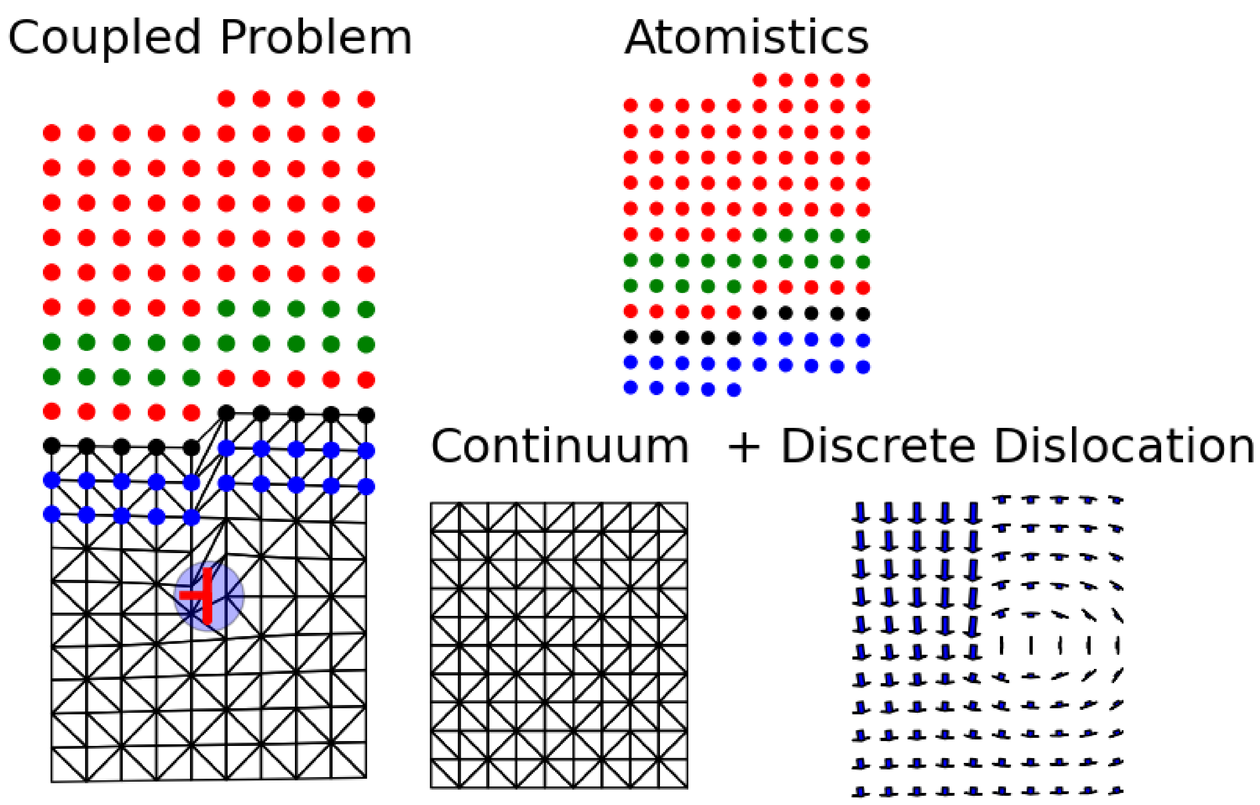
Coupling Atomistics and Discrete Dislocations in 3D: A Start

Till Junge, Jean-François Molinari, Guillaume Anciaux, William A. Curtin

Motivation

Coupled atomistics and discrete dislocations (CADD) is a concurrent multiscale method for modeling of plasticity. The computational domain is split into atomistic and continuum regions and dislocations are seamlessly converted between an atomistic and discrete description at the interface. CADD allows the study of systems far too large for full atomistic treatment.

Problem: Only 2D implementations of CADD exist to date.



