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Multibillion-atom Molecular Dynamics Simulations on BlueGene/L[1] PETER S. LOMDAHL, TIMOTHY C. GERMANN, KAI KADAU, Los Alamos National Laboratory — The IBM BlueGene/L supercomputer at Lawrence Livermore National Laboratory, with 65,536 CPU processors connected by multiple high-performance networks, enables a completely new class of physical problems to be investigated. Using either pairwise interactions such as the Lennard-Jones potential, or the embedded atom method (EAM) potential for simple metals, system sizes up to 160 billion atoms (or a cube of copper a micron on each side) can be modeled. 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. We will describe the performance scaling and initial results obtained for 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.

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