A Framework for Continuum-Atomistic Simulations of Crack Tip Plasticity

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1 ABSTRACT

Multiscale simulations of crack tip plasticity suffer from one significant limitation - as these simulations progress, large regions of the simulation domain are converted from continuum to atomistics to accommodate the evolution of dislocations. We will describe a new continuum-atomistic framework for modeling dislocations which allows one to retain atomic resolution in the near core region, without significantly increasing the number of degrees of freedom in the system. The framework combines the Bridging Domain Method (BDM) with the eXtended Finite Element Method (XFEM). The XFEM-BDM framework allows the coarse-graining of both regions where the atomistic displacements are homogeneous and where they are discontinuous by replacing large portions of the atomistic domain along the glide planes and crack by XFEM approximations. The framework will be compared to several direct numerical simulations and its advantages and limitations will be discussed.

2 INTROCUTION

Analyses of ductile fracture in which individual dislocations are resolved are leading to a more fundamental understanding of how materials fail. We describe here a continuum-atomistic model which maintains atomistic resolution at the dislocation cores while significantly reducing the number of atoms in the simulation by coarse-graining a significant portion of the dislocation slip. Our framework is depicted in Figure 1, which shows a dislocation emanating from a crack tip. The subdomains near the crack tip and the dislocation core are modeled by atomistics while the rest of the domain is modeled by a continuum. What is new about our framework is that the material separating the dislocation core and the crack tip subdomains is modeled by a continuum even though the displacement field is discontinuous.

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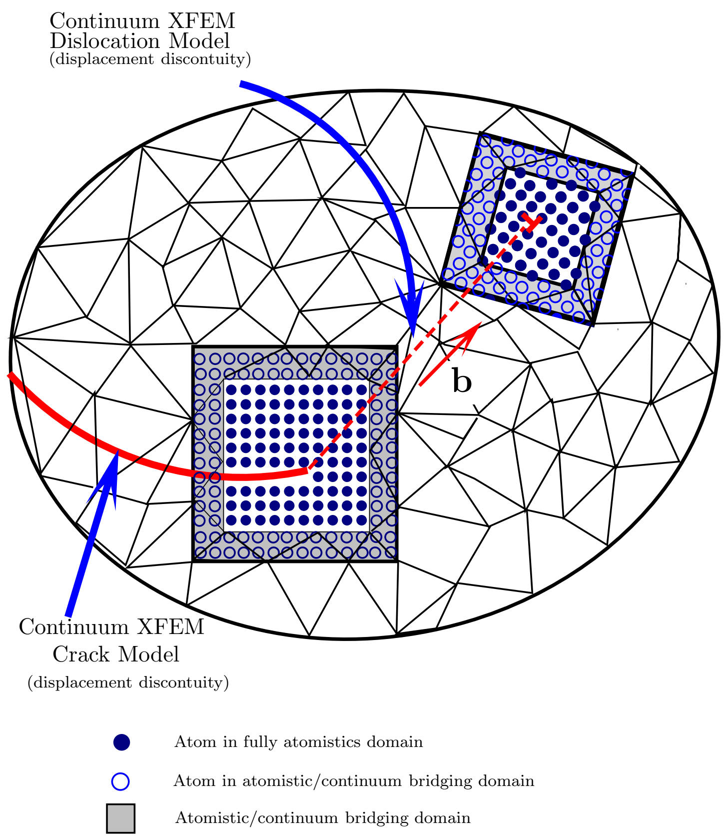

Figure 1 - Illustration of the continuum-atomistic model of crack tip plasticity [1].

At the mesoscale, dislocation dynamics simulations have provide useful insight into the dislocation networks which form near the crack tip of both single and poly-crystals. However, these models have been based on the superposition of isotropic linear elastic solutions of dislocations in infinite domain and as a result the behaviour at the dislocation cores is singular.

Fully atomistic simulations of fracture have lead to a better understanding of the early stages of ductile fracture. These simulations are computationally expensive an often rely on atomistic potential which are qualitative rather than quantitative. Further more, the domain sizes, of even the largest atomistic simulations performed to date, are too small to simulate the entire crack tip process zone.

