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An Efficient Multigrid Method for Molecular Mechanics Modeling in Atomic Solids

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Abstract. We propose a multigrid method to solve the molecular mechanics model (molecular dynamics at zero temperature). The Cauchy-Born elasticity model is employed as the coarse grid operator and the elastically deformed state as the initial guess of the molecular mechanics model. The efficiency of the algorithm is demonstrated by three examples with homogeneous deformation, namely, one dimensional chain under tensile deformation and aluminum under tension and shear deformations. The method exhibits linear-scaling computational complexity, and is insensitive to parameters arising from iterative solvers. In addition, we study two examples with inhomogeneous deformation: vacancy and nanoindentation of aluminum. The results are still satisfactory while the linear-scaling property is lost for the latter example.

AMS subject classifications: 65B99, 65N30, 65Z05, 74G15, 74G65, 74S05

Key words: Multigrid method, linear-scaling algorithm, Cauchy-Born rule, nanoindentation.

1 Introduction

Molecular mechanics model is an important tool for studying static properties of atomic solids. At zero temperature (or lower temperature), the equilibrium state is obtained by minimizing the total energy subject to certain boundary condition and external loading. The most popular approach is the lattice statics proposed by Born and Huang [3]. Recent development of this method can be found in [39] and the references therein. The lattice statics has been widely used to study the equilibrium configurations and many other properties of solids. This method considers a harmonic perfect crystal with an

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eigendeformation as the defect, and solves the equilibrium equations arising from the minimization problem. Therefore, the solution obtained represents the equilibrium state, which may be a local minimum, a metastable state or even a global minimum.

In contrast, we turn to the direct minimization of the molecular mechanics model. By [11, 12, 38], the elastically deformed states are only local minima of the total energy at zero temperature. Therefore, we seek for relevant local minimum. The principal difficulty arises from the nonconvexity of the total energy. There are two sources of nonconvexity. On the one hand, the potential energy function is usually nonconvex; on the other hand, the translation invariance of the underlying crystal naturally imposes nonconvexity on the total energy even though the potential energy function is convex [18]. A crucial step for the success of the traditional minimization algorithms is to find a good initial guess, which places the crystal in the right energy well nearby the configurations of interest.

By [12], under certain stability conditions on the phonon spectra of the crystal, there is a unique local minimum of the atomistic model sitting nearby the elastically deformed state. This motivates us to employ the elastically deformed state as the initial guess for the minimization algorithms of the atomistic model. First, we solve the Cauchy-Born (CB) elasticity model over the successively refined meshes. Next we interpolate the solution to the atomic sites and take the interpolant as the initial guess for the atomistic model. Finally, the atomistic model is minimized with the given initial guess. Similar ideas can be found in many atomistic simulations of fracture and dislocation, where explicit solutions of elasticity model over the whole space, such as the solution obtained by Sin and Liebowitz [32] and the Stroh's formalism [36], are employed.

We demonstrate the efficiency of the current method by a set of representative examples. The method is applied to crystals under either homogeneous deformation or inhomogeneous deformation. For crystals under homogeneous deformation, the total CPU time scales linearly with respect to the total number of the atoms. Hence, the proposed method is a linear-scaling algorithm. For crystals under inhomogeneous deformation, the method still gives satisfactory results. The linear-scaling property is even recovered for a problem with vacancy by an additional local correction step.

It is worth mentioning that the method automatically bypasses many irrelevant local minima since the elastically deformed state is relatively smooth. It is a notorious fact that there are enormous local minima for the molecular mechanics models. For example, there are 1467 different local minima for Lennard-Jones cluster problem [9] that is closely related to the problem in study. Another interesting aspect of this method is that it is insensitive to parameters in the nonlinear iterative solvers, which may be due to the hierarchical structure of the method.

In contrast to the quasicontinuum method [34] that combines the macroscopic model and the microscopic model in a concurrent way, our method is a sequential multiscale method in the terminology of multiscale modeling and multiscale methods [4, 10].

Compared with our method, the commonly used quasistatic process also gives satisfactory results if the increment of the deformation is sufficiently small. During the pro-