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Peridynamic State-Based Models and the Embedded-Atom Model

Pablo Seleson[1*], Michael L. Parks[2] and Max Gunzburger[3]

[1] *Institute for Computational Engineering and Sciences, 201 East 24th St, Stop C0200, Austin, Texas 78712-1229, USA.*
[2] *Sandia National Laboratories, Computing Research Center, P.O. Box 5800, MS 1320, Albuquerque, NM 87185-1320, USA.*
[3] *Department of Scientific Computing, 400 Dirac Science Library, Florida State University, Tallahassee, FL 32306-4120, USA.*

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Abstract. We investigate connections between nonlocal continuum models and molecular dynamics. A continuous upscaling of molecular dynamics models of the form of the embedded-atom model is presented, providing means for simulating molecular dynamics systems at greatly reduced cost. Results are presented for structured and structureless material models, supported by computational experiments. The nonlocal continuum models are shown to be instances of the state-based peridynamics theory. Connections relating multibody peridynamic models and upscaled nonlocal continuum models are derived.

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1 Introduction

Multibody potentials were proposed in molecular dynamics (MD) to overcome some of the limitations of pair potentials [1, Section 4.3]. One such multibody potential is the *embedded-atom model* (EAM) [2, 3], commonly used for metallic systems, in which the potential energy of the system is expressed as a combination of volume-dependent and

*Corresponding author. *Email addresses:* seleson@ices.utexas.edu (P. Seleson), mlparks@sandia.gov (M. L. Parks), gunzburg@fsu.edu (M. Gunzburger)

pair potential energy terms. Other common multibody potentials include the Stillinger-Weber potential [4], frequently used for modeling semiconductors, and the Tersoff potential [5], which utilizes two- and three-atom contributions and is based on the idea that the strength of a bond between two atoms is environment dependent.

MD models are computationally expensive and even intractable at large scales. In contrast, continuum models can be discretized on coarse meshes, resulting in efficient numerical implementations. Consequently, attempts to replace MD models by continuum models, capable of preserving important features of MD, have been proposed. One such approach, based on higher-order gradient continuum models, is given in [6]. A different approach, using nonlocal continuum models (NCMs) appears in [7]. These methods attempt to use continuum models for the *continuous upscaling*[†] of MD. By replacing MD models with their corresponding upscaled continuum models, we can simulate length scales not tractable by MD alone. In [7], the continuous upscaling of pairwise MD models is derived within the peridynamics theory of solid mechanics [8,9], recovering characteristic dispersion relations of discrete models at the continuum level. That work is related to coarse-graining, but differs from the phase-space average approach presented in [10]. In this paper, we extend the techniques of [7] to multibody potentials of the form of the MD EAM. We derive upscaled nonlocal continuum models inspired by peridynamics, and we demonstrate that all of the nonlocal continuum models we derive are instances of the peridynamics theory.

Alternative approaches for efficient and accurate simulation of systems exhibiting MD phenomena include concurrent multiscale modeling. These methods appear in the literature under so-called atomistic-to-continuum coupling methods, attempting to couple classical continuum models and MD models [11–13].

The organization of this paper is as follows. In Section 2, we review the multibody MD EAM. The continuous upscaling of MD models to NCMs is shown for a structureless EAM in Section 3 and for a structured EAM in Section 4, with supporting computational examples. Concluding remarks are presented in Section 5. Appendix A includes an overview of the peridynamics theory and its multibody models, their connections, and their relations to upscaled NCMs.

2 Embedded-atom models in molecular dynamics

The MD EAM was proposed in [2, 3] based on density functional theory and, in particular, on the earlier quasiatom [14] and effective medium [15] theories. By utilizing a volume-dependent energy, this model overcomes existing difficulties of pair potentials in the description of elastic properties of materials.

In a solid, each atom can be viewed as an impurity embedded in a host composed by all other atoms. As the energy of an impurity is a functional of the electron density of the

[†]By *continuous upscaling*, we refer to the process of deriving a continuum model from a discrete one, so that the continuum model preserves certain quantities of interest of the discrete model.