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Enabling strain hardening modeling via efficient time-integrators in dislocation dynamics simulations

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ABSTRACT

Dislocation dynamics (DD) provides a systematic framework for the simulation of metal plasticity and strain hardening. DD models follow the motion of a network of dislocation lines discretized into segments and connected by a set of nodes, which are the degrees of freedom of the system. In order for DD simulations to provide insight into the strain hardening process, they must be able to reach plastic strains on the order of experimental values (>10%). Despite the development of massively parallel algorithms and codes, this level of plastic strain has been out of reach thus far. A major cause of this computational gap is inefficient time integration. In order to remove this limitation, we have developed advanced time integration algorithms for 3D DD simulations. We show that DD simulations contain unstable modes, which force explicit time-integrators to take very small time stepswhile implicit time-integrators offer much better performance. Unfortunately, there also exist unstable and highly nonlinear modes that require a very small time step even when an implicit integrator is used. A significant speed-up is then achieved by the subcycling algorithm, in which nodes involved in the unstable and nonlinear modes are time integrated with small time steps while the remaining nodes are integrated with larger time steps. The performance of these advanced algorithms in large-scale DD simulations is evaluated.