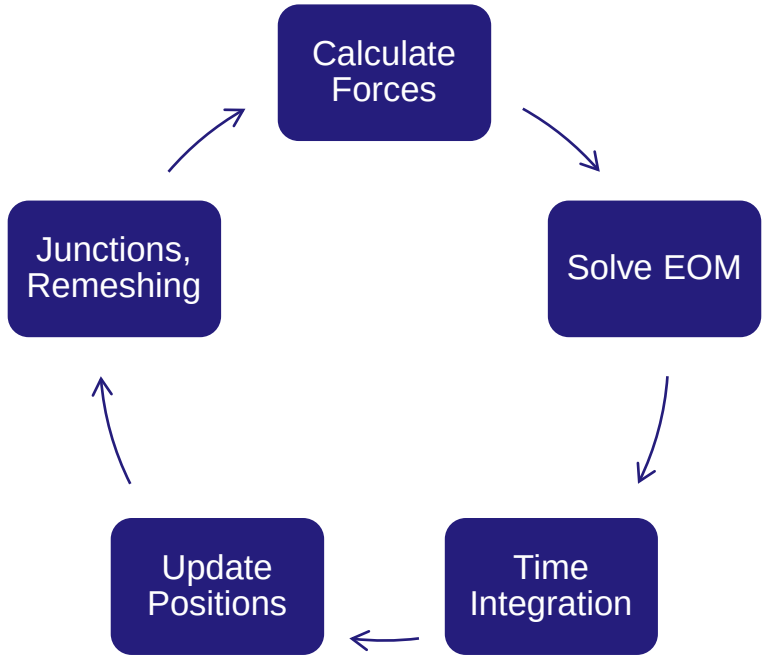
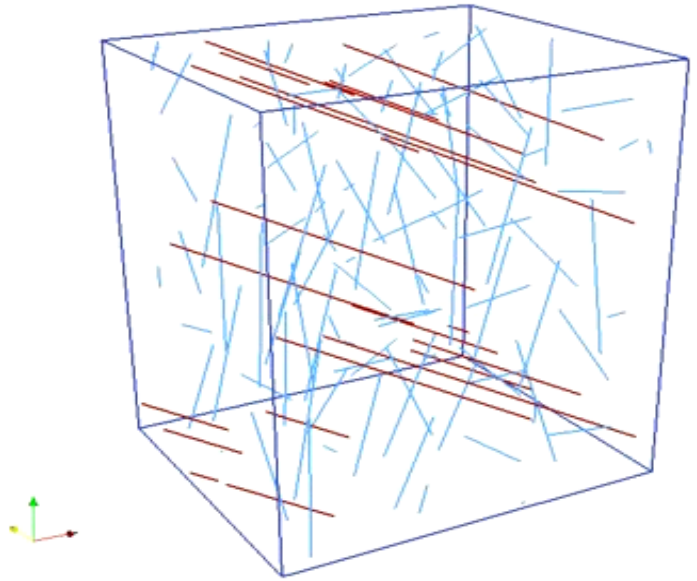
GD^3: Discrete Dislocation dynamics

Request code

The Generalized discrete defect dynamics toolkit simulates the collective interaction of line defects (dislocations) in a fully three dimensionally resolved fashion. It predicts both microstructure evolutions and mechanical response in single crystals and polycrystals over moderate strain amplitudes. Furthermore the toolkit generates virtual diffractions peaks resulting from the defected microstructures. Finally, minimum energy pathways across obstacle forests can be found.





Principle: SGD^3 tracks the evolution of every line defect in the system by solving the equation of motion (EOM) acting on each dislocation segment. The EOM is fitted against atomistic simulations. Further short- range defect interactions leading to dislocation annihilation, junction formation, slip transfer across grains are determined according to maximum dissipation criteria

