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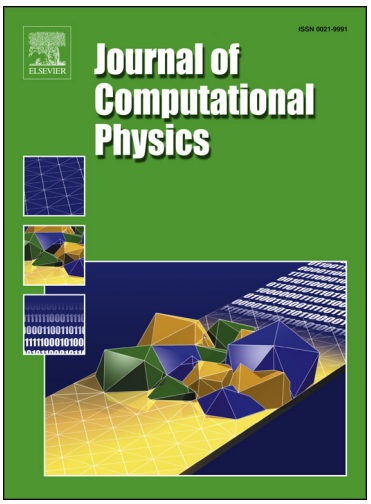

An efficient multigrid strategy for large-scale molecular mechanics optimization

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AN EFFICIENT MULTIGRID STRATEGY FOR LARGE-SCALE MOLECULAR MECHANICS OPTIMIZATION

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Abstract. Static mechanical properties of materials require large-scale nonlinear optimization of the molecular mechanics model under various controls. This paper presents an efficient multigrid strategy to solve such problems. This strategy approximates solutions on grids in a *quasi-atomistic* and *inexact* manner, transfers solutions on grids following a coarse-to-fine (oneway) schedule, and finds physically relevant minimizers with linear scaling complexity. Compared to the full multigrid method which has the same complexity, the prefactor of this strategy is orders of magnitude smaller. Consequently, the required CPU time of this strategy is orders of magnitude smaller than that of the full multigrid method, and is smaller than that of the brute-force optimization for systems with more than $200,000$ atoms. Considerable savings are found if the number of atoms becomes even larger due to the super-linear scaling complexity of the brute-force optimization. For systems with $1,000,000$ atoms (over three million degrees of freedom), on average a more than 70% reduction of CPU time is observed regardless of the type of defects, including vacancies, dislocations, and cracks. In addition, linear scalability of the proposed strategy is tested in the presence of a dislocation pair for systems with more than 100 million atoms (over 400 million degrees of freedom).

1. Introduction

In the classical picture, atoms constitute matter and their interaction is described by a potential energy function. For a given system of atoms at zero (low) temperature, its equilibrium configuration is obtained by minimizing the potential energy with respect to atomic positions, known as the molecular mechanics (atomistic) model (see, e.g., [8]). The potential energy is highly nonlinear and the number of minimizers grows exponentially [46]

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