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Reflection-free atomistic-continuum coupling for solid mechanics employing spacetime discontinuous finite element method B. KRACZEK, D.D. JOHNSON, R.B. HABER, Depts. of Physics, Materials Science and Theoretical and Applied Mechanics, U. of Illinois, Urbana, IL 61801 — We present a means for coupling dynamic atomistic and continuum simulations via a spacetime discontinuous Galerkin (SDG) finite element method. Our scheme allows the SDG method to couple a general MD simulation using Verlet time-stepping through the flux conditions on the element boundaries at the interface. These flux conditions ensure weak balance of momentum and energy to achieve reflection-free transfer of disturbance across the interface. Our work is supported by the National Science Foundation (ITR grant DMR-0121695) on Process Simulation and Design and, in part, by the Materials Computation Center (FRG grant DMR-99-76550)

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