

# **A Multigrid Method for Molecular Mechanics**

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**Abstract:** We present a multigrid method for molecular mechanics. The approach is based on the one-way multigrid method, and take the Cauchy-Born nonlinear elasticity as the coarse grid operator. Due to the hierarchical structure, the method is insensitive to parameters in the nonlinear solvers and exhibits linear scaling computational complexity. We demonstrate the efficiency of the algorithm by performing the computation for the one dimensional chain under tension and aluminum under tension in three dimension. In addition, we study an example with inhomogeneous deformation: nanoindentation of aluminium. This is a joint work with Weinan E(Princeton University) and Pingbing Ming(ICMSEC and LSEC, AMSS, CAS).