

## End of Year Summary

**PINAME : Aidan Thompson and Tzu-Ray Shan**

**YEAR : 2014**

**PROGRAM : ALCC / 80 Million Core-Hours**

### Project Usage

#### Report on Project Milestones

- Milestones
  - Simulate shock localization at nano-scale voids and entrained solvent in HNS
    - Status: Complete
  - Simulate the effect of relief wave passing through shocked HNS
    - Status: Complete
  - Simulate shock localization at micron-scale voids and entrained solvent in HNS
    - Status: Complete
- Additional major accomplishments
  - Ported Kokkos-enabled version of the ReaxFF potential as implemented in LAMMPS to Mira (thanks to Nichols Romero for the assistance).

#### Project Productivity

- List Papers from work at ALCF and include a sentence about how this is related to the project.
  - H. M. Aktulga, P. Coffman, W. Jiang, C. Knight, T.-R. Shan, "Implementation and Performance Optimization of the LAMMPS/ReaxC Package for Multi-core Architectures", to be submitted to J. Comp. Chem,
    - "An award of computer time was provided by ALCF's program. This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357."
  - T.-R. Shan, A. P. Thompson, "Micron-scale Reactive Atomistic Simulations of Void Collapse and Hotspot Growth in Pentaerythritol Tetranitrate", Proc. 15th International Detonation Symposium, Accepted for publication (2014)
    - "This research used resources of the Argonne Leadership Computing Facility at Argonne National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357."

- List Presentations work at ALCF
  - T.-R Shan, “Enabling Performance Portability for Large-scale Simulations on Next-Generation Computing Architectures”, 2nd Workshop on Enabling Methods for Materials Innovation from Quantum to Mesoscale, Gainesville, Florida, June 2-4, 2015
  - T.-R. Shan, R. R. Wixom, C. D. Yarrington, A. P. Thompson, “Atomistic Simulation of Initiation in Hexanitrostilbene”, 19th Biennial Intl. Conference of the American Physical Society Topical Group on Shock Compression of Condensed Matter, Tampa, Florida, July 14-19, 2015
  - T.-R. Shan, R. R. Wixom, A. P. Thompson, “Micron-scale Reactive Atomistic Simulations of Void Collapse and Hotspot Growth in PETN”, 2015 American Physical Society March Meeting, San Antonio, Texas, March 2-5, 2015.
  - T.-R. Shan, A. P. Thompson, “Micron-scale Reactive Atomistic Simulations of Void Collapse and Hotspot Growth in PETN”, 15th International Detonation Symposium, San Francisco, California, July 13-18, 2014
- List any other awards, honors, media coverage, etc
  - ALCF annual brochure *2015 Science Highlights*

### Code Description

In addition to the hybrid OpenMP/MPI version of ReaxFF potential in LAMMPS that was used in this work (see the first publication listed above by H. Aktulga et al.), we have also ported the Kokkos version of ReaxFF (work in progress) in LAMMPS to ALCF’s Mira. Sandia’s Kokkos C++ library was developed to provide codes with a user accessible manycore performance portable programming model. Kokkos library allows users to run on various many computing architectures including Intel MIC, NVIDIA GPU, and multithread CPUs such as IBM BG/Q. Under the DOE ASC program, we are porting many features in the LAMMPS software to Kokkos, including the Reactive Force Field (ReaxFF). Thanks to Nichols Romero for his assistance in compiling the code.

### Next Steps

- We have been allocated 10 million core-hours under ALCF’s Director’s Discretionary program to continue the work of porting and testing the Kokkos version of ReaxFF.

### Other Comments

Please answer as applicable: Has the support received from the following been beneficial to your project team? Cite examples if possible

- User Assistance Center
- Catalysts or Performance Engineering
- Visualization and Analysis Team
- Operations

Yes, we have received help from our Catalyst partner Nichols Romero in porting/compiling LAMMPS with Kokkos/ReaxFF.

Any additional feedback from your project team for the ALCF?

Please include any other comments or requests you have about the facility, allocation program, etc



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