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A Constrained Cauchy-Born Elasticity Accelerated Multigrid Method for Nanoindentation

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Abstract. We introduce a new multigrid method to study the lattice statics model arising from nanoindentation. A constrained Cauchy-Born elasticity model is used as the coarse-grid operator. This method accelerates the relaxation process and considerably reduces the computational cost. In particular, it saves quite a bit when dislocations nucleate and move, as demonstrated by the simulation results.

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1 Introduction

As a way of probing mechanical properties of materials in small volumes, nanoindentation has attracted great attention in last few decades [11,21]. It is a flexible characterization technique by varying indentor geometry and indentation direction in experiments. Compared to the uniaxial tension, the strain field under an indentor is more complicated

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and highly heterogeneous even for a specimen with isotropic materials. Although the timescale issue is crucial in many indentation tests [13], (quasi-)static properties, such as hardness and modulus, are also of great interest for different materials. During nanoindentation, different length scales coexist in the problem due to indenter size, sample size, dislocation nucleation and dislocation propagation. The atomistic-level simulation tools are necessary for nanoindentation. However, the computationally intensive nature of atomistic simulations of these phenomena restricts the simulation cell to a size which is many orders of magnitude smaller than the typical size of the solid in an experiment. Thus, many multiscale approaches have been proposed to exploit the nanoindentation problem. On the other hand, its multiscale nature also supplies a benchmark problem for multiscale methods [4, 5, 12, 17, 23].

From a numerical point of view, multiscale methods can be divided into two categories. One is based on the domain decomposition method [24], which combines lattice statics and continuum model in a concurrent manner [17]. The other is based on the multigrid method [3, 25], where models are combined in a sequential manner [5, 12].

In this paper, we will focus on the latter. Brandt [4] highlighted many possible applications of the multigrid method, including molecular statics. Goedecker *e*t al. [12] employed the linear elasticity as the coarse-grid operator in the two-grid method. The efficiency of the method is verified by the silicon crystals with some point defects. A more general approach was proposed by Chen and Ming [5]. They used the one-way multigrid method [7], which can automatically bypass many unphysical local minimizers. The coarse-grid operator was constructed by the Cauchy-Born (CB) rule [2]. The consistency between the CB elasticity model and lattice statics has been proven under some stability conditions [8]. Efficiency of the method is demonstrated by FCC Aluminium crystals under different homogeneous deformations. Moreover, this method gives qualitatively reasonable results for nanoindentation with quite a bit cost.

To overcome this issue, we introduce a constrained CB elasticity model as the coarse-grid operator to accelerate the convergence of the multigrid method. In nanoindentation, collective motion of atoms in the strain field formally can be separated into two parts: one is induced by loading applied on boundaries and the other is by dislocation structures after nucleation. It has been shown in [5] that the former can be effectively captured by CB elasticity model on coarse grids. It will be shown in the present work that the constrained CB elasticity model can capture the latter in an effective manner. This will be done by updating the local strain field around dislocations at the atomistic scale and then transmitting updated information globally on grids.

In the following, we first briefly review the one-way multigrid method for lattice statics, and then introduce a constrained CB elasticity model, based on which we propose an accelerated multigrid method. We show its efficiency by studying the lattice statics model in nanoindentation. A heuristic explanation of the constrained model will be given in the appendix.