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# Multiresolution molecular mechanics: A unified and consistent framework for general finite element shape functions

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## Highlights

- This paper presents a generalized framework of multiresolution molecular mechanics.
- The framework is unified and consistent for general finite element shape functions.
- An optimal summation rule is derived by analytically determining energy distribution.
- The optimal summation rule outperforms Gauss quadrature rule.

## Abstract

We present a general mathematical framework for the newly proposed energy-based concurrent atomistic/continuum method Multiresolution Molecular Mechanics (MMM) (Yang et al., 2013). The main features of the generalized framework are: (1) Consistency with the atomistic framework by directly employing the interatomic potential to calculate force and energy; (2) Simple procedure for analytically deriving the optimal summation rule for any given finite element shape function employed in the coarse-grained region. The procedure for obtaining the optimal summation rule is developed based on deriving and then fitting the atomic energy distribution within an element under the constraint of a given shape function. To validate the generalized framework, test problems including non-local harmonic and anharmonic models undergoing tensile, shear and bending deformations will be solved using linear, bilinear and quadratic elements, respectively. Results obtained using the proposed optimal summation rules for the different element types will be compared with Gauss quadrature for accuracy. Through error structure analyses, it is found that the proposed summation rule always outperforms Gauss quadrature, even when the latter employs more quadrature points than the former. It is argued that widely-used numerical quadrature techniques such as Gauss quadrature are not optimal for coarse-grained atomic energy approximation because they do not account for the discrete nature of the atoms. In contrast, the present summation rule is derived consistently from the underlying atomic energy distribution, and thus has better accuracy and smaller computational cost.



*Keywords:* Multiscale modeling; Multiresolution molecular mechanics; Finite element method; Gauss quadrature; Summation rule

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## 1. Introduction

With the development of faster computers, complex systems spanning a wide range of scales once thought to be intractable can now be simulated by continuum methods such as the finite element method (FEM). However, due to the prohibitive computational cost, fully resolved atomistic and molecular simulations are still out of reach with current computer resources for engineering problems of practical interest [1–3]. On the other hand, models based on continuum mechanics are inadequate for understanding deformation mechanisms of material defects such as cracks, dislocations and grain boundaries. The promise of multiscale modeling is that by coupling atomistic and continuum models, the accuracy of full atomistic simulations can be obtained at a much reduced computational cost.

Many multiscale methods have been developed to bridge different spatial and time scales from Angstroms and femtoseconds to meters and seconds [4–44]. Capturing interaction between different scales is of main concern to multiscale modeling. Sequential or hierarchical multiscale models perform the simulations from bottom-up in a step-by-step fashion [13,45–48]. The simulations are performed independently at each scale and a complete separation of both length and time scales is achieved. Iterative parameter passing between different length scale simulations are employed in sequential methods which is best suited for coupling scales with weak dependence [46]. Concurrent multiscale methods employ the domain decomposition strategy and couple the atomistic region and continuum domain simultaneously [48]. The continual information exchange between the two scales is ensured by the consistency of the field variables between the subdomains.

Concurrent methods can be further classified into energy-based approaches and force-based schemes. Energy-based methods generally have a well-defined energy functional consisting of energy contributions from each subdomain to minimize to derive the force equilibrium equations analytically. This category contains the bridging domain method (BDM) [11,18], the bridging scale method (BSM) [12,20,21,49], the atomic-scale finite element method (AFEM) [14], the coupling of length scale method (CLS) [8], the original quasicontinuum method [5] and its energy-based variants [29,44,50] and the newly presented multiresolution molecular mechanics (MMM) [38,40,51], to name a few. Force-based approaches, in contrast, generally derive the force equilibrium equations directly on carefully chosen set of degrees of freedom without minimizing a corresponding energy functional. Among the force-based coupling schemes are the coupled atomistic and discrete dislocations (CADD) [10,17], the atomic-to-continuum method (Atc) [24,25], the finite element-atomistic method (FEAt) [4], the force-based variants of the quasicontinuum method [9,41,52], and the recently proposed atom collocation method (ACM) [35], just to name a few. Several excellent review papers [37,45–48,53–56] address the details of various multiscale models and the existing challenging issues.

The constitutive model employed in the coarse-grained region plays a key role of determining the performance of a specific multiscale model since it is directly related to the treatment of interface between subdomains and thus to the information exchange. One popular approach to construct the constitutive model is the well-known Cauchy–Born (CB) rule [5]. However, there are three main disadvantages: (1) in nature, CB rule is a local description of continuum constitutive model that is incompatible with the non-locality of atomic interaction; thus it causes the local–nonlocal mismatch at the interface [55]; (2) CB rule requires sufficiently homogeneous deformation of the underlying crystal and is no longer valid (and thus inaccurate) if the deformation becomes inhomogeneous [57]; (3) CB rule is unable to capture surface effects [58]. The local–nonlocal mismatch causes the so-called “ghost” force problem and has motivated the development of many ghost force correction techniques and the force-based multiscale models [48]. The inaccurate description of nonhomogeneous deformation has motived the development of high-order CB rules [28,59,60] and the inability to capture surface effect has motived the well-known surface Cauchy–Born rule (SCB) [58].

On the other hand, the direct employment of the atomic constitutive model or the interatomic potential in the coarse-grained region can avoid the aforementioned drawbacks of the CB rule [9,29–32,35,36,38–40,44]. Since the constitutive models employed in the atomistic and coarse-grained domains are the same, the interface mismatch does not exist. Since the atomic constitutive model has no requirement of the deformation smoothness of underlying crystal and it can directly capture the surface effects, the last two disadvantages are overcome. However, the main challenging issue arises when using the atomic constitutive model in the coarse-grained region is that an accurate summation rule is needed to approximate the energy contribution from the coarse-grained domain. The main merit of employing CB rule in the coarse-grained area is that the energy calculation can be put into the continuum framework that is rather mature and convenient to accurately estimate the energy contribution. To overcome this challenging issue with using the atomic constitutive model, Ortiz first proposed the node-based summation rule. However, it caused