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Accelerating Molecular Dynamics Simulations to Investigate Shock Response at the Mesoscales. AVINASH DONGARE, GARVIT AGARWAL, University of Connecticut, RAMAKRISHNA VALISETTY, RAJU NAMBURU, US Army Research Laboratory, ARUNACHALAM RAJENDRAN, University of Mississippi — The capability of large-scale molecular dynamics (MD) simulations to model dynamic response of materials is limited to system sizes at the nanoscales and the nanosecond timescales. A new method called quasi-coarse-grained dynamics (QCGD) is developed to expand the capabilities of MD simulations to the mesoscales. The QCGD method is based on solving the equations of motion for a chosen set of representative atoms from an atomistic microstructure and retaining the energetics of these atoms as would be predicted in MD simulations. The QCGD method allows the modeling of larger size systems and larger time-steps for simulations and thus is able to extend the capabilities of MD simulations to model materials behavior at mesoscales. The success of the QCGD method is demonstrated by reproducing the shock propagation and failure behavior of single crystal and nanocrystalline Al microstructures as predicted using MD simulations and also modeling the shock response and failure behavior of Al microstructures at the micron length scales. The scaling relationships, the hugoniot behavior, and the predicted spall strengths using the MD and the QCGD simulations will be presented. This work is sponsored by the US Army Research Office under Contract# W911NF-14-1-0257.

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