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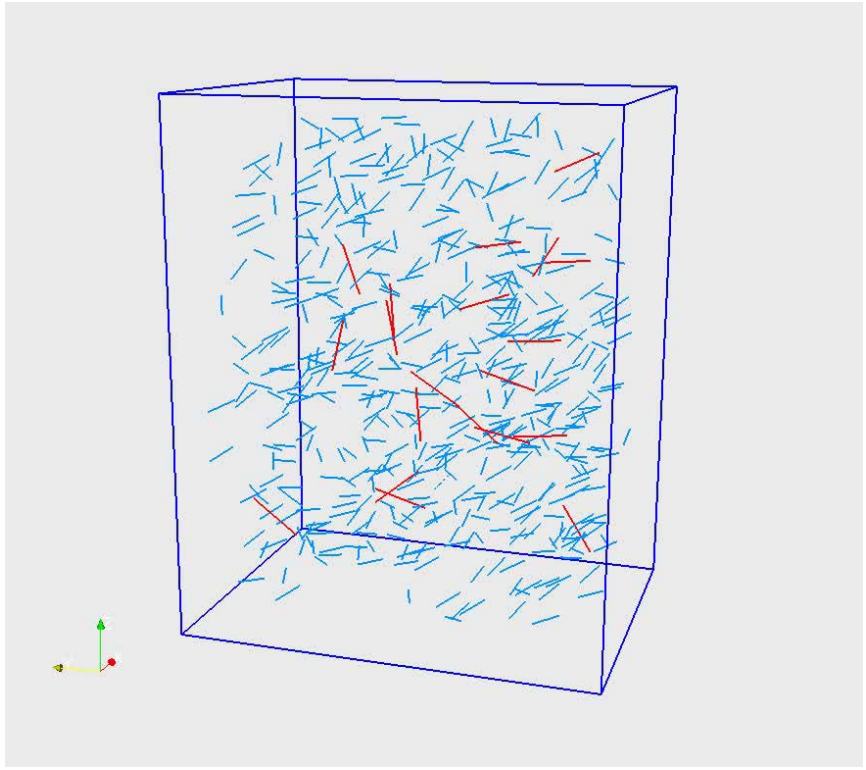
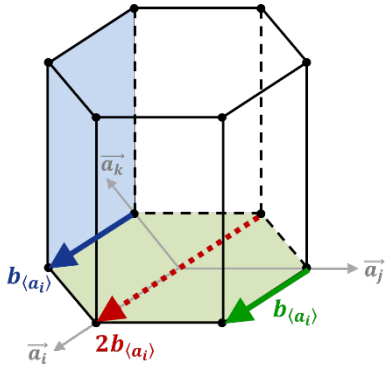
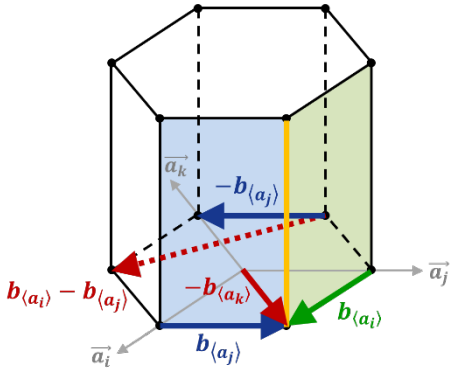
Problem: In low crystal symmetry metals, Plasticity is accommodated by the simultaneous activation of several slip modes

Goal: parameterize a constitutive law to account for latent slip system interactions

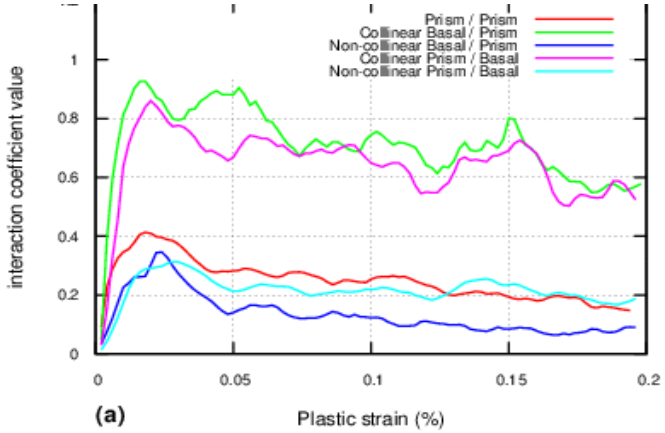




Basal/Prismatic: Collinear



Prismatic/Prismatic



$$\tau_c^s = \tau_0^s + \mu b \sqrt{\sum_u a^{su} \rho^u}$$

a^{su} denotes the latent interaction matrix which coefficient are quantified with DDD