# Interfacial Conditions in Seamless Multiscale Simulations

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## Summary

Several alternate time-dependent interfacial conditions, between the atomistic and continuum regions, are studied systematically for the seamless multiscale simulation, by decomposing the displacement of atoms in continuum region into macro-average and thermal fluctuation components. Multiple length scale, multiple time step, and meshless local Petrov-Galerkin (MLPG) method are used in the numerical examples.


## Introduction

Systems with multiple length scales are ubiquitous in science. When the length-scale in a system in question cannot be accessed by either the continuum methods because it is too small for averaging, or by the atomistic methods because it is too large for simulations on the present day computers, these two approaches become inadequate; and this has stimulated the research in multiscale simulation to couple the atomistic and continuum methods in a seamless way [1]. In the multiscale simulation, the atomistic method is employed where the displacement field varies on an atomic scale, and the continuum approach is employed elsewhere. For the seamless multiscale simulation, it is important to ensure that the elastic waves generated in the atomistic region can propagate into the continuum region. The continuum region cannot support modes of short wavelength, which is less than the spacing of the nodes. One source of finite size effects is the short waves which are reflected back unphysically from an artificial interface or boundary, which may also produce uneven heating across the interface. In order to minimize such reflections, some interfacial conditions are proposed [3][4][5]. In this paper, alternate interfacial conditions between atomistic and continuum regions are proposed, and are studied systematically. Their effectiveness in ensuring the accurate passage of information between atomistic and continuum regions is discussed.

## Interfacial Conditions

We consider a multiscale system, including an atomistic region A, which may contain inhomogeneities, and an outer domain B, which is defect-free. In region B, the deformation is homogeneous, and thus can be approximated by an equivalent continuum mechanics model (ECM) as in [2], where the individual atomic displacements are not being solved using molecular dynamics. The atomic environment is characterized by the deformation gradient there. Similar to the quasicontinuum method proposed in [2], the constitutive response in this region is obtained from the atomistic energy calculations. The material in ECM is discritized into a set of nodes, which are not necessarily coincident with the atoms. The positions of the atoms in this region can be interpolated from those of the nodes. Effectively, the ECM model involves an averaging over the atomic degrees of the

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freedom that are missing from the node. In this paper, MLPG5 is used in the ECM region B, with the local radial basis functions being used as the interpolats.

Assume that there are $N_1$ atoms in region A (MD), and $N_2$ in region B (ECM). The displacement of atom $\alpha$ in Region A is denoted as $\mathbf{q}_\alpha$ $(1 \le \alpha \le N_1)$. The displacement of atom $i$ in Region B is denoted as $\mathbf{u}_i$ $(1 \le i \le N_2)$, which is interpolated from the displacements of the nodes in region B. The displacement $\mathbf{u}_i$ of an atom in region B implies an average value of the atomistic displacement, and can not catch the thermal fluctuations. To describe it more accurately, we assume that the "real" displacement $\mathbf{q}_i$ of the atom in the region B can be expressed as: $\mathbf{q}_i = \mathbf{u}_i + \Delta\mathbf{u}_i$, where $\Delta\mathbf{u}_i$ denote the atomistic thermal fluctuations, and it is assumed that $\Delta\mathbf{u}_i << \mathbf{u}_i$ in region B. Now, the total potential energy of the system (A+B) can be written as:

$$\begin{aligned} &\Pi(\mathbf{q}_1, \cdots, \mathbf{q}_{N_1+N_2}) \approx \Pi(\mathbf{u}_i; \mathbf{q}_\alpha) + \sum_{i=1}^{N_2} \left.\frac{\partial \Pi}{\partial \mathbf{q}_i}\right|_{\mathbf{q}_i=\mathbf{u}_i} \Delta\mathbf{u}_i \\ &= \Pi_0 + \sum_{i=1}^{N_2} \frac{\partial \Pi_0}{\partial \mathbf{u}_i} \Delta\mathbf{u}_i = \Pi_0(\mathbf{u}_B; \mathbf{q}_A) + \frac{\partial \Pi_0}{\partial \mathbf{u}_B} \cdot \Delta\mathbf{u}_B \end{aligned} \tag{1}$$

