On a new method for modelling dislocations

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1. Introduction

A newly developed method, [1], for modelling dislocations is applied to problems involving the interaction of dislocations with arbitrary interfaces. Dislocations are modeled in a manner akin to the Volterra dislocation model where a dislocation is defined by cutting the material, displacing the two sides of the cut and reattaching the two surfaces. The method is based on the extended finite element method (XFEM), [2]. Discontinuities are explicitly introduced into the domain through a prescribed enrichment of the standard finite element approximation.

In contrast to the behaviour of dislocations in bulk materials, the behaviour of dislocations in micro and nano scale systems depends greatly on the interaction of dislocations with both domain boundaries and material interfaces. Most dislocation models are base on Green's functions for a dislocation in an infinite isotropic domain. It is known that the use of isotropy versus anisotropy can introduce errors of about 20-30% in many applications, [3]. However, there are a limited number of Green's functions for dislocations in anisotropic material for systems with material interfaces. The difficulty of applying existing dislocation models in applications involving material interfaces is the motivation for this work.

Here we will limit ourselves to isotropic materials however the method can be easily adapted for anisotropic materials, simply by using an anisotropic elasticity tensor. We will also only consider examples with edge dislocations; however, the method may equally be applied to other types of dislocations in 3 dimensions.

2. Model and Governing Equations

We define the geometry of an edge dislocations by two affine functions, $f(x)=\alpha_o+\alpha_i x_i$ and $g(x)=\beta_o+\beta_i x_i$, such that the glide plane of the dislocations is defined by $f(x)=0$ and $g(x)>0$.

In XFEM the standard finite element approximation is extended by what is known locally about the solution. In this case the discontinuity across the glide plane. In what follows we consider only a single dislocation for simplicity. The general formulation for n_D dislocations can be found in [1]. We decompose the displacement field approximation into a continuous part $\mathbf{u}^C(x)$ and a discontinuous part $\mathbf{u}^D(x)$, i.e.

$$\mathbf{u}(x)=\mathbf{u}^C(x)+\mathbf{u}^D(x) \tag{1}$$

where $\mathbf{u}^C(x)$ is the standard finite element approximation and

$$\mathbf{u}^D(x)=\mathbf{b}\sum_{I\in S} N_I H\left(f(x)\right)H\left(g(x)\right) \tag{2}$$

where N_I are the standard finite element shape functions, $\mathbf{b}$ is Burgers vector and $H(\bullet)$ is the Heaviside step function

$$H(z)=\begin{cases} 0, & z<0 \\ 1, & z>0 \end{cases} \tag{3}$$

S is the set of all nodes with supports cut by the glide plane of the dislocation. Note that S is a small subset of the total nodes in the domain so the additional computational cost of including the discontinuity is small. The enrichment (2) introduces a tangential jump across the glide plane with magnitude and direction of Burgers vector.

The discrete finite element equations are then determined by the substitution of (1), (2) and (3) into the standard weak form of the equilibrium equation. In the case of linear elasticity this yields a system of equations of the form

$$\mathbf{Ku}=\mathbf{f}^{ext}-\mathbf{f}^{D} \tag{7}$$

where $\mathbf{K}$ is the standard finite element stiffness matrix, $\mathbf{f}^{ext}$ is the nodal forces due to the external tractions and $\mathbf{f}^{D}$ is the nodal forces due to the dislocation. The effect of the dislocations is reduced to a nodal force because the Burgers vector $\mathbf{b}$ is known for a given dislocations and material. So the discontinuous enrichment introduces no additional degrees of freedom. As a result, the model is easily incorporated into most existing linear FEM commercial codes because only an addition nodal force needs to be defined. Note, that no limitations have been place on the elasticity matrix; it can be either isotropic or anisotropic.

3. Examples

3.1 Dislocation near a Bimaterial Interface

To demonstrate the numerical accuracy of the method we consider an edge dislocation near a bimaterial interface between two semi-infinite domains, as shown in Figure 1.

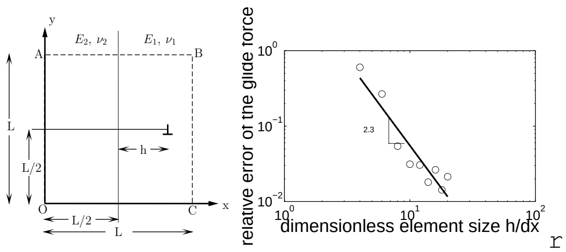

Figure 1. Left: edge dislocation near a bimaterial interface. Right: convergence of the proposed method.

The bimaterial interface is located along the plane $x=L/2$. An edge dislocation with Burgers vector $b=0.8551$ nm and with a glide plane along the plane $y=L/2$ is considered. The core is located at $x=L/2+h$. In the subdomain $x>L/2$ the elastic modulus $E_1=121$GPa and Poisson's ratio $\nu_1=0.34$; in the subdomain $x<L/2$ $E_2=0.1E_1$ and $\nu_2=0.3$.

Figure 1 (right) shows the convergence of the method for 3-node constant stress elements. An excellent convergence rate is obtained.

3.2 Interaction of Dislocations with an Inclusion

In this example the ability of the method to model the interaction of many dislocations with an arbitrary material interface without the need to introduce additional assumptions is illustrated. For this purpose, we consider a body with an inclusion, as shown in Figure 2. The inclusion is centered in a domain with dimensions $1\mu\text{m}\times 1\mu\text{m}$ and has a radius of $0.1\mu\text{m}$. The material parameters of the inclusion are $E_1=121$GPa and $\nu_1=0.3$ and of the bulk material are $E_2=10$GPa and $\nu_2=0.2$.

We consider 40 dislocations with Burgers vector $b=0.3$ nm distributed randomly on 8 evenly distributed horizontal slip planes. The domain is discretized by 13000 linear triangular elements. We rigidly constrain the bottom surface of the domain and apply a shear displacement $u_x = 0.01\mu m$ to the top surface. The resulting shear stress contours are shown in Figure 2.

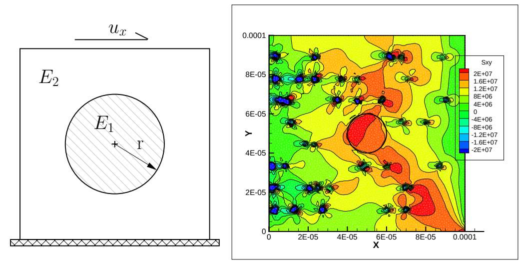

Figure 2. Left: Illustration of the problem of a body with an inclusion. Right: Shear stress contours showing the interaction of 40 dislocations with an inclusion.

4. Conclusions

A method for modelling dislocations based on the extended finite element method (XFEM) has been applied to problems involving material interfaces. In the method dislocations are modeled by prescribed discontinuities on internal surfaces. Here edge dislocations in two dimensions and isotropic materials were modeled; however, the method can equally be applied to more complicated dislocation loops in three dimensions and to anisotropic materials.

The simulation of an edge dislocation near a bimaterial interface shows that the method has an excellent rate of convergence. The modelling of an inclusion in a bulk material illustrated the application of the method to problems of dislocation interaction with arbitrary interfaces.

The integration of XFEM based dislocation models into dislocation dynamic simulations is expected to be beneficial for the simulation of dislocations interaction with material interfaces between anisotropic materials.

Acknowledgements

This work was supported by a Graduate Scholarship from the Natural Sciences and Engineering Research Council of Canada.

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