Multiscale models, which concurrently combine continua and atomistics, have the potential to circumvent the limitations of both the dislocation dynamics and fully atomistic models. To date multiscale models of fracture have been largely focused on brittle fracture because dislocations which are nucleated at the crack tip tend to propagate towards the continuum-atomistic boundary. So, multiscale models of ductile materials must have the ability to adaptively expand the atomistic domain to follows the motion of the dislocations. This leads to a situation where the number of atoms in the model quickly becomes prohibitive.

Our framework combines the Bridging Domain Method (BDM) [1][2] with the eXtended Finite Element Method (XFEM) [3]. The BDM is a hierarchical overlapping domain decomposition scheme where compatibility between the atomistic and continuum domains is enforced using Lagrange Multipliers. Material far from dislocations cores is modeled as a continuum using the XFEM whereas Molecular Mechanics is used to resolve the near core behaviour and dislocation reactions. The XFEM-BDM framework allows the coarse-graining of both regions where the atomistic displacements are homogeneous and where they are discontinuous by replacing large portions of the atomistic domain along the glide planes by the XFEM dislocation approximation developed by Gracie et al. [4].

3 MODEL, DISCRETIZATION AND APPROXIMATION

Consider a domain Ω, decomposed into overlapping subdomains Ω^C and Ω^A, where a continuum and atomistic model are used, respectively. The coupling domain is denoted by $\Omega^B = \Omega^C \cap \Omega^A$. Let $\mathbf{u}^C(\mathbf{x})$ be the displacement field in Ω^C, W be the strain energy density of the continuum and W^{ext} be the work of external forces. Let $\mathbf{u}_i^A$ be the displacement of atom i, r_{ij} be the distance between atoms i and j and V_{ij} be the potential energy of the bond between atoms i and j. Furthermore, let $\boldsymbol{\lambda}(\mathbf{x})$ be the Lagrange multiplier field in Ω^B which enforces compatibility between Ω^C and Ω^A. The energies of the continuum and atomistic models are weighted in Ω^B, by a weight function $\alpha^C(\mathbf{x})$, which ensures that energy is not counted twice in Ω^B. The total energy of the system is given by

$$\Pi = \Pi^C - W^{ext} + \Pi^A + \left(\boldsymbol{\lambda}, \mathbf{u}^C - \mathbf{u}^A\right), \tag{1}$$

where

$$\Pi^C = \int_{\Omega^C} \alpha^C(\mathbf{x}) W\left(\mathbf{u}^C(\mathbf{x})\right) d\Omega, \tag{2}$$

$$\Pi^A = \sum_i \sum_{i \neq j} \left(1 - \alpha^C(\mathbf{x})\right) V_{ij}\left(r_{ij}\right) \tag{3}$$

and

$$\left(\boldsymbol{\lambda}, \mathbf{u}^C - \mathbf{u}^A\right) = \sum_{i \in \Omega^B} \boldsymbol{\lambda}\left(\mathbf{x}_i^A\right) \cdot \left(\mathbf{u}^C(\mathbf{x}) - \mathbf{u}_i^A\right). \tag{4}$$

The weight function $\alpha^C(\mathbf{x})$ ranges between 0 and 1; $\alpha^C(\mathbf{x})=1$ in $\Omega^C \setminus \Omega^B$ and $\alpha^C(\mathbf{x})=0$ in $\Omega^A \setminus \Omega^B$. In Ω^B, $\alpha^C(\mathbf{x})$ decreases monotonically from 1 in the fully continuum domain to 0 in the fully atomistic domain.

We now further consider that the domain contains several dislocations and cracks. We will assume that all dislocation cores and crack tips are located in the fully atomistic domain $\Omega^A \setminus \Omega^B$. Let the surfaces where dislocation slip has occurred be denoted by Γ_D. It is convenient to define Γ_D in terms of two level set $f(\mathbf{x})$ and $g(\mathbf{x})$, i.e.

$$\Gamma_D = \{\mathbf{x} \mid f(\mathbf{x}) = 0 \text{ and } g(\mathbf{x}) < 0\} \tag{5}$$

This definition is illustrated for a dislocation loop in Figure 2. The slip plane of the dislocation loop is defined by $f(\mathbf{x})=0$ and the portion of the slip plane where slip has occurred is defined by $f(\mathbf{x})=0$ and $g(\mathbf{x})<0$.

