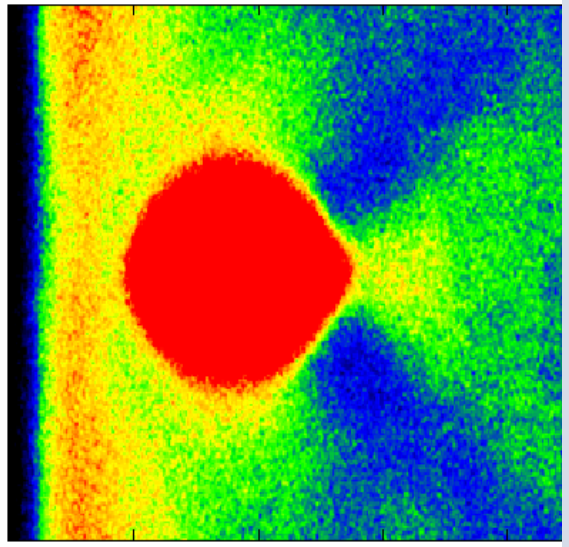
- The purpose of this work is to understand how defects control initiation in energetic materials used in stockpile components.
- Sequoia gives us the core-count to run very large-scale simulations of up to 10 million atoms.
- Using an OpenMP threaded implementation of the ReaxFF package in LAMMPS, we have been able to get good parallel efficiency running on 16k nodes of Sequoia, with 1 hardware thread per core.

Principal Investigator: Aidan Thompson
Platform and Campaign ID: Sequoia CCC7-119
Usage: *1.6 days*

Hotspot Formation in Energetic Materials



Temperature map from MD simulation showing hotspot formation and growth around a collapsed cylindrical void in PETN under shock loading. After 0.450 ns, secondary heating zone is radiating outward from site of initial void collapse. Simulation size is roughly 0.2 microns and 10 million atoms.

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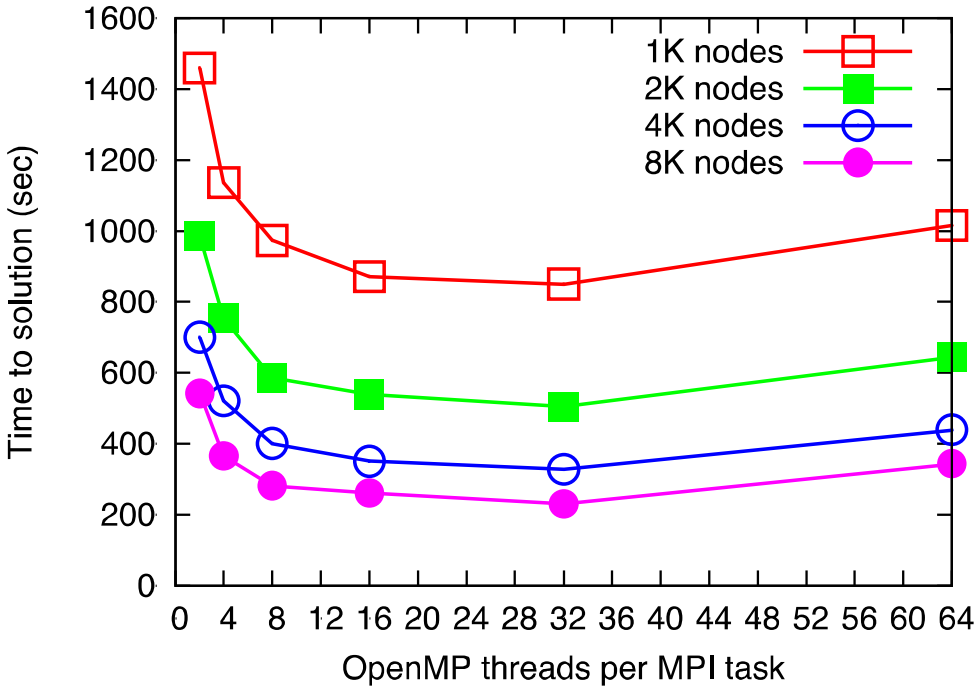
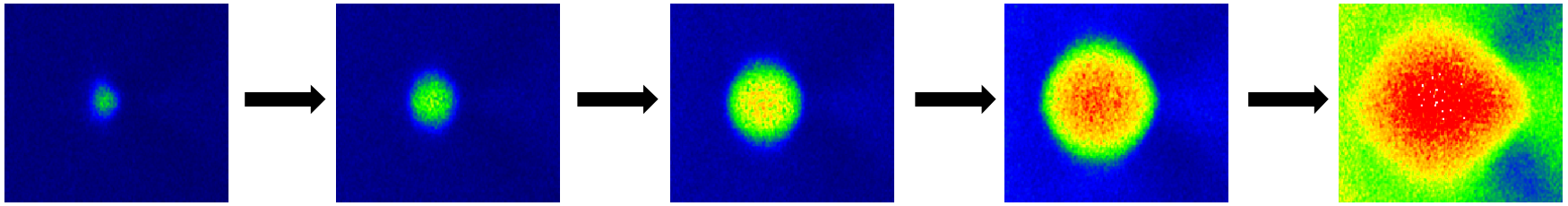
Thread-scaling on BGQ Processors