Here $\Pi_0$ denotes the zeroth-order approximation of the potential energy; $\mathbf{q}_A$and $\mathbf{u}_B$ are the atomic displacement vectors with dimensions $3N_1$ (for 3 dimensions) in region A, and $3N_2$ in region B, respectively; $\Delta\mathbf{u}_B$ is atomistic thermal fluctuation vector with dimension $3N_2$. In many of the existing multiscale modeling methods, the thermal fluctuation is generally neglected, as in [1]. In this case, in region A, the Newton's Second law can be written in a matrix form as

$$\mathbf{M}_A \ddot{\mathbf{q}}_A = \mathbf{f}_A^0; \quad \mathbf{f}_A^0 = -\partial \Pi_0 / \partial \mathbf{q}_A \tag{2}$$

where the atomic mass matrix $\mathbf{M}_A$ is a diagonal matrix of size $3N_1$ with the atomic masses on the diagonal, and the force vector $\mathbf{f}_A^0$ is of dimension $3N_1$. Eq. (2) is valid only for classical $0^\circ$K. We denote the solution of eq. (2) as "Solution Method 1". Thus, in Solution Method 1, which is computationally inexpensive, has the potential drawback that higher frequencies waves will reflect back from the interface between A and B. To improve the performance at higher frequencies and assure that the energy in region A can pass through the interface between A and B, the thermal fluctuation of atoms in region B must be considered. Thus, we will use the first-order approximation of the potential energy,

$$\mathbf{M}_A \ddot{\mathbf{q}}_A = \mathbf{f}_A^0 - \mathbf{K}_{AB} \Delta\mathbf{u}_B \tag{3}$$

where $\mathbf{K}_{AB} = \partial^2 \Pi_0 / \partial \mathbf{u}_B \partial \mathbf{q}_A$. It is noted that the tangent stiffness matrix $\mathbf{K}_{AB}$ is of order $3N_1 \times 3N_2$, and its entries are nonzero, only when the atoms in region A are directly coupled to atoms in region B. $\Delta\mathbf{u}_B$ can be obtained from the equation of motion in region B, viz.,

$$\mathbf{M}_B \Delta\ddot{\mathbf{u}}_B = \mathbf{f}_B^0 - \mathbf{M}_B \ddot{\mathbf{u}}_B \tag{4}$$

where the atomic mass matrix $\mathbf{M}_B$ is a diagonal matrix of size $3N_2$, and the force vector $\mathbf{f}_B^0$ of dimension $3N_2$ is approximated as $\mathbf{f}_B^0 = -\partial\Pi_0/\partial\mathbf{u}_B$. *In eqs. (3) and (4), we note that* $\mathbf{f}_A$ *in A is approximated as* $\mathbf{f}_A = -\partial\Pi/\partial\mathbf{q}_A \approx -\partial\Pi_0/\partial\mathbf{q}_A - \partial^2\Pi_0/\partial\mathbf{u}_B\partial\mathbf{q}_A$*; that in B is approximated as* $\mathbf{f}_B = -\partial\Pi/\partial\mathbf{q}_B$. By integrating eq. (4) twice, $\Delta\mathbf{u}_B$ can be solved for, and substituting this solution into eq. (3), we have

$$\mathbf{M}_A\ddot{\mathbf{q}}_A = \mathbf{f}_A^0(\mathbf{u}_B, \mathbf{q}_A) - \mathbf{K}_{AB}\int_0^t (t-\tau)\,\mathbf{Y}(\tau)\,d\tau - \mathbf{R}(t) \tag{5}$$

where

$$\mathbf{Y}(t) = \mathbf{M}_B^{-1}\mathbf{f}_B^0(\mathbf{u}_B, \mathbf{q}_A) - \ddot{\mathbf{u}}_B(t) \tag{6}$$

$$\mathbf{R}(t) = \mathbf{K}_{AB}[\Delta\mathbf{u}_B(0) + t\Delta\dot{\mathbf{u}}_B(0)] \tag{7}$$

$\mathbf{Y}(t)$ simply represents $\Delta\ddot{\mathbf{u}}_B$. $\mathbf{R}(t)$ represents the effects on region A due to the initial thermal fluctuation, and the velocity in region B and is usually treated as a vector of random forces to describe the effects of statistical fluctuation in region B at nonzero temperature. The solution of eq. (5), which is originally proposed here, is denoted as "Solution Method 2". It is noted that only a few of the entries in vector $\mathbf{Y}(t)$ are necessary, since the matrix $\mathbf{K}_{AB}$ is nonzero only for the atomic pairs in the cutoff of the interface. That makes presently proposed Solution Method 2 is computationally inexpensive.