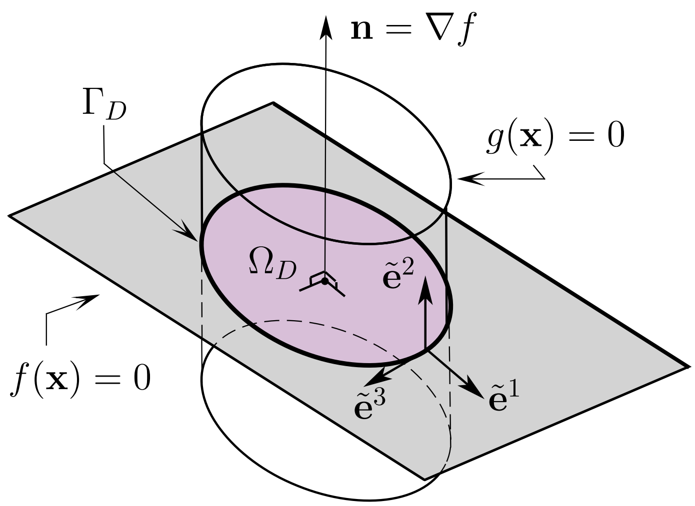

Figure 2 - Description of a dislocation loop by two level sets $f(\mathbf{x})$ and $g(\mathbf{x})$.

Similarly, cracks will be defined by the level sets $\phi(\mathbf{x})$ and $\psi(\mathbf{x})$ such that

$$\Gamma_C = \{\mathbf{x} \mid \phi(\mathbf{x}) = 0 \text{ and } \psi(\mathbf{x}) < 0\} \tag{6}$$

The continuum displacement approximation is decomposed into the standard finite element part $\mathbf{u}^{FE}(\mathbf{x})$ and an enrichment part $\mathbf{u}^{ENR}(\mathbf{x})$:

$$\mathbf{u}^C(\mathbf{x}) = \mathbf{u}^{FE}(\mathbf{x}) + \mathbf{u}^{ENR}(\mathbf{x}) \tag{7}$$

The standard finite element part is given by

$$\mathbf{u}^{FE}\left(\mathbf{x}\right)=\sum_{\forall I}N_I\left(\mathbf{x}\right)\mathbf{u}_I \tag{8}$$

where $N_I\left(\mathbf{x}\right)$ are the finite element shape functions and $\mathbf{u}_I$ are the nodal displacements. The enriched part of the approximation is given by

$$\begin{aligned}\mathbf{u}^{ENR}\left(\mathbf{x}\right)=\mathbf{b}\sum_{J\in \mathrm{S}^D}N_J\left(\mathbf{x}\right)\left[H\left(f\left(\mathbf{x}\right)\right)-H\left(f\left(\mathbf{x}_J\right)\right)\right]\\+\sum_{K\in \mathrm{S}^C}N_K\left(\mathbf{x}\right)\left[H\left(\phi\left(\mathbf{x}\right)\right)-H\left(\phi\left(\mathbf{x}_K\right)\right)\right]\mathbf{a}_K\end{aligned} \tag{9}$$

where $\mathbf{b}$ is Burgers vector, $\mathbf{x}_J$ is the position of node J, S^D and S^C are the nodes with supports cut by Γ_D and Γ_C, respectively. We note that the sets S^D and S^C are small subsets of all nodes on the mesh.

Remark 1: The enriched part of the continuum displacement Eq. (9) is the critical addition to the standard Bridging Domain Method, which allows the discontinuities of cracks and dislocations to be smoothly transferred from the atomistic domain to the continuum domain.

