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Molecular Dynamics Simulations of Hot Spots and Detonation on the Roadrunner Supercomputer SUSAN MNISZEWSKI, MARC CAWKWELL, TIMOTHY GERMANN, Los Alamos National Laboratory — The temporal and spatial scales intrinsic to a *real* detonating explosive are extremely difficult to capture using molecular dynamics (MD) simulations. Nevertheless, MD remains very attractive since it allows for the resolution of dynamic phenomena at the atomic scale. We have studied the effects of spherical voids on the build up to detonation in three dimensions (3D) in a *model* explosive using the reactive empirical bond order (REBO) potential for the A-B system. This force field is attractive because it has been shown to support a detonation while being simple, analytic, and short-ranged. The transition from 2D to 3D simulations was facilitated by our port of the REBO force field in the parallel MD code SPaSM to LANL's petaflop Roadrunner supercomputer based on previous work by Swaminarayan and Germann [T. C. Germann et al. Concurrency Computat.: Pract. Exper. **21**, 2143 (2009)]. We will provide a detailed discussion of the challenges associated with computing interatomic forces on a hybrid Opteron/Cell BE computational architecture. We will compare and contrast our results in 3D from Roadrunner with earlier 2D simulations of hot-spot assisted detonations by Heim, Herring, and co-workers [S. D. Herring et al. Phys. Rev. B, **82**, 214108 (2010)].

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