Atomistic Materials Modeling on Petascale Platforms Using SNAP[1] AIDAN THOMPSON, LAURA SWILER, CHRISTIAN TROTT, STEPHEN FOILES, Sandia National Laboratories, GARRITT TUCKER, Drexel University — The growing availability of capacity computing for atomistic materials modeling has encouraged the use of high-accuracy computationally intensive interatomic potentials, such as SNAP. These potentials also happen to scale well on petascale computing platforms. SNAP has a very general form and uses machine-learning techniques to reproduce the energies, forces, and stress tensors of a large set of small configurations of atoms, which are obtained using high-accuracy quantum electronic structure (QM) calculations. The local environment of each atom is characterized by a set of bispectrum components of the local neighbor density projected on to a basis of hyperspherical harmonics in four dimensions. The computational cost per atom is much greater than that of simpler potentials such as Lennard-Jones or EAM, while the communication cost remains modest. We discuss a variety of strategies for implementing SNAP in the LAMMPS molecular dynamics package. We present scaling results obtained running SNAP on three different classes of machine: a conventional Intel Xeon CPU cluster; the Titan GPU-based system; and the combined Sequoia and Vulcan BlueGene/Q.

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