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**Machine Learning of Interatomic Potentials for Shock Compression Phenomena**[1] BENJAMIN NEBGEN, KIPTON BARROS, LEONID BURAKOVSKY, SARYU FENSIN, TIMOTHY GERMANN, NICHOLAS LUBBERS, JUSTIN SMITH, Los Alamos National Laboratory — As classical molecular dynamics simulations have become a widely used tool for investigating shock loading and release, the need for transferable interatomic potentials that are valid across a wide range of temperatures and pressures has become increasingly urgent. Machine learning is emerging as a powerful tool to emulate electronic structure calculations. Deep neural networks can now predict atomic interactions with accuracies exceeding density functional theory, at a tiny fraction of the computational cost. We will describe recent methods for building interatomic potentials relevant to chemistry, materials science, and biophysics applications. A key concept is active learning, which facilitates optimal training dataset generation using uncertainty quantification built into the neural network. Active learning fills in gaps of the machine learning model without saturating the dataset with similar structures, leading to a surprising level of transferability. Using the recently deployed Sierra supercomputer, we have applied these concepts to develop neural network-based interatomic potentials for aluminum and tin. We will describe these results, and their initial implementation in parallel large-scale non-equilibrium molecular dynamics simulations of shock compression and release.

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