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A Consistency Study of Coarse-Grained Dynamical Chains through a Nonlinear Wave Equation of Mixed Type

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Abstract. A dynamical atomistic chain to simulate mechanical properties of a one-dimensional material with zero temperature may be modelled by the molecular dynamics (MD) model. Because the number of particles (atoms) is huge for a MD model, in practice one often takes a much smaller number of particles to formulate a coarse-grained approximation. We shall mainly consider the consistency of the coarse-grained model with respect to the grain (mesh) size to provide a justification to the goodness of such an approximation. In order to reduce the characteristic oscillations with very different frequencies in such a model, we either add a viscous term to the coarse-grained MD model or apply a space average to the coarse-grained MD solutions for the consistency study. The coarse-grained solution is also compared with the solution of the (macroscopic) continuum model (a nonlinear wave equation of mixed type) to show how well the coarse-grained model can approximate the macroscopic behavior of the material. We also briefly study the instability of the dynamical atomistic chain and the solution of the Riemann problem of the continuum model which may be related to the defect of the atomistic chain under a large deformation in certain locations.

AMS subject classifications: 65M06, 35L20, 35L67, 74J40, 74H15, 35Q74

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1 Introduction

Modelling and simulation of material motion plays an important role in understanding and predicting material defect behaviors, such as dislocation and dynamic fracture [6,13,

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14, 21, 32, 44]. An atomistic level model is necessary since the atomistic bond is a crucial factor in such behaviors. However, a full atomistic system is too large to handle even using the most powerful computers available. This is where coarse-grained methods are particularly useful. Problems in this area are very challenging to analysts and many theoretical studies so far are about steady state models. In this paper, we shall consider a dynamical atomistic model and its coarse-grained approximation.

Several approaches have been studied in recent years, most notably the quasicontinuum method [28, 35, 38, 44], the virtual internal bond method [13, 14, 21, 25, 46], the coarse-grained molecular dynamics [5, 22–24, 30–32, 48, 49], the heterogeneous multiscale method [8–11], and the bridging scale method [26, 45]. Related approaches have also been proposed for simulations involving stochastic systems [3, 18, 19]. In this paper, we consider only the deterministic, dynamical atomistic (or so-called molecular dynamics) model. However, because the number of atoms under consideration is huge, in practice, a coarse-grained model formulated by a relatively small number of particles is involved in simulation. The question is whether the simulation result is consistent with respect to the grain (or mesh) size and whether such a coarse-grained model could still be able to reproduce macroscopic properties of a material. Here, macroscopic properties may be represented through the continuum model associated with the atomistic or coarse-grained model.

It is pointed out in [13, 21] and [14] that the prospects for this type of model in numerical simulations of material properties are highly promising. There are not many theoretical studies available. As an early attempt for theoretical justification, we analyze a one-dimensional model with the nearest neighbor interaction at zero temperature, and utilize the Lennard-Jones potential as the atomic interacting potential. It is believed that considering the interaction of one atom with its nearest neighbors is a good approximation to the original finite range interaction problem. We will see that fundamental mathematical problems associated to this simple case are still far from being solved.

A defect of a large deformation may probably lead to a fracture in a material. One of such fundamental problems is that in the case of a large deformation, the type of the associated continuum model may change from hyperbolic to elliptic. Owing to this change, the model may be called a nonlinear wave equation of mixed type and is ill-posed as indicated in [34]. There is almost no mathematical analysis for such mixed type continuum equations associated with the atomistic model interacted with the Lennard-Jones potential. There are some incomplete results in the sense of measure-valued solutions, but only for the case where the interacting potential is close to quadratic [7, 27]. Fortunately, a defect under a large deformation may be formulated as a specific initial value problem, which is usually called a Riemann problem of the nonlinear wave equation. Therefore techniques in analyzing the Riemann problem can be used in the analysis.

Our main goal is to study the consistency of the coarse-grained solutions with various grain (mesh) sizes. However, according to [1] we may find that the characteristic frequencies of the atomistic MD model and its coarse-grained approximation are variant at different grain sizes. So under a standard error measure, e.g. maximum norm,