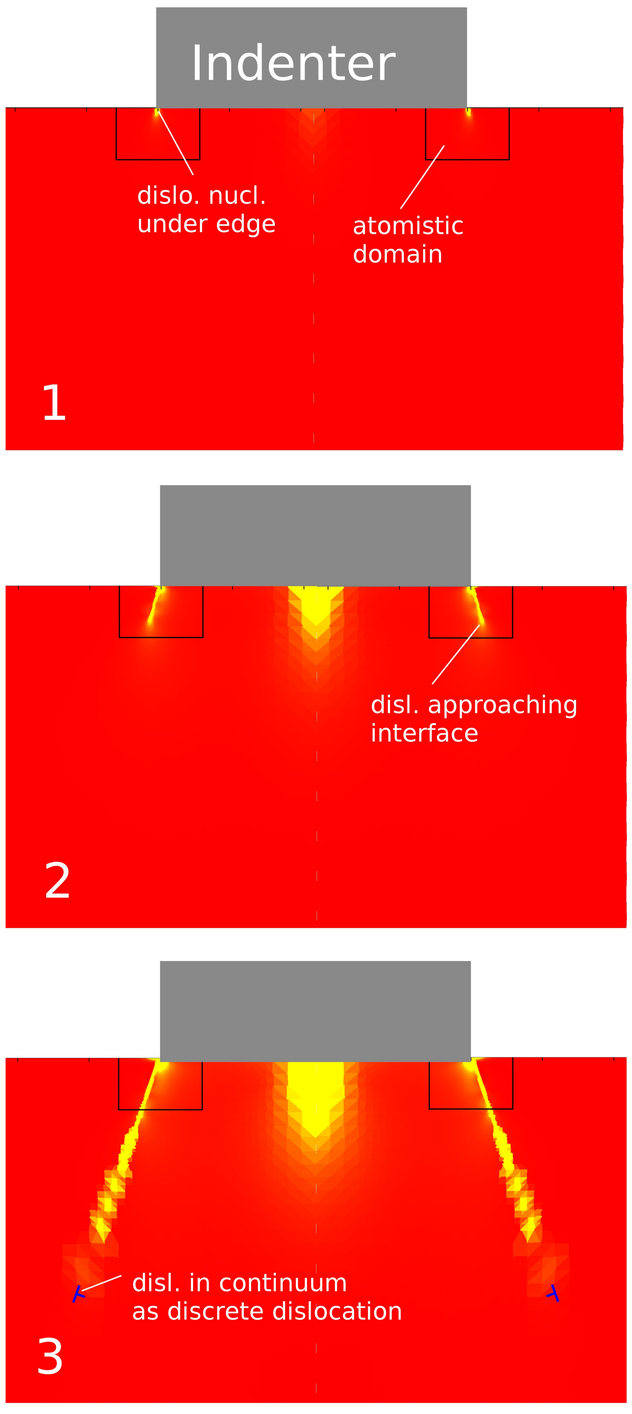
← Method

- The atomistic domain is modeled by **molecular dynamics** (MD)
- The continuum solution is the superposition of the **finite elements** (FEM) solution and the **discrete dislocations** (DD) dynamics solution

Interface conditions:

- FEM displacement boundary conditions given by interface atom postitions (black)
- Ghost atoms (blue) on FEM nodes serve as boundary atoms for MD
- Displacement discontinuities due to dislocations are handled by DD

Microindentation in 2D



From ← 2D to 3D → the mixed dislocation

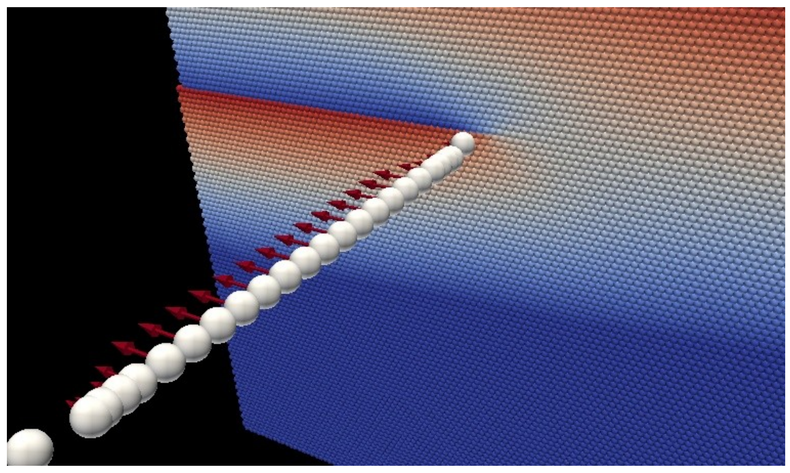
In 2D, dislocations are **point entities**, a single dislocation is either in the atomistic or the continuum domain.

Dislocation cores do not linger on the interface, their nonlinearity can be neglected.

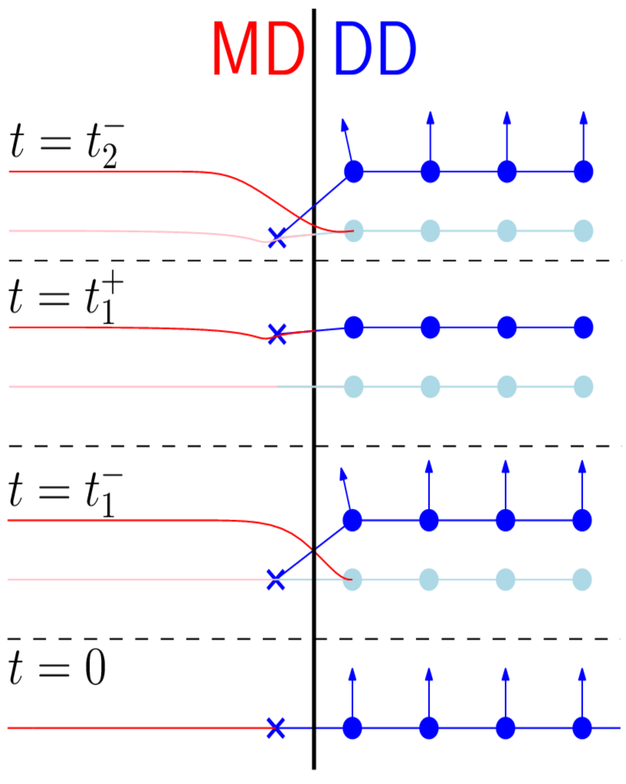
In 3D, dislocations form **networks**, and dislocation segments can intersect the interface resulting in hybrid dislocations.

The cores of hybrid dislocations intersect the interface, the nonlinearity cannot be neglected.

Traveling hybrid edge dislocation



Coupling sequence for hybrid disl.



To-do list for CADD 3D

- ~~Hybrid edge dislocation~~ done
- Hybrid arbitrary character angle dislocation
- Automatic dislocation network detection

References:

- R. E. Miller, L. E. Shilkrot, and W. A. Curtin. *Coupled Atomistic and Discrete Dislocation Plasticity*. Phys. Rev. Lett., 89(2):025501, 2002
- L.E. Shilkrot, R. E. Miller, W. A. Curtin, *Multiscale plasticity modeling: coupled atomistics and discrete dislocation mechanics,* J. Mech. Phys. Solids, 52 (2004), pp. 755–787
- J. P. Hirth, J. Lothe, *Theory of dislocations*, 2nd edition, Krieger Publishing, 1992
- V. Bulatov, W. Cai, *Computer Simulations of Dislocations*, Oxford University Press, 2006

till.junge@epfl.ch
Computational Solid Mechanics Laboratory
Swiss Federal Institute of Technology Lausanne