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An enhanced bridging domain method for linking atomistic and continuum domains

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ABSTRACT

Bridging domain method (BDM) is a multiscale method which couples molecular dynamics (MD) with finite element simulations. In this paper, using numerical study we show that time integration step size and the discretization of Lagrange multipliers can highly impact the capability of BDM in removing spurious reflections. We present a technique to enhance the performance of bridging domain method and to alleviate the effects of the two aforementioned factors on the BDM. In our technique, the total displacement field of the atoms located in the overlapping zone is decomposed into a coarse and a fine field. The equations of motion of fine scale oscillations are first obtained and then modified to include a damping term. The damping condition effectively filters out and removes the fine scale oscillations that cannot pass into the continuum domain; hence eliminates the spurious wave reflections. Using numerical examples, we show that the proposed enhancement significantly improves the performance of bridging domain method. This is specially significant when discontinuities such as cracks are present in the domain or when the integration time step is small.

1. Introduction

Molecular dynamics simulations provide vast amount of information about material behavior at nanoscale. They have been particularly used to study how defects such as cracks, grain boundaries or dislocations affect macroscale processes such as elasticity or plasticity. However, the high computational costs associated with atomistic simulations limit their applicability to systems made of limited number of atoms. Coupled atomistic-continuum methods have been introduced as a remedy to this limitation. In the coupled methods, full atomistic resolution is maintained where deformations are highly inhomogeneous (e.g., at the vicinity of defects) and continuum models are used elsewhere [1–16]. The challenge lies in appropriate gluing of atomistic and continuum zones such that the atomistic region behaves as if the entire domain is atomistic. To achieve this objective, the effects of the atomistic-continuum interface should be minimized. In static problems ghost forces can be generated at the coupling interface [17] and a number of techniques have been developed to overcome this issue [9,11]. In dynamic problems an additional difficulty related to the passage of the propagating wave from atomistic to continuum across the interface is encountered; the change of the constitutive equations from inherently nonlocal atomistic to local continuum along with the change of the resolution from atomistic to continuum lead to spurious wave reflection at the interface. Since in the coupling methods atomistic zone usually has a small size, the spuriously reflected wave can quickly increase the temperature of atomistic zone, whereby destroys the simulation.

To avoid the spurious wave reflections, the interface between the atomistic and continuum should be such that coarse scale information (low frequency waves) can be accurately transmitted in both directions, whereas the fine scale oscillations which cannot be transmitted into the continuum zone should be eliminated at the interface. Several such interfaces have been developed in the past, among those are coarse-grained molecular dynamics (CGMD) method [4,5], macroscopic-atomistic-ab initio dynamics (MAAD) method [6,7], bridging scale method (BSM) [8,18], bridging domain method (BDM) [9,10], concurrent AtC coupling method [11,19], embedded statistical coupling method (ESCM) [12] and heterogeneous multiscale method (HMM) [20,21]. Reviews on concurrent atomistic-continuum multiscale methods can be found in [22–25].

Belytschko et al. [9,10] developed a bridging domain method (BDM) to couple continuum mechanics with molecular models. Bridging domain method lies in the category of overlapping domain decomposition coupling methods, or Arlequin method, which has been developed earlier by Ben Dhia [26–28]. This

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method has been used for modeling cracks and defects in graphene and carbon nanotubes [9,10,29,30] and has been combined with extended finite element method (XFEM) [31] to study crack propagation and dislocation emission in nanomaterials [32,33]. More recently, BDM applications are extended to multiscale analysis at finite temperature [34,35].

In the bridging domain method, continuum and atomistic domains overlap in a bridging (handshaking) domain where a weight function is used to partition the atomistic and continuum energy. In the overlapping domain, the positions of atoms and nodes are not necessarily coincident and the compatibility between atomistic and continuum domain is imposed by Lagrange multipliers. This allows to use a uniform mesh in the entire domain and removes the need for mesh refinement in the overlapping region.

In this paper, we first numerically show that the type of the discretization of Lagrange multipliers and the time integration step size significantly impact the success of BDM method in suppressing spurious reflections. Then, we present a new technique to enhance the performance of BDM and to alleviate the effects of the two aforementioned factors. In this method, the total displacement field of atoms located in the overlapping zone is decomposed into a fine and a coarse scale displacement field. The fine scale displacements corresponds to the oscillations which cannot be resolved by the finite element mesh and need to be damped. The elimination of fine scale oscillations is accomplished by deriving their equations of motion and inserting a damping term into their equations of motion.

The outline of this paper is as follows. In Section 2, we review the bridging domain method. In Section 3, we numerically study the performance of the BDM method and will provide the motivation of the proposed enhancement. The formulation of the new enhancement is presented in Section 4. The effectiveness of the method in removing spurious reflections and in modeling crack propagations will be investigated using numerical examples in Section 5. Some conclusions are made in Section 6.

