Accelerated Molecular Statics Based on Atomic Inertia Effect

Fei Shuang[1,2], Pan Xiao[1,*], Yilong Bai[1] and Fujiu Ke[3]

[1] *LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China.*
[2] *Department of Mechanical and Aerospace Engineering, University of Florida, Gainesville, FL, 32611, USA.*
[3] *School of Physics and nuclear energy engineering, Beihang University, Beijing 100191, China.*

Abstract. Molecular statics (MS) based on energy minimization serves as a useful simulation technique to study mechanical behaviors and structures at atomic level. The efficiency of MS, however, still remains a challenge due to the complexity of mathematical optimization in large dimensions. In this paper, the Inertia Accelerated Molecular Statics (IAMS) method is proposed to improve computational efficiency in MS simulations. The core idea of IAMS is to let atoms move to meta positions very close to their final equilibrium positions before minimization starts at a specific loading step. It is done by self-learning from historical movements (atomic inertia effect) without knowledge of external loadings. Examples with various configurations and loading conditions indicate that IAMS can effectively improve efficiency without loss of fidelity. In the simulation of three-point bending of nanopillar, IAMS shows efficiency improvement of up to 23 times in comparison with original MS. Particularly, the size-independent efficiency improvement makes IAMS more attractive for large-scale simulations. As a simple yet efficient method, IAMS also sheds light on improving the efficiency of other energy minimization-based methods.

1 Introduction

Over the past two decades, intensive research interests have been dedicated in nanomechanics and nanomaterials to uncover underlying deformation mechanisms resulting

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*Corresponding author. *Email addresses:* `xiaopan@lnm.imech.ac.cn` (P. Xiao), `shuangfei@ufl.edu` (F. Shuang), `baiyl@lnm.imech.ac.cn` (Y. Bai), `kefj@lnm.imech.ac.cn` (F. Ke),

from individual atoms [1–4]. In particular, well-developed atomistic simulation methods such as molecular dynamics (MD) [5], molecular statics (MS) [6], Monte Carlo (MC) [7] and nudged elastic band (NEB) calculation [8] are of great importance to predict material properties and explain deformation mechanisms, which provide alternative research tools besides in situ experiments. Among these methods, empirical-based methods greatly reduce the computational cost and make simulations with millions of atoms possible [9]. Currently, empirical-based MD and MS are two of the most commonly used methods which are capable of dealing with more than 10^8 atoms with simple potential models like Lennard-Jones (LJ) and embedded atomic model (EAM), achieving the great accomplishment in studying nanomaterials [10] and manipulating their properties [11]. Despite the successful development of modern computer technology and new numerical algorithms, it is always important to improve computational efficiency as much as possible in order to shorten research period and increase simulation dimension.

Various methodologies have been developed to improve simulation efficiency from the perspectives of physics and mathematical optimization. Physically, one can develop new methods to bridge across length and time scale gap between MD and continuum theory. Long timescale dynamics such as EON [12] and diffusive MD [13] can be used in simulations of experimental timescale events. One of the extreme situations is quasi-static simulation at finite temperature without strain rate effect. Molecular Statistical Thermodynamics (MST) [14] and Engineering Molecular Mechanics (EMM) [15] are two representative work. Based on the local harmonic approximation [16], MST uncouples atomic motion from thermal vibration with high frequency. The Helmholtz free energy instead of potential energy is minimized to search local stable configuration at finite temperature. MST shows excellent efficiency improvement and reliable results in simulations of copper nanowire tensile, thin film nanoindentation and phase transformation of ZnO nanowires [14]. For EMM method, parameters of interatomic potential are considered temperature-dependent and are modified as functions of simulating temperature. EMM shows good agreement with conventional MD when simulating elastic properties and thermal stress with 100 times improving efficiency, but the feasibility of EMM on plastic deformation simulation is unknown.

On the other hand, several multi-scale methods based on energy minimization have been proposed in the last few decades to decrease the computational cost of ultra-large atomistic systems [17]. Hierarchically, FE2AT utilizes information from finite element calculation to provide appropriate initial and boundary conditions for atomistic simulations, such that large parts of the elastic loading process can be accelerated [18]. Concurrently, atomistic representation is used in regions under inhomogeneous deformation dominated by dislocation evolutions, whereas quasi-continuum representation is used in regions under homogeneous deformation to reduce computational cost. One of the typical multi-scale methods is the quasi-continuum (QC) method which searches for the positions of representative nodes by minimizing the coarse-grained potential energy [19]. By introducing discrete dislocation line in QC framework, coupled atomistics and discrete dislocation mechanics (CADD) was put forward further to improve the efficiency