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A Brief Description of the Kokkos implementation of the SNAP potential in ExaMiniMD

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Within the EXAALT project, the SNAP [1] approach is being used to develop high accuracy potentials for use in large-scale long-time molecular dynamics simulations of materials behavior. In particular, we have developed a new SNAP potential that is suitable for describing the interplay between helium atoms and vacancies in high-temperature tungsten[2]. This model is now being used to study plasma-surface interactions in nuclear fusion reactors for energy production. The high-accuracy of SNAP potentials comes at the price of increased computational cost per atom and increased computational complexity. The increased cost is mitigated by improvements in strong scaling that can be achieved using advanced algorithms [3].

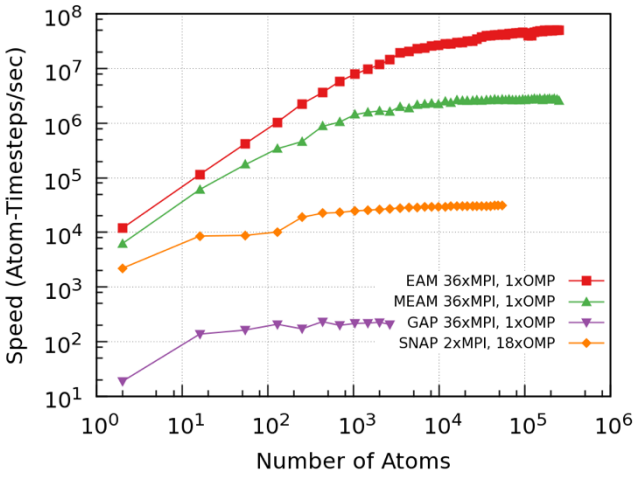

Figure 1 Computational speed of MD using the SNAP potential for tungsten as a function of problem size. We compare SNAP to two simpler tungsten potentials (EAM, MEAM) and another high-accuracy data-driven potential (GAP). The peak speed for SNAP is about 100x slower than MEAM, but 100x faster than GAP. All timings were obtained from LAMMPS running on a single node with 36 Intel Broadwell 2.1 GHz CPUs [2].

The current production implementation of SNAP in LAMMPS [4] uses OpenMP multithreading for on-node parallel calculation of atom forces, while MPI-based parallel spatial decomposition and halo exchange enables MD simulations of typical size (10^5-10^6) to be disbributed across large numbers of compute nodes. This works well for conventional multicore processors (see Fig. 1), but there is no ability to run on GPUs. One of the goals of the EXAALT project is to enable LAMMPS simulations (running under ParSplice) using SNAP interatomic potentials to run efficiently on a range of computer platforms, including GPU-based architectures. The ExaMiniMD proxy application being developed within the CoPA ECP co-design project provides an ideal framework for prototyping different SNAP algorithms and testing them on a range of hardware. ExaMiniMD uses the Kokkos library for all low-level data structures and computational kernels, which enables a single code base to be compiled for different node architectures without sacrificing performance portability.

To achieve this, the LAMMPS OpenMP SNAP code base was first integrated into ExaMiniMD and converted to use the Kokkos library. The validity of the new code was verified by comparing the ExaMiniMD output (forces and energies) against LAMMPS reference outputs for the SNAP tantalum potential. This was followed by performance benchmarking against LAMMPS. Finally, some basic optimization of the algorithms and code was performed.

Compared to the LAMMPS implementation, the new ExaMiniMD implementation exposes greater parallelism which is necessary for reasonable performance on GPU nodes. In LAMMPS, the force contributions due to the full set of bispectrum components associated with an interaction pair are all computed by the same thread, whereas in ExaMiniMD, the bispectrum components are distributed over a team of threads.

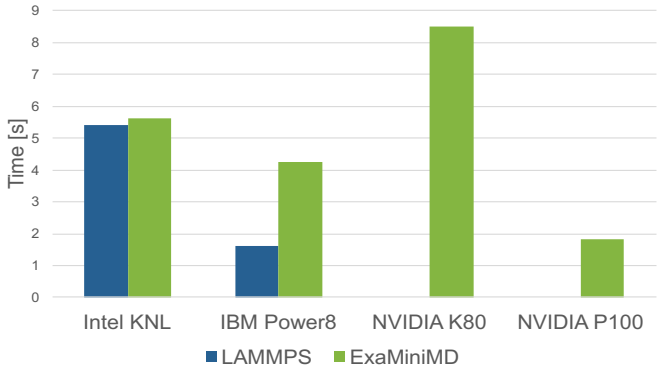

Figure 2 LAMMPS and ExaMiniMD execution times for SNAP benchmark running on 4 different node architectures.

The results are summarized in Figure 2, which compares the LAMMPS and ExaMiniMD execution times for a standard SNAP benchmark running on an Intel KNL node and an IBM power8 node. Also shown are ExaMiniMD timings on NVIDIA K80 and P100 GPUs, where LAMMPS can not run. The timings for the NVIDIA K80 indicate a substantial speed-up on the ORNL Titan machine will be realized by migrating from the current LAMMPS implementation running on the Titan CPUs to the new code running on the Titan GPUs.

The next step is to explore further optimizations, such as testing out different memory access strategies. Once this has been completed, the ExaMiniMD SNAP implementation will be ported back to LAMMPS for use in production simulations.

References

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[3] C.R. Trott, S.D. Hammond, A. P. Thompson, "SNAP: Strong scaling high fidelity molecular dynamics simulations on leadership-class computing platforms," *Supercomputing, (Lecture Notes in Computer Science)*, **8488** 19 (2014).

[4] *http://lammps.sandia.gov*

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