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# A Comparative Study of General Finite Element Techniques in Atomistic-to-Continuum Coupling

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## ABSTRACT

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, are invalid beyond the scope of their calibration. In regions containing dislocations, mobile defects, or nonlinear material, these numerical methods have to be modified to capture important phenomena. Molecular dynamics (MD) is an excellent means for predicting interactions on an atomic scale as well as predicting the response when sub-micron scale phenomena occur. However, MD can be computationally expensive beyond small sample sizes and has difficulty implementing boundary conditions applied at a continuum scale. Therefore, to alleviate these problems multiscale methods have been developed in recent years 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]. 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.

In this presentation, 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 [7], and moving least squares [8] – 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.

The results of our study show that using partition of unity interpolation functions in the continuum produces accurate results compared to finite elements and moving least squares interpolation functions. For example, in figure 1 we demonstrate the effectiveness of partition of unity shape functions by simulating a Gaussian wave

propagating throughout a 1D domain with a harmonic potential between neighbouring atoms. As the wave moves through the atomistic-continuum interface and through the graded mesh, the effectiveness of the partition of unity shape functions are clearly seen. In spite of the higher computational costs, the improvement in accuracy appears beneficial in practice.

The final presentation will also include comparisons of these interpolation functions for nonlinear problems using the Lennard-Jones potential between atoms in three-dimensional examples. To explain these differences, we will also review the theoretical aspects of the numerical methods.

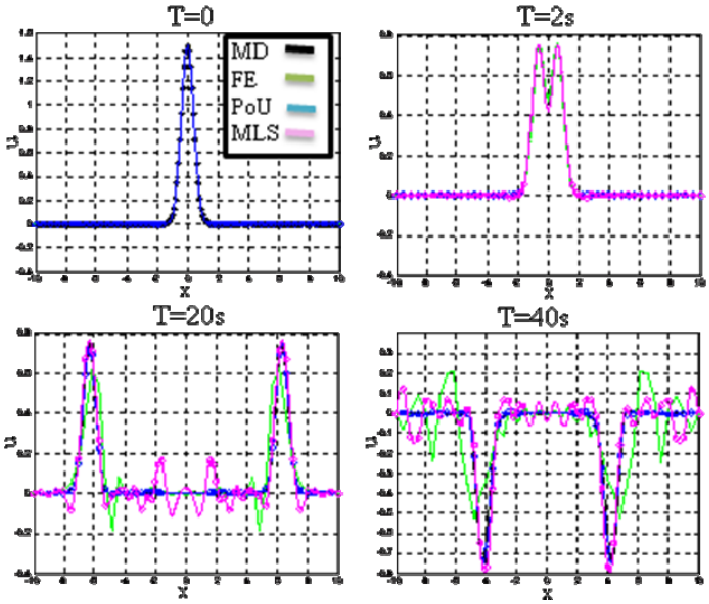


**Figure 1: Gaussian wave through harmonic continuum. Comparison of full MD, MD/FE, MD/Partition of Unity (PoU), and MD/Moving Least Squares (MLS) using snapshots of the solution at different time steps. In these images, the full MD solution is indistinguishable from the blue MD/PoU solution.**

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