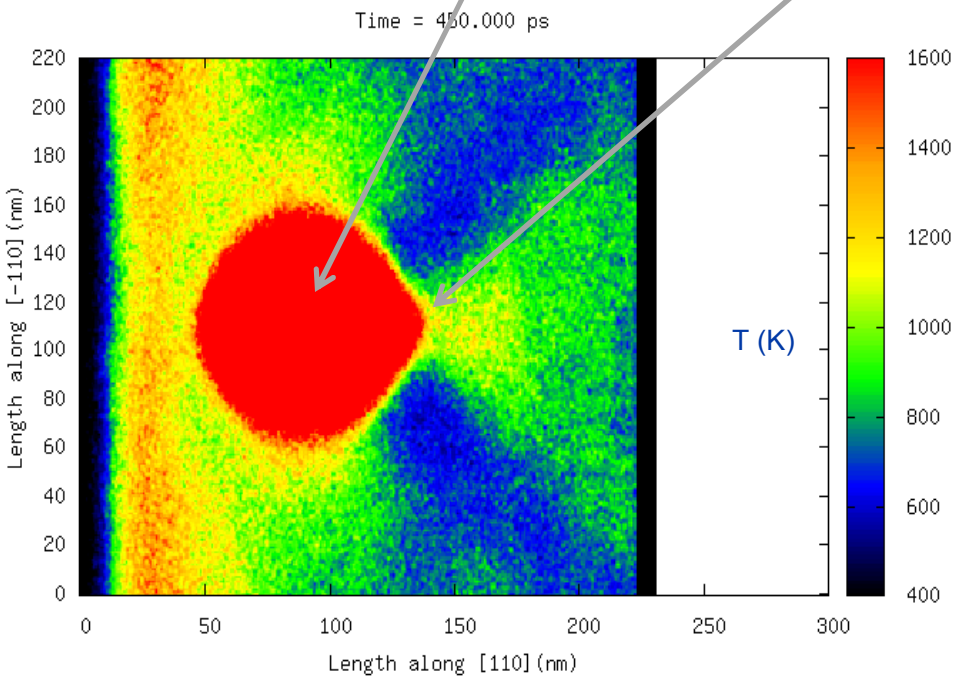
Strong scaling benchmark for the optimized OpenMP version of the ReaxFF package in LAMMPS on 1 to 8 racks of IBM BGQ nodes. All tests were performed with 64 hardware threads per node; as the number of OpenMP per MPI task was increased from 1 to 64, the number of MPI tasks was accordingly decreased.

Evolution of Hot Spot Morphology



100 ps 200 ps 300 ps 400 ps 500 ps

- Asymmetry developed after 400 ps.
- Due to interaction between primary hot spot and secondary hot zone.



Paragraph

Quantifying margins of operation for detonators requires a detailed scientific understanding of how detonation is initiated in energetic materials. The response to shock impact of high explosive molecular crystals such as pentaerythritol tetranitrate (PETN) depends strongly on the material microstructure. A defect-free single crystal requires a higher initiation pressure than a polycrystalline powder of the same substance.

While the basic physics of how voids and other defects localize energy leading to initiation is understood, much remains to be learned. For example, what size of void has the greatest effect? Large-scale reactive molecular dynamics simulation provides a unique tool for studying hot spot formation and growth, without making strong assumptions about the material properties. Instead, the observed behavior emerges from the collective interaction of millions of atoms, as they exchange momentum and energy, compress to high density, and participate in exothermic chemical reactions. Using the power of the LAMMPS molecular dynamics code and a significant subset of the entire the Sequoia supercomputer, we have been able to push the time and length scales of these simulations out farther than ever before, observing a variety of phenomena that help provide a better understanding of the behavior of explosives. Advancing this understanding of energy transfer mechanisms may enable the use of more insensitive materials in detonators, which has great implications for safety.