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Modeling of slow time-scale behavior of fast molecular dynamic systems

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ABSTRACT

This paper aims to apply a recently developed numerical scheme toward multi-time scale modeling, which we refer to as 'Practical Time Averaging' (PTA), to molecular dynamical (MD) systems. In the first part, we investigate the fine-scale dynamics of a one-dimensional chain of identical particles under cyclic loading. Assuming a double-well interatomic potential among adjacent particles leads to a phase transition between two distinct equilibrium states. Specifically, we study the macroscopic stress–strain behavior of the dynamical chain in three settings, i.e. Newtonian MD, Newtonian MD with viscous dissipation and Newtonian MD with thermostat. Rate-independent high frequency oscillations are observed in Newtonian MD due to an instability that is related to the non-convexity of the strain energy. This is stabilized by adding viscosity or a thermostat, which leads to strong hysteresis that is consistent with quasi-static results (i.e. lattice statics). In the second part, we first define coarse variables as finite time averages of phase functions in MD. Then we apply the technique of PTA developed in Tan et al. (2013) to numerically approximate the coarse dynamics for the time averaged quantities. The tested model problems include a two-dimensional lattice made of stoichiometric Nickel–Manganese undergoing detwinning and a three-dimensional atomic chain made of face-centered cubic (FCC) Nickel under uniaxial tension. The macroscopic features (such as space-time averaged strain/stress) are obtained from coarse dynamics. It is also shown that the time savings become significant when the loading rate is small.

1. Introduction

Molecular dynamics (MD) has become an important simulation tool in understanding material behaviors in a vast variety of settings. This method is based on a particle description of atoms or molecules and treats the interaction between the particles using Newtonian dynamics. However, a key difficulty in using MD for engineering applications is the extremely large separation between the timescales of atomic bond vibrations (femtoseconds) and even the smallest timescales of engineering interest (nano- to microseconds). This limits MD to unrealistically small time intervals for many applications. This situation is even worse for materials under extremely slow loading rates. When the loading rate tends to zero, the equations of motion become a singularly perturbed system of Ordinary Differential Equations (ODE). The objective of this paper is to apply and evaluate the temporal coarse-graining strategy developed in Tan et al. (2013) to such singularly perturbed problems in the mechanics of materials.

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In the first part of the paper, we study the macroscopic stress–strain behavior of a one-dimensional dynamical chain of atoms joined by springs with a non-monotone stress–strain relation. A sinusoidal loading with small loading rate is applied at one end of the chain. The magnitude of the external loading is large enough so that the chain will go from one equilibrium state to the other during this dynamical process. Due to the non-monotonicity in the constitutive relation (or equivalently, the non-convex interatomic potential), the dynamics will lead to rate-independent high frequency vibration of the atoms beyond a certain critical strain as a result of an instability of the system (reported before in Balk et al., 2001 and called the 'inner instability') that is insensitive to external excitation. This finding is quite different from the observation under quasi-static dynamics that ignores inertia, which is normally associated with a hysteresis indicating energy dissipation at the macroscopic level. It is also suggested in Balk et al. (2001) that the inner vibrations of the atoms can be stabilized by a small dissipation, which leads to a strong hysteresis rather than a steady state stress–strain dependence. We test two cases in order to dissipate the high kinetic energy of the system. One is by adding viscosity and the other is by thermostating. The effects in both cases are essentially the same and thus give rise to quite similar results. Furthermore, the hysteresis converges to the quasi-static result as the loading rate tends to zero.

In the second part of the paper, a numerical strategy developed in Tan et al. (2013) and referred to as 'Practical Time Averaging'(PTA) is applied to two MD problems. The approach may be viewed as a natural extension of the method of averaging motivated by practical considerations, naturally for systems whose limiting fast flows may not converge to an equilibrium. The theory of Artstein and Vigodner (1996) and Artstein et al. (2007) is utilized here, where the limit behavior of the fast flow (parameterized by the slow variable) in a singulary perturbed system is characterized by an invariant measure rather than algebraic equations in the standard reduced order approach. However, this theory requires that variables that can be averaged be 'slow', i.e. orthogonal to the fast flow in a precise sense, but does not provide a prescription for generating such 'orthogonal observables'. Following Slemrod and Acharya (2012) (which makes rigorous some of the ideas presented in Acharya, 2007, 2010) and Tan et al. (2013), a natural class of slow variables based on time averaged coarse observables and their evolution are defined and practically implemented.

Two model problems are investigated with the implementation of PTA. One is a two-dimensional infinite strip of a Ni–Mn lattice with two variants of martensite coexisting in the lattice. A twin boundary is located within the strip in a stress-free initial configuration. The two variants have the same free energy. When the body is subjected to an applied cyclic loading, the free-energies of the different variants are no longer equal and one variant becomes energetically more favorable than the other. This leads to the motion of the twin boundary and the dynamics of detwinning. We study the macroscopic stress–strain behavior of the two-dimensional lattice. The other tested example is a three-dimensional dynamical chain system made of FCC Ni undergoing uniaxial tension. The macroscopic stress–strain behavior with different loading rates is studied. We define the overall stress and strain as coarse variables. The averaged response of fine-scale dynamics and PTA is found to be in broad agreement. Moreover, in the range of slow loading rate, we show that the time savings from PTA is significant in both examples. This paper is organized as follows. In Section 2, we construct a one-dimensional atomic dynamical chain under cyclic loading and study the stress–strain behavior in three different settings. Section 3 is excerpted from Tan et al. (2013), which shows the procedures of PTA to write down the coarse evolution equation for singularly perturbed systems based on the Young measure theory (i.e. Artstein and Vigodner, 1996; Artstein et al., 2007; Slemrod and Acharya, 2012; Tan et al., 2013). In Sections 4 and 5, we implement the idea of PTA on a two-dimensional Ni–Mn system and a three-dimensional atomic chain made of FCC Ni, respectively. The stress–strain relations from fine dynamics and from PTA are investigated in both cases. We end in Section 6 with summarizing the main findings from the various numerical tests and discussing the advantages as well as the limitations of the proposed multi-scale modeling technique.

2. Atomistic study

2.1. Model description

The dynamics of interest is adopted from Purohit (2002). This problem is chosen since the set-up is quite similar to large scale MD.

Fig. 1 shows a chain of atoms interacting with each other through non-linear springs with two states of equilibrium. The relation between the potential energy and the distances of atoms is also plotted in Fig. 1. The interactions are limited to the first nearest neighbors.

In this example, we assume double-well potential energy, i.e.,

$$\phi = \sum_{i=1}^{N-1} \phi^1(x_{i+1}-x_i) = \sum_{i=1}^{N-1} (x_{i+1}-x_i-a_s)^2(x_{i+1}-x_i-a_l)^2, \tag{1}$$

where x_i denotes the position of mass i at any time. a_s is the equilibrium separation between two adjacent masses in the low strain phase and a_l is the equilibrium separation between them in the high strain phase. The initial configuration of the atoms is chosen to be in the low strain phase, so the displacement of atom i can be written as

$$u_i = x_i-(i-1)a_s. \tag{2}$$