 ICCES, vol.7, no.2, pp.77-82

Comparisons of coupling General Finite Element Techniques with Molecular Dynamics

M. Macri[1], P. Chung[1]

Summary

In this paper, we compare three interpolation functions in a discretized continuum when used in coupled dynamic atomistic-to-continuum simulations. The focus is on assessing the ability of the discrete continuum model to capture and accurately represent transient effects, namely a travelling longitudinal wave, through both the mixed atomistic-continuum interface and the non-uniform continuum mesh beyond. We specifically examine the differences among Bubnov-Galerkin, partition of unity, and moving least squares finite element methods, which generally fall under the framework of the meshless Petrov-Galerkin Finite Elements, in the continuum part of the multiscale model, where the key technical distinction is in the penalty formulation we presently adopt for matching at the interface. Our study shows that using partition of unity interpolation functions in this context for the continuum produces superior results compared to the other two approaches.

Introduction

It is well known that continuum based techniques such as Lagrangian or Eulerian numerical methods, which use constitutive relations that do not account for the atomistic structure, have questionable accuracy beyond the scope of their calibration. In regions containing cracks, fractures or nonlinear material, modifications to these numerical methods have to be implemented to capture the phenomena. Molecular dynamics (MD) is an excellent means for predicting the reactions on an atomic scale as well as predicting the response of when phenomena such as cracks occur. However, MD can be computationally expensive beyond small sample sizes and has difficulty implementing boundary conditions applied a continuum scale. Therefore, to alleviate these problems multiscale methods have been developed to couple the continuum and atomistic scales together.

There has been extensive work on developing novel coupling techniques for linking atomistic and continuum scales. These techniques include the quasicontinuum method [1], bridging domain method [2], bridging scale method [3] and homogenization techniques [4,5], among others. A thorough review of several recent techniques is given in [6]. In [7], technique was developed which couples a meshless method, MLPG, with the atomic scale using a bridging scale technique. These techniques have been developed using the finite element method within the continuum scale. Though seemingly well known, to our knowledge, an examination of the level of approximation and choice of interpolation in the continuum region in and around the discrete atomistic domain has not been shown.

[1]Computational and Information Sciences Directorate, US Army Research Laboratory

In this paper we show a comparative study of the quality of interpolation that best suits continuum methods in regions at and near the interface with a molecular dynamics region. We specifically examine interpolation functions prominent in general finite element methods and meshless methods – Bubnov-Galerkin, partition of unity [8], and moving least squares [9] – and assess their ability to capture a travelling wave through a discrete/continuum interface and a graded finite element mesh (increasing element size away from the MD region). Within the interface region, where the continuum and atomistic scales overlap, the displacements on the continuum are dictated by the atomistic results generated from MD. In this study, the forces between the domains are communicated from the atoms to the continuum through ghost nodes.

Continuum Formulation

We begin by reviewing the governing equations on the continuum scale. The conservation of momentum can be defined as:

$$\nabla_0 (V_0 \mathbf{P}) + \rho_0 V_0 \mathbf{f}_0 = \rho_0 V_0 \ddot{\mathbf{u}} \tag{1}$$

where $\mathbf{P}$ is the first Piola-Kirchoff stress tensor, $\mathbf{f}_0$ is the body force, $\rho_0$is the density, A_0 is the area and $\ddot{u}$is the acceleration.

From classical continuum mechanics we can define the first Piola-Kirchoff stress as:

$$\mathbf{P} = \frac{\partial W}{\partial \mathbf{F}} \tag{2}$$

where W is the potential energy density, and $\boldsymbol{F}$ is the deformation gradient defined as:

$$\mathbf{F} = \frac{\partial x}{\partial \mathbf{X}} = \frac{\partial u}{\partial \mathbf{X}} + 1 \tag{3}$$

where $\mathbf{X}$ denotes the reference configuration and $\mathbf{x}$ denotes the spatial or current configuration. In order to use equation (1) for numerical techniques such as general finite elements we need to use the principal of virtual work on (1) to obtain the variational form:

$$\int_\Omega \delta \mathbf{u} \left[\nabla_0 (V_0 \mathbf{P}) + \rho_0 V_0 \mathbf{f}_0 - \rho_0 V_0 \ddot{\mathbf{u}}\right] \partial \Omega = 0 \tag{4}$$

where $\delta \mathbf{u}(\mathbf{x})$ is the virtual displacement. We define two different approaches to approximating the displacement and virtual displacement, such that:

$$\mathbf{u}(\mathbf{x}) = \mathbf{h}(\mathbf{x}) \alpha \tag{5}$$

where $\mathbf{h}$ is a vector interpolation functions and α is a vector of coefficients.

For the partition of unity paradigm [8], the first step of is to define a weighting function, W, on each node that is compactly supported on $\bar{B}(\mathbf{x}_I, r_I)$ with the following properties:

1. $W_I(\mathbf{x}) \in C_0^s(\bar{B}(\mathbf{x}_I, r_I))\ s \geq 0$
2. $W_I(\mathbf{x}) \geq 0\ \forall \mathbf{x} \in \bar{B}(\mathbf{x}_I, r_I)$
3. $W_I(\mathbf{x}) = 0$ elsewhere

The symbol $C_0^s(\bar{B}(\mathbf{x}_I, r_I))$ stands for the space of functions that are compactly supported on$\bar{B}(\mathbf{x}_I, r_I)$, where in the case of general finite elements $\bar{B}(\mathbf{x}_I, r_I)$ is generated using neighboring elements, which have continuous derivatives of order s. We define the Shepard partition of unity function at each node I as:

$$\phi_I^0 = \frac{W_I}{\sum_{J=1}^N W_J} \tag{6}$$

From the partition of unity property it follows that the functions satisfy zeroth order consistency, i.e. they ensure that rigid body modes are exactly satisfied. The next step is to develop, at each node I, a local approximation space

$$V_I^{h,p} = span_{m\in\zeta}(p_m(\mathbf{x})) \subset H^1(\bar{B}(\mathbf{x}_I, r_I) \cap \Omega) \tag{7}$$

where h is a measure of the size of the spheres, p is the polynomial order, ζ is an index set, H^1 is the first order Hilbert space, and $p_m(\mathbf{x})$ is a polynomial or other function. Finally, the global approximation space is defined by pasting together the local spaces as follows:

$$V^{h.p} = \sum_{I=1}^N \phi_I^0 V_I^{h,p} \subset H^1(\Omega) \tag{8}$$

Hence, any function $v^{h,p} \in V^{h,p}$ can be written as:

$$u^{h,p}(\mathbf{x}) = \sum_{I=1}^N \sum_{m\in\zeta} h_{Im}\alpha_{Im} \tag{9}$$

$$h_{Im}(\mathbf{x}) = \phi_I^0 p_m(\mathbf{x}) \tag{10}$$

and h_{Im} the shape function at node I corresponding to the mth degree of freedom.

In moving least squares we set the approximation to:

$$u^h(\mathbf{x}) = \mathbf{p^T}(\mathbf{x})\mathbf{a}(\mathbf{x}) \tag{11}$$

where $\mathbf{p}$ is a vector composed of the monomial basis functions as in equation (7) and $\mathbf{a}(\mathbf{tx})$ is a vector composed of their coefficients. These coefficients are obtained by using a weighted least square fit for the local approximation. We can derive this by minimizing the difference between the local approximation and the function, such that:

$$\mathbf{A}(\mathbf{x})\mathbf{a}(\mathbf{x}) - \mathbf{B}(\mathbf{x})\mathbf{u} = \mathbf{0} \tag{12}$$

$$\mathbf{A} = \mathbf{P^T}\mathbf{W}(\mathbf{x})\mathbf{P} \tag{13}$$

$$\mathbf{B} = \mathbf{P}^{\mathbf{T}}\mathbf{W}(\mathbf{x}) \tag{14}$$

where $\mathbf{P}$ is a matrix composed of the monomial basis functions and $\mathbf{W}$ is a matrix composed of the weighting functions having the same properties as those used in partition of unity interpolation functions. This results in:

$$\mathbf{a}(\mathbf{x}) = \mathbf{A}^{-\mathbf{1}}(\mathbf{x})\mathbf{B}(\mathbf{x})\alpha \tag{15}$$

