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Analysis of Coarse-Grained Lattice Models and Connections to Nonlocal Interactions

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Abstract. We study coarse-grained models of some linear static lattice models with interactions up to second nearest neighbors. It will be demonstrated how nonlocal interactions, as described by a nonlocal kernel function, arise from a coarse-graining procedure. Some important properties of the nonlocal kernels will be established such as its decay rate and positivity. We also study the scaling behavior of the kernel functions as the level of coarse-graining changes. In addition, we suggest closure approximations of the nonlocal interactions that can be expressed in local PDE forms by introducing auxiliary variables.

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1 Introduction

Coarse-graining of finest scale models has become an important methodology in computer simulations of complex systems in the last two decades. For example, despite rapidly growing computing power, all-atom simulations of materials still remain challenging due to the computational complexity, which has been a major motivation for the development of coarse graining methodology. Reduced models (a.k.a., coarse-grained models) have been shown to be more effective in practice. Starting with a relatively small number of representative degrees of freedom, e.g., local averages, the goal in developing a reduced model is to begin with the many-body atomic interactions and derive a model

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that only involves the preselected degrees of freedom, see [13, 14, 23, 24] for various perspectives and recent progress.

One remarkable success, in the study of solids with crystal structures, has been the quasi-continuum (QC) method [30]. By assuming the smoothness of the deformation field away from defects and employing a finite-element approximation of the elastic energy, a reduced model is constructed that describes the deformation of pre-selected representative atoms. The key ingredient in such an approach is the Cauchy-Born rule, which obtains the local energy density by considering a unit cell under uniform deformation gradient. Effectively, the reduced model, known as the local quasi-continuum approximation, is expressed in terms of the finite element nodal values.

Most QC type of methods have been motivated by continuum mechanics, and inevitably, they lead to modeling error, which can be quantified when the underlying atomic displacement has certain smoothness, see, for example [6, 18, 33], the analysis for one-dimensional models. In this paper, however, we will first derive an *exact* reduced model, with an attempt to understand various properties of the exact interactions among the representative atoms resulting from the coarse-graining process. As an illustration, we consider a one-dimensional lattice system with the interactions being among the first and second neighbors. By assuming that the interaction is linear, we can obtain the exact reduced model explicitly in the form of nonlocal difference equations. Several properties regarding the kernel function that characterizes the coarse-grained interactions can be established. Our first observation is that, in general, this kernel function has no compact support, i.e., the interaction is nonlocal. This observation reflects a strong motivation for the current work, that is, to connect model reduction with nonlocal modeling [7]. It also allows us to draw similarities of the reduced models using nonlocal integral operators to nonlocal peridynamics models, see [15, 29]. We show that the reduced nonlocal model, through rescaling, has a characteristic interaction range, even though the kernel decays exponentially. The latter observation provides a justification for the finite-ranged interactions that are often used in the parameterization of reduced models [14, 23].

Furthermore, we suggest a new approach to approximate the *nonlocal* continuum formulation of the reduced models, by using a Padé approximation of the dispersion relation. More specifically, the nonlocal operator can be approximated by an integral operator with the kernel function consisting of double exponential functions and delta functions. In the physical domain, these models can be rewritten as higher order PDEs, and we prove the stability of these PDEs. It is our hope that this result sheds some light on the origins and selections of interaction kernel functions in nonlocal continuum models. In particular, this approach associates atomic interactions, in the form of force constants, to the kernel functions in the nonlocal models, and hence leading to kernel functions that are material specific and dependent of the coarse-graining procedure.

The rest of the paper is organized as follows. Section 2 will provide a demonstration of the model reduction procedure of some lattice models, including a model with nearest neighbor interactions, followed by one with next nearest neighbor interactions that leads naturally to nonlocal reduced models. In Section 3, we present a Fourier representation