Remark 2: The first term on the right hand side of Eq. (9) allows dislocations to be modeled in the continuum independently of the mesh. Burgers vector $\mathbf{b}$ is assumed to be known, and so the dislocation part of the enrichment does not lead to any additional degrees of freedom in the continuum model. This is a standard assumption in mesoscale models of dislocations and is reasonable here since the near core slip which is non-constant in magnitude is modeled by the atomistic domain.

Remark 3: The second term on the right hand side of Eq. (9) allows cracks to be modeled in the continuum independently of the mesh. The parameters $\mathbf{a}_K$ are addition degrees of freedom at the nodes in S^C and the magnitude of the parameters is directly related to the crack opening displacement of the element connected to the nodes.

We will weakly enforce the compatibility constraint Eq. (4) by approximation the Lagrange Multiplies by a field, i.e.

$$\boldsymbol{\lambda}\left(\mathbf{x}\right)=\sum_{L}N_L^{\lambda}\left(\mathbf{x}\right)\boldsymbol{\lambda}_L,\mathbf{x}\in\Omega^B. \tag{10}$$

The discrete equations are obtained by finding the stationary point of Eq. (1) with respect to $\mathbf{u}_I,\mathbf{a}_k,\boldsymbol{\lambda}_L$ and $\mathbf{u}_\alpha^A$.

4 NUMERICAL EXAMPLES

We will student the problem of an edge crack in a grapheme sheet. Other examples of evolving dislocations will be presented at the conference; however, due to space limitations and in the interest of clearly describing our framework, we have restricted ourselves to a single illustrative example. Multiscale simulations of graphene sheets are well suited to demonstrate the usefulness of the overlapping domain decomposition scheme since the generation of meshes which conform to the lattice is difficult. Furthermore, the simulation of defected graphene with the coupled Bridging Domain Method and Extended Finite Element Method framework will demonstrate its robustness for complex lattice structures.

The second generation Tersoff-Benner REBO potential [5] is used to model the graphene at the atomic scale. Under a small displacement assumption, graphene is isotropic and the Lame constants are μ=5.428 eV and λ=7.148 eV .

We will compare the accuracy of the coupled XFEM-BDM method to a fully atomistic direct numerical simulations. For this purpose, the change in energy of the atoms in the fully atomistic domain due to applied loads relative to pristine unloaded sheets is considered. Let the relative error in the change in energy per atom be defined as

$$e_\alpha^U = \frac{\left|U_\alpha^A - U_\alpha^{DNS}\right|}{\max\limits_\alpha\left(U_\alpha^{DNS}\right)} \tag{11}$$

and the relative error in the change in energy in the subdomain $\Omega^A \setminus \Omega^B$ be defined as

$$e^U = \frac{1}{n^{AB}}\sqrt{\sum_{\alpha\in\Omega^B}\left(e_\alpha^U\right)^2} \tag{12}$$

where n^{AB} is the number of atoms in Ω^B and U_α^A is the change in the energy of atom α computed by the coupled model. U_α^{DNS} is the change in the energy of atom α from the direct numerical simulation, and $\max\limits_\alpha\left(U_\alpha^{DNS}\right)$ is the maximum change in the energy of an atom in the direct numerical simulation. We also examine the error in the displacements using similar measures of error

Consider a 247.18Å x 208.03Å graphene sheet as shown in Figure 3a; the origin of the domain is located at the center of the sheet. The sheet is oriented such that the zig-zag direction corresponds to the x-axis. A crack is created by deleting the bonds from the atomistic model which are cut by the line $y = 9.5$ Å for $x \in (\text{-}123.59, 10)$. The bottom edge of the domain is fully constrained. Displacement boundary conditions are applied to the top edge: $\bar{u}_x = 0.01 L_x$ and $\bar{u}_y = 0.01 L_y$, where $L_x = 247.18$ Å and $L_x = 208.03$ Å.

