Example: dislocation glide in Ni-based superalloys

MD simulation of dislocations in γ phase Ni

- Aleatoric and epistemic uncertainties
- Model uncertainty: how accurate is interatomic potential? Parameters and functional form
- Random microstructures, limited data
- Algorithmic uncertainty in solvers
- Limited transferability: can we model chemical complexity, e.g. impurities?

EAM, 5% Al, T = 300 K, 100 MPa shear stress


F Bianchini, A Glielmo, JRK and A De Vita, Submitted (2019)