And the shape function is defined as:

$$h_I(\mathbf{x}) = \mathbf{p}^{\mathbf{T}}\mathbf{A}^{-\mathbf{1}}(\mathbf{x})\mathbf{B}(\mathbf{x}) \tag{16}$$

Molecular Dynamics

For the atomistic scale the governing equation for MD is Newton's equation of motion defined as

$$M_I\ddot{\mathbf{u}}_I = \mathbf{f}_I \tag{17}$$

where M_I is the mass, $\ddot{\mathbf{u}}_I$ is the acceleration and $\mathbf{f}_I$ is the force acting on discrete atoms, I. For our study we will only examine short range interactions. The force can be defined as:

$$\mathbf{f}_I = -\nabla\varphi(r_{IJ}) \tag{18}$$

Where $\varphi(r_{IJ})$ is the interatomic potential, which we can relate to the potential defined in (2) as $W = \varphi/r_{IJ}$.

In this paper we specifically examine a linear harmonic potential and a nonlinear Lennard-Jones potential, where the harmonic potential is given as:

$$\varphi = \tfrac{1}{2}k\left(r_{IJ} - r_0\right)^2 \tag{19}$$

where k is a constant and r_0 is the zero potential distance between two atoms. The Lennard-Jones potential is defined as:

$$\varphi = 4\varepsilon\left(\left(\frac{\sigma}{r_{IJ}}\right)^{12} - \left(\frac{\sigma}{r_{IJ}}\right)^{6}\right) \tag{20}$$

where ε and σ and constants.

Coupling

In figure 1 we define the domain as discretized into a region in which the continuum equations are applied, Ω^C, and a region in which MD is applied, Ω^A. There is a overlap between these two regions defined as the interface region Ω^I.

The constraint that matches atoms to nodes in the interface is applied through a penalty formulation. The result is a modified variational form of (4):

$$\int_\Omega \delta\mathbf{u}\left[\nabla_0\left(V_0\mathbf{P}\right) + \rho_0 V_0\mathbf{f}_0 - \rho_0 V_0\ddot{\mathbf{u}} - \gamma\left(\mathbf{u}^h - \mathbf{u}^{MD}\right)\right]\partial\Omega = 0 \tag{21}$$

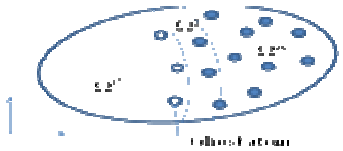

Figure 1: Coupling Domain

Where γ is the penalty constant which is generally a large positive number. To enforce the boundary conditions for MD, ghost atoms are placed in the continuum region (see figure 1) to avoid a surface layer or unphysical termination in he interface.

Numerical Example

We present an example of a Gaussian wave propagating through a 1D domain to illustrate the preliminary results. The fully atomistic domain is comprised of 201 atoms. For the comparative study, the domain is discretized such that for $-2 \leq x \leq 2$ each atom is individually resolved and from $-10 \leq x \leq 1.6$ and $1.6 \leq x \leq 10$ the different numerical interpolation schemes are applied. The interface regions are defined in $-2 \leq x \leq -1.6$ and $1.6 \leq x \leq 2$. In the regions $-10 \leq x \leq -1.6$ and $1.6 \leq x \leq 10$ the discrete continuum is represented with a grid of increasing element size as one moves away from the atomistic core. We compare the use of Bubnov-Galerkin, partition of unity and moving least squares interpolation functions to full MD throughout the domain.

We use a harmonic interatomic potential for this example. The results of the displacements at different time steps are shown in figure 2.

