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Multi-scale dynamical simulations of steady shock waves using moleculardynamics and analytical equations of state EVAN REED[1], LAURENCE FRIED, WILLIAM HENSHAW, M. RIAD MANAA, CHRISTOPHER MUNDY, CRAIG TARVER, Lawrence Livermore National Laboratory, JOHN JOANNOPOULOS, Massachusetts Institute of Technology — We have deveoped a multi-scale simulation method and applied it to the study of steadily propagating shock waves in materials. The method combines molecular dynamics and the Euler equations for compressible flow to provide up to 8 demonstrated orders of magnitude of computational savings over non-equilibrium molecular dynamics simulations of steady shock waves. Utilizing a recently developed coarse-grained approach with analytical equations of state, we explicitly show that spatial profiles of shock waves yielded by the method are identical to those of fully hydrodynamic simulations of steady shock waves in chemically reactive systems.

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