Absorbing boundary conditions for molecular dynamics and multiscale modeling S. NAMILAE, D.M. NICHOLSON, P.K.V.V. NUKALA, Computer Science and Mathematics Division, Oak Ridge National Laboratory, C.Y. GAO, Department of Chemical Engineering, University of Tennessee, Y.N. OSETSKY, Computer Science and Mathematics Division, Oak Ridge National Laboratory, D.J. KEFFER, Department of Chemical Engineering, University of Tennessee — We present an application of differential equation based local absorbing boundary conditions to molecular dynamics. The absorbing boundary conditions result in the absorbtion of the majority of waves incident perpendicular to the bounding surface. We demonstrate that boundary conditions developed for the wave equation can be applied to molecular dynamics. Comparisons with damping material boundary conditions are discussed. The concept is extended to the formulation of an atomistic-continuum multiscale scheme with handshaking between the regions based on absorbing boundary conditions. The multiscale model is effective in minimizing spurious reflections at the interface.

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