Comput. Methods Appl. Mech. Engrg. 237–240 (2012) 67–77

Contents lists available at SciVerse ScienceDirect

Comput. Methods Appl. Mech. Engrg.

journal homepage: www.elsevier.com/locate/cma

Atom collocation method

Qingcheng Yang [a], Emre Biyikli [a], Pu Zhang [a], Rong Tian [b], Albert C. To [a,*]

[a] Department of Mechanical Engineering and Materials Science & Center of Simulation and Modeling, University of Pittsburgh, Pittsburgh, PA, USA
[b] Institute of Computing Technology, Chinese Academy of Science, Kexueyuan Nanlu 6, Haidian 100190, China

ARTICLE INFO

Article history:
Received 29 February 2012
Received in revised form 5 May 2012
Accepted 6 May 2012
Available online 19 May 2012

Keywords:
Multiscale modeling
Surface relaxation
Point defect
Crack propagation
Collocation method
Molecular statics

ABSTRACT

This paper presents a new concurrent atomistic-continuum method called the atom collocation method (ACM). By adopting the framework of continuum collocation method, ACM aims at overcoming the current difficulties in interfacial mismatch, adaptive analysis, and parallel implementation of existing atomistic-continuum methods. The proposed ACM is truly meshfree and generalizes the full atomistic description, which naturally yields a perfectly compatible atomistic/continuum interface that eliminates any ghost forces. A unique feature of ACM is that the collocation atoms can be turned on or off freely at any time without the need to reconstruct interpolation functions, which greatly enhance the ability to perform adaptive analysis. The proposed ACM is applied to solve problems involving point defect and crack propagation as well as surface, edge, and corner effects and demonstrates excellent accuracy and efficiency compared to molecular statics.

1. Introduction

The development of concurrent atomistic-continuum methods [1–16] to tackle computationally inaccessible number of atoms in a simulation came from the realization that full atomistic description of the material is required only in the localized regions of the material, which contain the essential physics that affect the overall mechanical behavior. These physical phenomena usually involve large atomic rearrangements, bond breaking, and thus require full atomistic treatment because they are more complicated deformations. Examples of these are nucleation of dislocations during ballistic impact, nanoindentation testing, and processes in the vicinity of a crack tip such as crack tip blunting and plasticity in the process zone. As a good approximation, the rest of the material can be thought of as a continuum where atomistic degrees of freedom can be integrated out or replaced by interpolation methods such as finite element method (FEM). This approach forms the basis for the development of hybrid computational schemes for coupling an atomistic region with a continuum region that are generally termed "multiscale methods".

All coupling schemes need to address the problem of passing information between the atomistic region and the surrounding continuum. Static methods are based on finding the configuration of mechanical equilibrium in the combined atomistic-continuum system and assume quasistatic application of a mechanical load. In statics, proper information passing is based on the assumption of continuity of the mechanical fields throughout the material at each load step. For static methods, generally there are two ways to determine the equilibrium of a multiscale model. The first approach is to define an approximate energy functional of the system to minimize rigorously, and hence is called the "energy-based" approach. The second way is to drive some physically-motivated forces on certain set of degrees of freedom to be zero. This is called the "force-based" approach. In concept, this classification is similar to the one we usually use to classify continuum methods. For instance, weak form approaches such as finite element method (FEM) and weak-form meshfree method such as RKPM [17], EFGM [18], etc., have a well-defined physical energy whereas strong form approaches such as continuum collocation method, which is truly meshfree, do not have a well-defined energy functional.

Among the energy-based coupling methods, there are several well-known approaches. These methods include bridging scale method (BSM) [5,6,19], quasicontinuum (QC) method [1,8], bridging domain method (BDM) [4,20], and atomic-scale finite element method (AFEM) [12], just to name a few. The BSM was first proposed for concurrent coupling in dynamic simulations [5] and then its static version was reported [6]. The static version of BSM is conceptually different from other energy-based methods. In BSM, a multiscale partition of the displacement field is proposed, which consists of a coarse scale component in the whole domain that is solved by a continuum approximation such as the meshfree method and a fine scale component present in the localized region that is solved by molecular statics. By introducing the projection properties of the partition, the governing equations of BSM can be

* Corresponding author. Address: 508 Benedum Hall, University of Pittsburgh, PA 15261, USA. Tel.: +1 (412) 624 2052.
E-mail address: albertto@pitt.edu (A.C. To).

0045-7825/$ - see front matter © 2012 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.cma.2012.05.010

decoupled and solved iteratively. It is also worth noting that, instead of using the well-known Cauchy–Born (CB) rule which is widely-used in other existing methods, a virtual atom cluster (VAC) model was proposed in BSM and applied to study the mechanical behavior of carbon nanotubes. For the relation between VAC and CB rule, readers are referred to the original paper by Qian et al. [6]. The QC method employs the CB rule and FEM in the continuum region coupled with the enriched atomistic region by a sharp interface to enforce the strong coupling boundary conditions. The strong coupling boundary conditions usually give better accuracy than the weak coupling boundary conditions [21], but it requires more effort to generate the mesh near the interface.

