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Multiscale Modeling using Molecular Dynamics and Dual Domain Material Point Method[1] TILAK DHAKAL, DUAN ZHANG, Los Alamos National Laboratory — For problems with very large material deformation rate, the time scale of material deformation can be shorter than the time that the material takes to reach a thermodynamic equilibrium. In these situations constitutive relation for the material becomes difficult to obtain. Furthermore, for these non-equilibrium problems, the history dependency of the material becomes important. A numerical method capable of tracking material deformation history is needed in a numerical simulation effort. In this work we use the dual domain material point (DDMP) method, which uses Lagrangian material points to track the history of the material where as Eulerian grids are used to calculate the gradients in continuum level. Molecular dynamics (MD) calculations are performed in the material points to calculate the closure quantities such as stress bypassing the need for a constitutive relation. Since the material points do not need to directly communicate among each other, the MD calculations can be done in parallel. In this work, GPUs are used to accelerate MD calculations. Examples of shock wave propagation in monoatomic gas and in Cerium metal are presented.

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Duan Zhang
Los Alamos National Laboratory

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