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Multibillion-atom Molecular Dynamics Simulations of Plasticity, Spall, and Ejecta[1]

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Modern supercomputing platforms, such as the IBM BlueGene/L at Lawrence Livermore National Laboratory and the Roadrunner hybrid supercomputer being built at Los Alamos National Laboratory, are enabling large-scale classical molecular dynamics simulations of phenomena that were unthinkable just a few years ago. Using either the embedded atom method (EAM) description of simple (close-packed) metals, or modified EAM (MEAM) models of more complex solids and alloys with mixed covalent and metallic character, simulations containing billions to trillions of atoms are now practical, reaching volumes in excess of a cubic micron. In order to obtain any new physical insights, however, it is equally important that the analysis of such systems be tractable. This is in fact possible, in large part due to our highly efficient parallel visualization code, which enables the rendering of atomic spheres, Eulerian cells, and other geometric objects in a matter of minutes, even for tens of thousands of processors and billions of atoms. After briefly describing the BlueGene/L and Roadrunner architectures, and the code optimization strategies that were employed, results obtained thus far on BlueGene/L will be reviewed, including: (1) shock compression and release of a defective EAM Cu sample, illustrating the plastic deformation accompanying void collapse as well as the subsequent void growth and linkup upon release; (2) solid-solid martensitic phase transition in shock-compressed MEAM Ga; and (3) Rayleigh-Taylor fluid instability modeled using large-scale direct simulation Monte Carlo (DSMC) simulations. I will also describe our initial experiences utilizing Cell Broadband Engine processors (developed for the Sony PlayStation 3), and planned simulation studies of ejecta and spall failure in polycrystalline metals that will be carried out when the full Petaflop Opteron/Cell Roadrunner supercomputer is assembled in mid-2008.

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