There is an unphysical phenomenon arising near the interface, usually termed "ghost force", whose definition is given according to [21] as follows. Consider a model where the atoms are initially at force equilibrium on their lattice structure. We then introduce a coarse-grained model (usually FEM) somewhere in the original system to reduce the degrees of freedom. Physically, the degree-reduced model should be able to reproduce the original equilibrium crystal structure, which means all the atoms and finite elements are unstressed and undeformed at the beginning. Therefore, any forces on atoms or nodes initially arisen in the coupled model are unphysical and will lead to spurious distortions of the body when relaxed. These unphysical forces are termed "ghost force". As pointed out by Miller [22], the origin of ghost forces lies precisely in the assumption of locality in the continuum region and the non-locality of interaction between atoms. There are some approaches proposed to correct the ghost force in QC method [7,21] and the accuracy is greatly improved with ghost force correction. To have a smooth transition, BDM employs, instead of a sharp interface, a handshake region where both atomistic description and continuum descriptions coexist. The displacement constraints are introduced into the handshake region using Lagrange multiplier. This introduces some parameters that need to be chosen to optimize computational efficiency. The BDM was first proposed to treat dynamic simulations [5] and then a static version was presented [20] and is discussed here. Like the QC method, BDM also use FEM with CB rule in the continuum region. Thus, it also suffers from ghost force problem. As pointed out in [21], the use of a finite handshake region has the effect of smearing out the ghost force, making the ghost force on a given atom or node smaller, but introduces ghost forces on more atoms and nodes. Another well-known method is the atomic finite element method (AFEM) proposed by Huang [12] to reduce the computational cost of original system for order-N^2 to order-N, where N is the total number of atoms in the system. The AFEM employs non-local elements, which is as accurate as molecular mechanics since no continuum assumption such as shape function is introduced. AFEM can be linked seamlessly with the continuum FEM by defining another new type of element, called transitional element to make it a concurrent coupling method. However, the transitional element requires the extrapolations of some atom positions and depends on the atomic structure of the material.

Among the force-based methods, there are several well-known approaches. These methods include the atomistic-to-continuum (AtC) method [10], the force-based cluster-based quasicontinuum method (CQC) [11], the force-based version of quadrature-rule type approximation to the quasicontinuum method (QC-QR) [23,24], just to name a few. The AtC method can be regarded as a force-based version of the BDM discussed before. It also employs FEM and CB rule in the continuum domain and the handshake region where, instead of blending a continuum and atomistic energy, the blending at the force level is employed. As pointed out in [21], AtC is not a truly ghost-force free method in general. Both the CQC and CQ-QR methods are variants of the original quasicontinuum method. In the CQC, different from other concurrent methods, a small cluster of atoms are chosen around each representation atom (or rep-atom) to approximate force of the missing atoms by employing summation rules, which directly utilize the interatomic potential to compute forces in the coarse-grained domain, thus eliminating the use of CB rule. This approach is supposed to eliminate the interfacial mismatch and also the ghost forces, but it was found that large clusters of atoms are needed to ensure good accuracy. There also exist substantial errors that cannot be removed by increasing the size of the clusters when graded mesh is used [25]. The QC-QR method is quite similar to the CQC method. The difference is that, instead of using the cluster summation rule, a new summation rule at the force level, called the quadrature-type approximation is introduced. It is worth noting that both the CQC and QC-QR methods have to calculate weights associated with the clusters or quadrature points and mesh generation is needed in the continuum domain.

As can be learnt from the discussion above, many of the existing multiscale methods employ FEM or needs mesh (or background mesh if weak-form meshfree method is used) generation for energy or force integral in the continuum domain. Some methods introduce some parameters that need to be chosen to optimize the performance or else suffer from the ghost force problem that has a great effect on the accuracy (at least for statics). However, as pointed out by Weinan E [26], the fundamental problem of utilizing FEM in concurrent methods is that the energy or force is strictly local to an element while atoms interact with each other in a nonlocal manner, and hence FEM and atomistic method are naturally incompatible. This is the very reason that special treatment is needed at the atomistic/continuum interface or handshake region in concurrent methods. For further details, readers are referred to the original papers and an excellent review paper on the comparison of 14 different concurrent methods by Tadmor and Miller [21].

Motivated by eliminating the mesh generation (even the background mesh generation) and interface mismatch without introducing any parameters and also facilitating large-scale adaptive analysis in concurrent atomistic-continuum analysis, we adopt the framework of continuum collocation method [27–32] combined with directly employing the interatomic potential to calculate forces between atoms in the coarse-grained region as used in CQC and QC-QR method in the formulation of a new approach called the atom collocation method (ACM). The first advantage of adopting the collocation framework is that it is naturally compatible with atomistic method since both methods solve their respective governing equations directly without resorting to the weak formulation. As such, no interfacial mismatch arises and ghost forces are eliminated when collocation method is adopted in the coarse-grained region to couple with the atomistic method in the full atomistic region, which will be proved in Section 2.3. Therefore, collocation method may be more accurate when utilized in concurrent atomistic-continuum simulations than when weak formulations such as FEM are employed in the coarse regions, though continuum collocation method is often found to be less accurate than FEM in continuum analysis [30,33,34].

The second advantage of adopting the collocation framework is that it is truly meshfree. It does not require any mesh, not even a background mesh as no integration is needed. In large-scale FEM simulations, the burden of mesh generation and mesh decomposition onto large number of processors becomes quite significant. This issue also motivates the recent development of more accurate continuum collocation methods by other researchers in the field [31–33,35]. Hence, adopting the collocation framework is timely and suitable for future large-scale coupled atomistic-continuum analysis of materials.

The third advantage of the proposed method is that ACM is amenable for adaptive analysis. Adaptive scheme will be utilized