Multibillion-Atom Molecular Dynamics Simulations of Ejecta Production and Transport using Roadrunner

Co-PIs: Timothy C. Germann, tcg@lanl.gov, and Guy Dimonte, dimonte@lanl.gov

Abstract
The SPaSM (Scalable Parallel Short-range Molecular dynamics) code will be used to investigate the physics of ejecta formation and transport from shocked copper surfaces. Recent (November 2007) simulations with a quasi-2D geometry on the full (212,992-CPU) BlueGene/L system at LLNL have provided insight into the production of ejecta from a roughened surface during the first nanosecond after impact; the proposed Roadrunner simulations are aimed at understanding the subsequent necking instabilities leading to jet breakup and 3D droplet formation at later times, including the resulting particle size and velocity distributions, and correlations between the two. In addition to the increased (by ~3x) performance of SPaSM that we expect on the full Roadrunner system over BlueGene/L, the radical redesign of the message-passing algorithm for the Roadrunner implementation of SPaSM enables us to load-balance problems with significant density variations, which will be especially important for the proposed problem of material jetting into vacuum or a low-density gas. We request 4.5 million hours (approximately two weeks of wall-clock time) of the full Roadrunner system for these simulations.