From these preliminary results, it can be observed that even in a one dimensional example, spurious oscillations occur in the atomistic-continuum multiscale problem when using Bubnov-Galerkin and moving least squares in the continuum part of the model. The partition of unity interpolation scheme is indistinguishable from the full-MD results in each of the frames depicted in Figure 2. Whereas the oscillations appear to grow as the wave travels through the graded part of the continuum mesh outside of the atomistic region, the partition of unity result maintains close agreement with the full MD.

The final presentation will also include comparisons of these interpolation functions for nonlinear problems using the Lennard-Jones potential, their subsequent extensions to three-dimensional examples, and a complete discussion of theoretical analyses that explain the observed differences.

References

1. Tadmor, E.B., Ortiz, M., Phillips, R., (1996) Phil. Mag., A73, 1529.
2. Zhang, S., Khare, R., Lu, Q. and Belytschko, T. (2007) *Int. J. Numer. Meth. Engng*, Vol. 70, pp. 913-933.

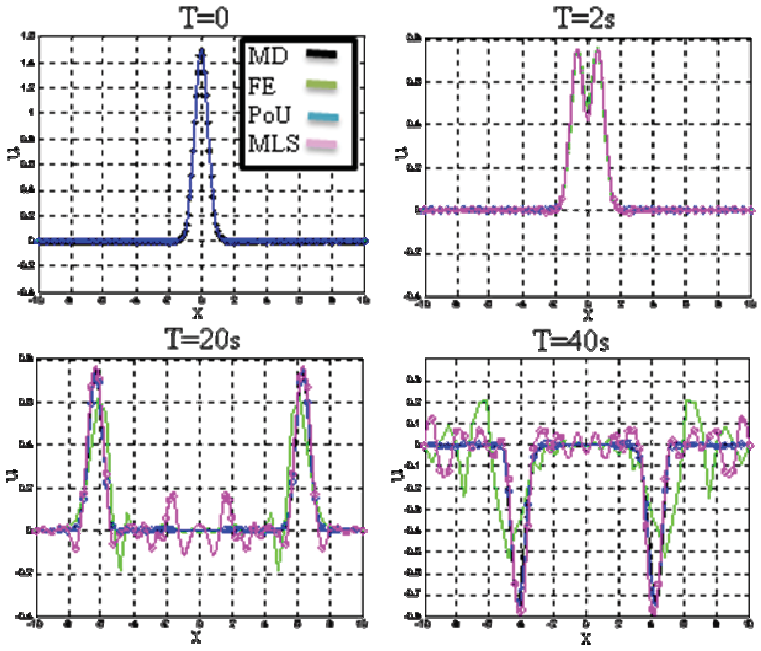

Figure 2: Gaussian wave through harmonic continuum. A molecular dynamics (MD) simulation is compared with multiscale schemes using interpolations based on Bubnov-Galerkin finite elements (FE), partition of unity (PoU), and moving least squares (MLS).

3. Tang, S., Hou, T.Y. and Liu, W.K. (2006) *Int. J. Numer. Meth. Engng*, Vol. 65, pp. 1688-1713.

4. Fish, J., Chen, W. and Li, R. (2007) *Comput. Methods Appl. Mech. Engrg.*, Vol. 196, pp. 908-922.

5. Chung, P. and Namburu, R. (2003) *International Journal of Solids and Structures*, Vol. 40, pp. 2563-2588.

6. Curtin, W.A. and Miller, R. (2003) *Modelling Simul. Mater. Sci. Eng.*, Vol. 11, pp. R33-R68.

7. Shen, S and Atluri, S.N. (2004) *CMES*, Vol. 5, pp. 235-255.

8. Melenk, J.M. and Namburu, I. (1996) *Comp Methds in App Mech and Engg*, Vol. 139, pp. 289-314.

9. Belytschko, T., Lu, Y.Y. and Gu, L. (1994) *Int. J. Numer. Meth. Engng*, Vol. 37, pp. 229.-256.