2. Brief review of bridging domain method

2.1. Reference model and notations

In the bridging domain method (BDM), the domain Ω is composed of an atomistic subdomain, Ω^{A}, and a continuum subdomain, Ω^{C}, which overlap in a bridging or handshaking subdomain, $\Omega^{\mathrm{B}}=\Omega^{\mathrm{A}}\bigcap\Omega^{\mathrm{C}}$, as shown in Fig. 1. The edges of the atomistic and continuum subdomains in the bridging subdomain are denoted by Γ^{A} and Γ^{C}, respectively. In this paper, the superscripts 'A', 'C', and 'B' identify the variables associated with the atomistic, continuum, and bridging subdomains respectively. Accordingly, Ω_0^{A}, Ω_0^{C}, and Ω_0^{B} denote the atomistic, continuum, and bridging subdomains in the initial configuration, respectively, where the subscript 0 refers to quantities defined at $t=0$. We denote the material coordinates by $\boldsymbol{X}$ or X_i, $i=1,\ldots,n_d$ in component notation, where n_d is the number of spatial dimensions, and the current coordinates by $\boldsymbol{x}$. We use subscripts I and J to refer to FE-nodes, and α and β to refer to atoms. The displacement of atom α is denoted by $\boldsymbol{d}_\alpha$ (or $d_{i\alpha}$ in component form). The continuum subdomain is spatially discretized by a finite element (FE) mesh and its displacement field is approximated by

$$u_i(\boldsymbol{X},t)=\sum_{J\in\mathcal{S}}N_J(\boldsymbol{X})u_{ij}(t), \tag{1}$$

where $\mathcal{S}$ is a set of finite element nodes, N_J is the FE shape function of node J and u_{ij} is the ith displacement component of node J.

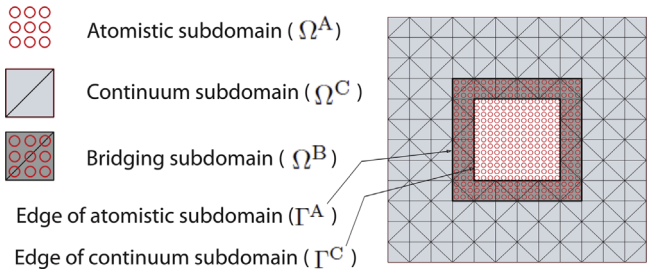

Fig. 1. Three subdomains in a BDM simulation: atomistic, continuum, and bridging subdomains.

2.2. Governing equations

In the bridging domain method, the total Hamiltonian of the entire domain is obtained by adding up the Hamiltonian of the continuum and atomistic domains. To avoid double counting in the overlapping domain, the Hamiltonian of continuum and atomistic domains are weighted by a scaling factor $\vartheta(\boldsymbol{X})$ defined as

$$\vartheta(\boldsymbol{X})=\begin{cases}0 & \text{in } (\Omega_0^{\mathrm{C}}-\Omega_0^{\mathrm{B}})\\ [0,1] & \text{in } \Omega_0^{\mathrm{B}}\\ 1 & \text{in } (\Omega_0^{\mathrm{A}}-\Omega_0^{\mathrm{B}})\end{cases} \tag{2}$$

In our numerical calculations, we use a linear scaling factor defined as [10]

$$\vartheta(\boldsymbol{X})=\frac{\|\boldsymbol{X}-\boldsymbol{X}_p\|}{\|\boldsymbol{X}_q-\boldsymbol{X}_p\|} \tag{3}$$

where $\boldsymbol{X}_p$ is the orthogonal projection of $\boldsymbol{X}$ onto Γ^A and $\boldsymbol{X}_q$ is the intersection point of line X_pX and Γ^{C}. The total Hamiltonian of the domain is given by

$$H(\boldsymbol{u},\boldsymbol{d},\lambda)=H^{\mathrm{C}}(\boldsymbol{u})+H^{\mathrm{A}}(\boldsymbol{d})+G^{B}(\boldsymbol{u},\boldsymbol{d},\lambda) \tag{4}$$

where H^{C} is the continuum domain Hamiltonian, H^{A} is Hamiltonian from the atomistic domain, and G^B is the Hamiltonian associated with the Lagrange multiplier constraint that imposes displacement compatibility of the atomistic and continuum domain at the overlapping domain.

The contribution of the continuum domain in the total Hamiltonian is given by

$$H^{\mathrm{C}}=\sum_{I,J\in\mathcal{S}}\int_{\Omega_0^{\mathrm{C}}}(1-\vartheta)\frac{p_{iI}^{\mathrm{C}}p_{ij}^{\mathrm{C}}N_IN_J}{2\rho_0}d\Omega + \int_{\Omega_0^{\mathrm{C}}}(1-\vartheta)W^{\mathrm{C}}(\boldsymbol{F})\,d\Omega, \tag{5}$$

where p_{iI}^{C} is the ith component of the linear momentum of node I, ρ_0 is the initial density of the continuum domain, W^{C} is the internal energy (strain energy) density and $F_{ij}=\partial x_i/\partial X_j$ is the deformation gradient. The Hamiltonian of the atomistic domain is

$$H^{A}=\sum_{\alpha\in\mathcal{M}}\left(\vartheta_\alpha\frac{p_{i\alpha}^{\mathrm{A}}p_{i\alpha}^{\mathrm{A}}}{2m_\alpha^{\mathrm{A}}}+\sum_{\beta\in\mathcal{M}>\alpha}\vartheta_{\alpha\beta}V_{\alpha\beta}\right) \tag{6}$$

where $\mathcal{M}$ is the set of all atoms, $p_{i\alpha}^{\mathrm{A}}$ is the ith component of the linear momentum of atom α, m_α^{A} is the mass of atom α, $V_{\alpha\beta}=V(r_{\alpha\beta})$ is the potential of the bond between atoms α and β which is a function of the bond length of two atoms (i.e. $r_{\alpha\beta}$), $\vartheta_\alpha=\vartheta(\boldsymbol{X}_\alpha)$ and $\vartheta_{\alpha\beta}=(\vartheta(\boldsymbol{X}_\alpha)+\vartheta(\boldsymbol{X}_\beta))/2$.

The compatibility of deformation between atomistic and continuum domain in the overlapping zone can be imposed in different ways [9,10,36,37]. For example, the compatibility of deformations can be obtained by requiring displacement of the atoms conform to the continuum subdomain displacement field at