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An Extended Bridging Domain Method for Continuum-Atomistic Simulations of Discontinuities

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ABSTRACT

In this presentation we will discuss a continuum multiscale framework which combines the Bridging Domain Method (BDM) of Xiao and Belytschko [1] with the eXtended Finite Element Method (XFEM) of of Moës et al. [2]. The BDM is a hierarchical overlapping domain decomposition scheme. Material in the coarse-scale domain is modelled as a continuum using XFEM and in the fine-scale domain by Molecular Mechanics. Compatibility between the atomistic and continuum domains is enforced in the overlap region using Lagrange Multipliers. The XFEM-BDM framework allows the coarse-graining of both regions where the atomistic displacements are homogeneous and where they are discontinuous, such as across cracks and dislocation glide planes. The combination of XFEM with BDM significantly reduces the number of degrees of freedom in the systems for problems involving cracks and dislocations. The proposed framework will be compared to direct numerical simulations and its advantages and limitations will be discussed.

Many multiscale methods suffer from one significant limitation; that is that, as the simulation progresses more and more of the simulation domain is converted from continuum to atomistics to accommodate the evolution of discontinuities. XFEM-BDM alleviates this problem by replacing large portions of the atomistic domain behind the crack tip with the XFEM crack approximation developed in [2]. In a similar manner, it is generally possible to replace atomistic degrees of freedom along the glide plane of a dislocation by the XFEM dislocation approximation developed by Gracie et al. [3,4].

The framework is schematically shown in Figure 1 for cracks, where only the domain near the crack tip is modelled by atomistics. The domain is decomposed into two overlapping subdomains Ω^C and Ω^A. In Ω^C the material is modelled as a continuum and in Ω^A it is modelled with Molecular Mechanics. The boundary of Ω^C is consists of an outer part Γ which is completely outside of Ω^A and an inner part $\partial\Omega^C$ which is inside of Ω^A. Essential and natural boundary conditions are only applied to Γ. The boundary of Ω^A is denoted as $\partial\Omega^A$. The coupling/overlap domain is given by $\Omega^\lambda = \Omega^C \bigcap \Omega^A$.

In the XFEM-BDM framework, the displacement approximation for a continuum subdomain with a crack defined by the zero of the level set function $f(\mathbf{x})$ is

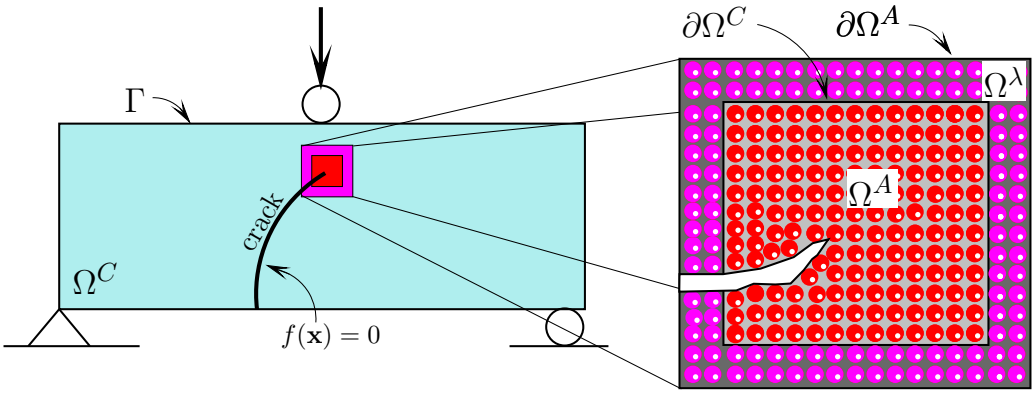

Figure 1: Schematic of the proposed atomistic-continuum hierarchical multicale method which is based on the Bridging Domain Method and the Extended Finite Element Method.

$$\mathbf{u} = \sum_{\forall I} N_I \mathbf{d}_I + \sum_{J \in \mathcal{S}} N_J H\left(f\right) \mathbf{b}_J \tag{1}$$

where $\mathcal{S}$ is the set of all nodes with supports cut by the crack, N_I are the standard FEM shape functions and $H(\cdot)$ is the Heaviside step function and $\mathbf{d}_I$ and $\mathbf{b}_J$ are the standard and enriched nodal degrees of freedom.

We define a weight function $w\left(s\right)$ which is unity in Ω^C/Ω^λ and zero in Ω^A/Ω^λ. The weight function decreases linearly from unity at $\partial\Omega^A$ to zero at $\partial\Omega^C$. Let Π^C and Π^A be the total energy of the continuum and atomistic subdomains, respectively. Let Π^λ be the total energy due to the coupling of the atomistic and continuum domains. The total energy, Π, of the system is

$$\Pi = w\left(s\right)\Pi^C\left(\mathbf{u}\right) + \left(1 - w\left(s\right)\right)\Pi^A\left(\mathbf{r}^A\right) + \Pi^\lambda\left(\boldsymbol{\lambda}, \mathbf{u}, \mathbf{r}^A\right) \tag{2}$$

where $\mathbf{r}^A$ are the positions of the atoms and $\boldsymbol{\lambda}$ are the Lagrange Multipliers which enforce compatibility in Ω^λ. The governing equations are determined by finding the minimum of (2) with respect to $\mathbf{u}$, $\mathbf{r}^A$ and λ.

REFERENCES

[1] S.P. Xiao and T. Belytschko "A bridging domain method for coupling continua with molecular dynamics". *Computer Methods in Applied Mechanics and Engineering.*, Vol. **193**, 1645–1669, 2004.

[2] N. Moës, J. Dolbow and T. Belytschko "A finite element method for crack growth without remeshing". *Int. J. Num. Meth. Eng..*, Vol. **46**, 131–150, 1999.

[3] R. Gracie, G. Ventura and T. Beltyschko "A new fast method for dislocations based on interior discontinuities". *Int. J. Num. Meth. Eng.*, Vol. **69**, 423–441, 2007.

[4] R. Gracie, J. Oswald and T. Beltyschko "On a new extended finite element method for dislocations: core enrichments". *J. Mech. Physics Solids.*, doi=10.1016/j.jmps.2007.07.010, in press.