Coupled 3D dislocation dynamics at nano- and micro-scales

Dislocation dynamics are important to understand material plasticity effects, e.g. size dependent strain hardening. Dislocations are nucleated at nano-scale, and interact with other defects including grain boundaries and other dislocations at micro-scale. 2D Coupled Atomistic Dislocation Dynamics (CADD) [1] is the only computational tool supporting such multiscale-physics as a concurrent coupling. In 2D CADD, only straight dislocations can be modeled, and these dislocations can only exist in either MD or DD domains. However, in 3D, curved dislocations (dislocation loops) are observed at any length scales. In this presentation, we propose a new method coupling MD and DD simulations in 3D (CADD3D) to solve such limitations of CADD. We will show its required building constituents (core templates [3] and mobility law). As shown in Figure 1, in CADD3D, an arbitrary dislocation structure can be modeled in MD and DD domains. While this dislocation consists of two different representations (hybrid dislocation), it can travel as one single dislocation thanks to proper communications between respective boundary conditions. After showing the methodology and building blocks of CADD3D, several applications including the coupled dislocation loop (Figure 1) will be presented.

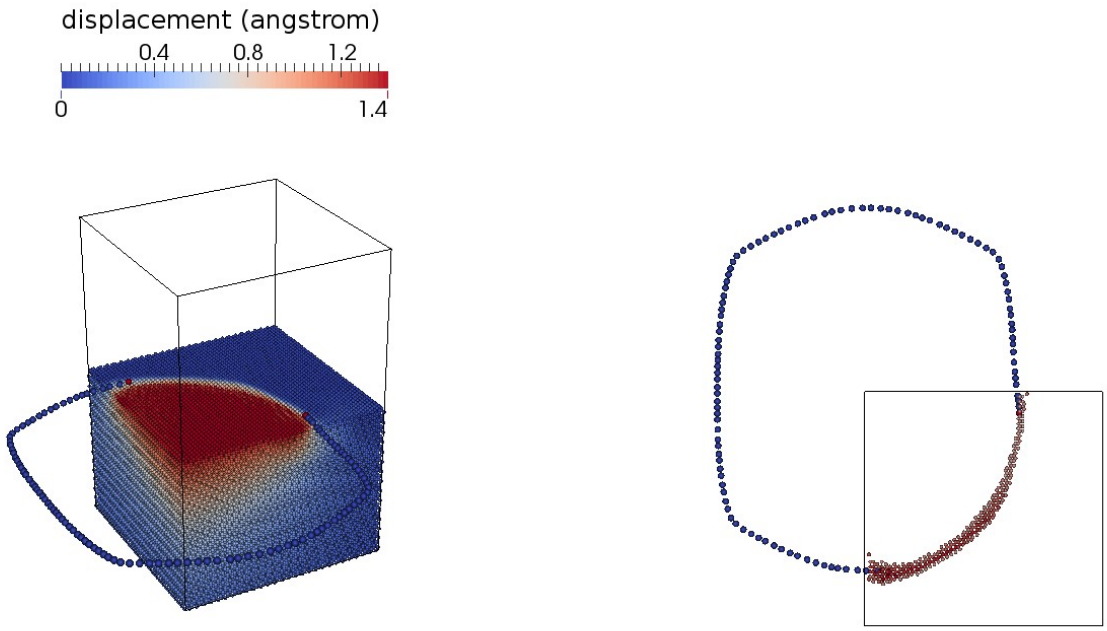

Figure 1: A snapshot of coupled dislocation loop dynamics implemented in CADD3D. The left figure shows DD dislocation and the atoms on the slip plane colored by the component of the displacement in the Burgers vector direction. In the right figure, this is a top view of the atoms having high centro-symmetry values and the DD dislocation.

[1] Shilkrot et.al. Journal of the Mechanics and Physics of Solids, 52(4):755-787, 2004
[2] Shiari et.al. Journal of Engineering Materials and Technology-Transactions of the ASME, 127(4):358-358, 2005
[3] Cho et. al. Advanced Modeling and Simulation in Engineering Sciences, 2(1):1-17, 2015