In equations (3) and (4), which are based on the potential energy, we note that the force in the region A is expanded to the first order of $\Delta\mathbf{u}_B$, while the force in the region B is only of the zeroth order. To increase the accuracy of the results, we can also expand the force in the region B to the first order, as $\mathbf{f}_B = \mathbf{f}_B^0 + \mathbf{K}_{BB}\Delta\mathbf{u}_B$, with the$3N_2 \times 3N_2$ tangent stiffness matrix $\mathbf{K}_{BB} = \partial^2\Pi_0/\partial\mathbf{u}_B\partial\mathbf{u}_B$. Then, eq. (4) can be rewritten as

$$\mathbf{M}_B\Delta\ddot{\mathbf{u}}_B = \mathbf{f}_B^0 + \mathbf{K}_{BB}\Delta\mathbf{u}_B - \mathbf{M}_B\ddot{\mathbf{u}}_B \tag{8}$$

Similar to [7], by means of Laplace transforms, the intermediate-variable $\Delta\mathbf{u}_B$ can be solved for, and substituting it back into eq. (3), we have

$$\mathbf{M}_A\ddot{\mathbf{q}}_A = \mathbf{f}_A^0(\mathbf{u}_B, \mathbf{q}_A) - \int_0^t \vartheta(t-\tau)\,\mathbf{Y}(\tau)\,d\tau + \mathbf{R}(t) \tag{9}$$

where

$$\vartheta(t) = L^{-1}\left\{\mathbf{K}_{AB}\left[s^2\mathbf{I} + \mathbf{M}_B^{-1}\mathbf{K}_{BB}\right]^{-1}\right\} \tag{10}$$

$$\mathbf{R}(t) = \dot{\vartheta}(t)\Delta\mathbf{u}_B(0) + \vartheta(t)\Delta\dot{\mathbf{u}}_B(0) \tag{11}$$

The matrix $\vartheta(t)$ denotes the time-dependent memory kernel. The Operator $L^{-1}$ indicates the inverse Laplace transform. Eq. (9) is similar to the Generalized Langevin Equation (GLE) boundary condition derived in [7] for the single-scale problem, and in [5] for the multiscale problem by using a "bridging scale" decomposition. We denote the solution of eq. (8) as "Solution Method 3". The second term on the right hand side of equations (5) and (9), the time history integral, implies the dissipation of energy from region A into region B, which results in non-reflecting boundary conditions, supporting short wavelengths that cannot be represented by the interpolations in region B. It is noted that the computation of the of the matrix $\vartheta(t)$ involves not only an inverse Laplace transform, but also the inversion of an $N_2 \times N_2$ matrix, which appears to be impractical, although only a few of the entries in this inverted matrix are necessary, since the matrix $\mathbf{K}_{AB}$ is nonzero only for atomic pairs in the cutoff of the interface. The necessary entries of the matrix $\vartheta(t)$ can be approximated as that in [7], or computed numerically as in [3]. However, the computation of the matrix $\vartheta(t)$ is costly. Here, we will not consider Solution Method 3. However, eq. (8) will play important role in static case for seamless multiscale simulations, which will be discussed in our future paper.

As a demonstration of the effectiveness of these interfacial conditions proposed here, we consider the same example as in [1]: one-dimensional chains of identical atoms with nearest-neighbor interactions. The spring constants, mass, and equilibrium distances are set equal to unity. There are 151 atoms in region A, which is bracketed by two semi-infinite chains (region B). The time integration uses multiple time steps: the equivalent continuum simulation in region B is advanced by a time step $\Delta t = 0.1$, while the MD simulation in region A is advanced by $\Delta t/5$. The distance between the nodes in region B is 7.8. The Solution Methods denoted as 1 and 2 earlier, are used to simulate the time evolution, after introducing initial displacements according to the wave packet [1], $u(X, t=0) = \cos(kX)\exp\left(-X_2/2\sigma^2\right)$. Here, $X$ denotes the equilibrium position of atoms. The center of region A is $X = 0$. A full MD simulation is also performed, in which the entire system is treated in atomistic scale. As a measure of the effectiveness of Solution Methods 1 and 2, the wave reflection at the interface between region A and B is evaluated. The reflectivity R is defined as the maximum difference between the instantaneous energies stored in region A during the simulation and the full MD run, divided by initial energy in region A [3].

