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Abstract for an Invited Paper
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Petascale Frontiers of Atomistic Materials Simulations[1]

TIMOTHY C. GERMANN, Los Alamos National Laboratory

Large-scale classical molecular dynamics simulations with 10^6 to 10^{12} atoms are providing unprecedented insight into material deformation processes under high strain-rate mechanical loading, and are increasingly being utilized to guide and interpret ultrafast *in situ* diffraction and microscopy experiments. I will describe our recent algorithm redesign motivated by the evolution towards hybrid multicore architechtures employing graphical processing unit (GPU) or Cell co-processors, specifically the heterogeneous petaflop Roadrunner platform at Los Alamos National Laboratory. I will then present the resulting performance achieved, as well as our approach to the challenges of terabyte data analysis and visualization on Roadrunner and Blue Gene systems. Finally, results from our initial scientific applications on Roadrunner to understand the response of copper single- and poly-crystals to shock compression and release, including material ejection and spall failure, will be described.

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