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Beyond the Harmonic Approximation: Lattice Dynamics and Thermal Conductivity on Massively Parallel Heterogenous Systems WESTON NIELSON, Univ of California - Los Angeles, FEI ZHOU, Lawrence Livermore National Laboratory, VIDVUDS OZOLINS, Univ of California - Los Angeles — The theory of lattice dynamics provides the mathematical foundation necessary to solve, exactly, the potential energy and interatomic forces of a system on a lattice, which can easily be written as functions of atomic displacements and so-called force constants. We have used this formalism to develop a highly-parallel algorithm that is capable of calculating the potential energy and interatomic forces across large computational clusters and on graphics processing units (GPUs). The necessary force constants are calculated well beyond the simple harmonic approximation (up to n-order), via a compressive sensing-based algorithm, which are then used in molecular dynamics simulations to study lattice thermal conductivity in a variety of crystal systems.

Weston Nielson
Univ of California - Los Angeles

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