Fig. 1 shows the variation of phonon reflectivity $R$ versus the wave number $k$ with $\sigma = 5$. In both cases shown, $R$ approaches to zero in the long wave-length limit. As the wave number increases, $R$ increases greatly, and is over 0.8 at the boundary of Brillouin zone in Solution Method 1, while it is less than 0.1 in all the Brillouin zone in Solution Method 2. Solution Method 1 obtains lower $R$ than that in [1], that means MLPG will be a better method for a seamless multiscale simulation than the finite element method. However, Solution Method 1 is much less effective than the Solution Method 2. Although lower $R$ can be reached in the Solution Method 3 [3], due to its high computational cost, Solution Method 3 should not be an appropriate choice among the three solutions in most

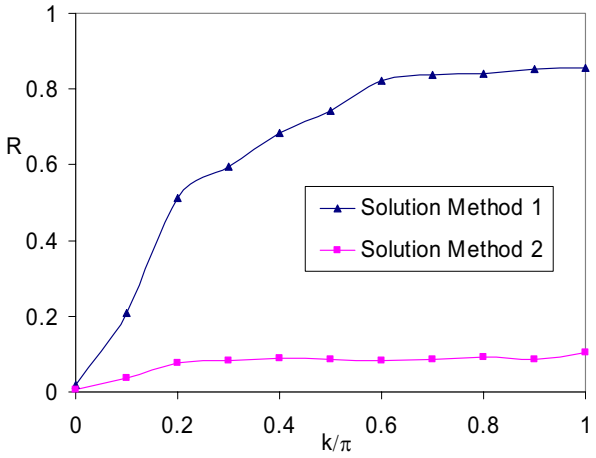


Figure 1: Comparison of the phonon reflectivity $R$ in two solution methods.

problems.

Another example is the same problem as in [5]. A short wave-length perturbation is multiplied to a Gaussian pulse. The resulting initial displacement is

$$u(X,t=0)=\frac{\left[\exp\left(-X^2/\sigma^2\right)-u_c\right]}{1-u_c}\left[1+0.1\cos(kX)\right] \tag{12}$$

Here, $u_c=\exp\left(-l^2/\sigma^2\right)$, $l=50$, $\sigma=20$, $k=0.4\pi$. All the other parameters are same as in the first example. Because of the configurational symmetry about $X=0$, only the right plane is plotted. Fig. 2 shows the displacements obtained by Solution Methods 1 and 2, and full MD at$t=18$. An internal reflection of the short wave-length perturbation appears in Solution Method 1, which looks like the mirror image of the short wave-length perturbation in full MD with the mirror located on the interface of region A and B ($X=75$). In Solution Method 2, the short wave-length waves almost pass out of region A at the same time as the long wave-length Gaussian pulse propagates into region B. In region B, both cases simulate the long wave-length Gaussian wave very well. Compared with the full MD solution, there is an apparent smoothing of the wave profile as the Gaussian pulse propagates in region B, due to the large node space.

In summary, three alternate interfacial conditions are derived, for the multiscale simulation, by considering the fluctuation of atoms in the continuum region. Solution Method 2, proposed in this paper, is found to be optimal in both reducing the reflection of phonons and in lowering computational cost. The MLPG method is also found to be very effective in seamless multiscale simulations.

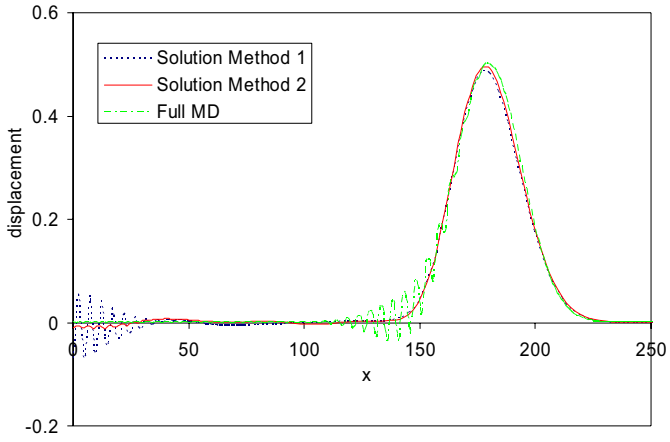


Figure 2: Comparison of the displacement profiles computed using the multiscale methods and the full MD, at $t$=18.

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