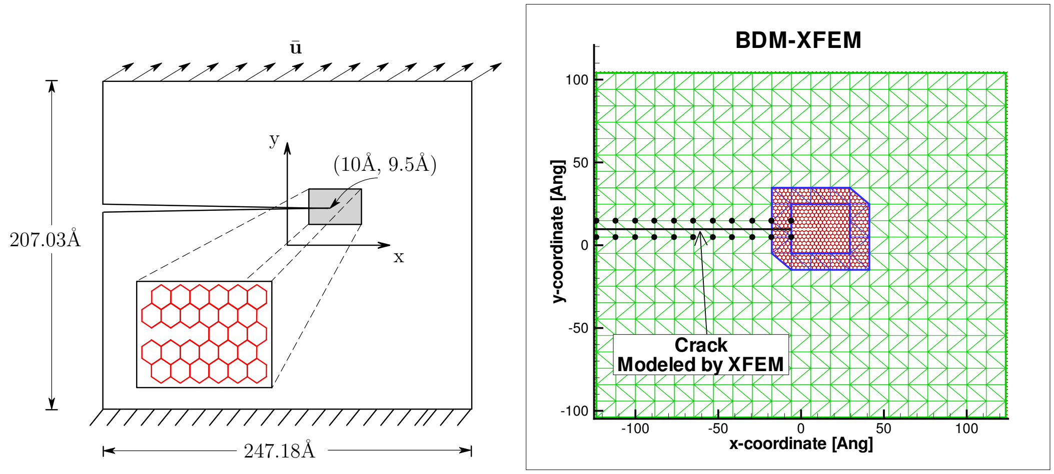

Figure 3 – a) Schematic of the problem of a graphene sheet with an edge crack. b) Domain decomposition and discretization of the problem of a graphene sheet with an edge crack for the combined Bridging Domain Method and Extended Finite Element Method model. Green and blue lines denote the FEM and the Lagrange multiplier meshes, respectively; Black disks represent Heaviside enriched nodes

The domain is discretized by a 21x21 triangular element mesh. We will compare the solution of the combined XFEM-BDM model to that obtained by direct numerical simulation using a fully atomistic model. Figure 3b shows the domain decompositions and discretization of the combined model; the purely atomistic subdomain, $\Omega^A \setminus \Omega^B$, consists only of the domain of the 18 elements surrounding the crack tip. So the bridging domain consists of the elements immediately surrounding the purely atomistic domain and the weight $\alpha^C(\mathbf{x})$ varies linearly from 0 to 1 within one element of the continuum.

In this example the zero contour of the function $\phi(\mathbf{x})$ which defines the location of the crack in the continuum is given by the problem description: $\phi(x, y) = \{x, y \mid x \in (123.59, 10), y = 9.5\} = 0$. In general, $\phi(\mathbf{x})$ must be determined from the atomistic displacements, i.e. from the location of the crack in the atomistic model, but in this problem it is straightforward. From $\phi(\mathbf{x})$ the set of Heaviside step function enriched nodes (those in set S^C) are determined. These are illustrated by black disks in Figure 3b.

We note that most concurrent multiscale models, such as the standard Bridging Domain Method and the Quasiconitnuum method, require atoms along the entire crack surface. In the combined XFEM-BDM model we can significantly reduce the number of atoms in the model by modeling a long portion of the crack by a discontinuity in the continuum model. This is accomplished by only 44 continuum enriched degrees of freedom. The enrichment of the continuum elements in the blending domain allows cracks to pass from the atomistic model to the continuum model.

Figure 4 shows the relative errors per atom from the combined XFEM-BDM model with respect to the direct numerical simulation for atoms in $\Omega^A \setminus \Omega^B$. The maximum relative error in the change in energy per atom is 5.5×10^{-2} and occurs at the crack tip while that the maximum relative error in the displacement of an atom is 7.8×10^{-2} and occurs at the bridging domain boundary. The error in the energy is highly localized while that in the displacements is more diffuse. The relative errors in the change in the energy and in the displacements of atoms in $\Omega^A \setminus \Omega^B$ are 3.6×10^{-4} and 4.2×10^{-3}, respectively. The displacement errors tend to localize at the coupling domain boundary likely because of ghost forces from the coupling constraint and because the strains in the continuum model are highest in the coupling domain and so the error induced by assuming that the continuum is linear elastic and isotropic are largest there. Other sources of error in the model come from free surface effects not captured by the continuum model. Theses occur along the vertical edges of the domain and along the crack surfaces. The loss in accuracy from the homogenization of the crack is not significant given the reduction in the number of degrees of freedom - the combined XFEM-BDM model uses only 1254 free atoms compared to the 19788 atoms used in the direct numerical simulation.

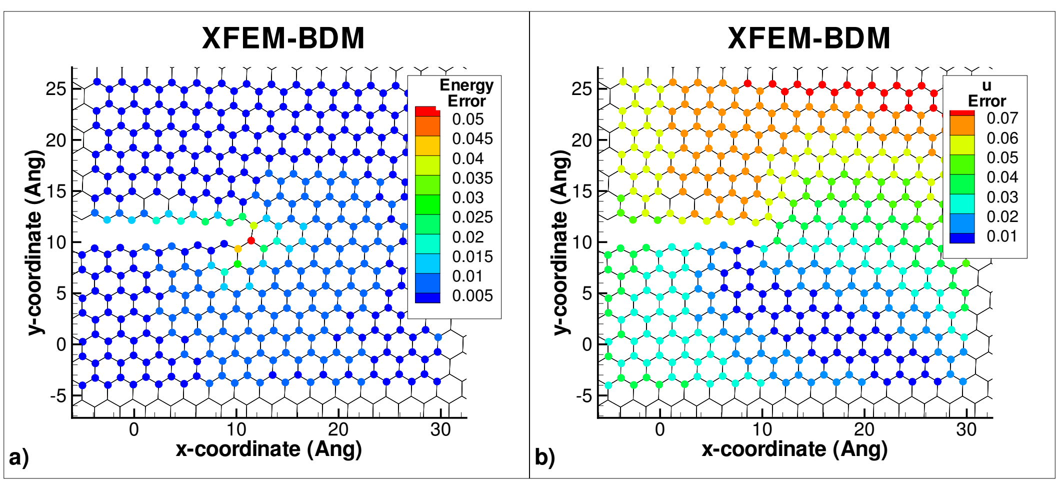

Figure 4 - Relative errors per atom of atoms in $\Omega^A \setminus \Omega^B$ of the combined Extended Finite Element Method and Bridging Domain Method model. a) Relative error in the change in energy per atom b) Relative error in the displacement per atom

5 Conclusions

We have developed a concurrent multiscale method for coupling atomistics and continua when the deformations at the continuum level corresponding to the atomistic phenomena are discontinuous, i.e. in the presence of dislocations and cracks. The framework is based on the Bridging Domain Method, where compatibility between overlapping continuum and atomistic domains is enforced by Lagrange multipliers. The key contribution of this work is the coupling of the Extended Finite Element Method with the atomistic model. This allows for discontinuities in the atomistic domain to be effectively passed into the continuum domain.

In our framework, atomistic models of material behaviour are used in the region near crack tips and dislocation cores; whereas a continuum model is adopted in the rest of the domain. The discontinuity due to a crack is incorporated into the continuum model by enrichment of the standard Finite Element Method approximation by the Heaviside step function. Similarly, slip across the glide plane in the continuum domain is modeled by a tangential step function enrichment.

Though we have applied the method to several problems; due to space limitations here, only the results for an edge crack under mixed mode loading are presented - further results will be present at the conference. The simulation using the combined Bridging Domain Method and Extended Finite Element Method (XFEM-BDM) was compared to direct numerical simulations (DNS) by fully atomistic models. It is shown that the accuracy of the XFEM-BDM is acceptable given the large reduction in the number of degrees of freedom. In the example considered here, the continuum model was linear but the XFEM-BDM model can be easily extended to a nonlinear hyperlastic constitutive model based on a Cauchy-Born approximation.

In traditional concurrent multiscale simulations, discontinuities from cracks and dislocation slip must be represented by the atomistic model. In contrast, the new method described here allows large portions of these discontinuities to be represented by a continuum. Therefore, a significant reduction in the number of atomistic degrees of freedom is possible. Furthermore, the numerical examples presented here show that this can be accomplished without compromising atomistic resolution and accuracy in the near crack tip or dislocation core regions.

6 REFERENCES

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