AN INVESTIGATION INTO THE METHODS FOR MODELLING PRE-EXISTING CRACKS IN PHASE FIELD PROBLEMS

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Abstract. Phase field (PF) models are an increasingly popular method of numerically modelling fracture problems. While research has focused on the practical applications and computational efficiency of PF methods, little discussion exists around the merits of different methods of prescribing initial cracks in PF fracture problems. This paper presents a comparison of three methods for modelling pre-existing cracks, through Dirichlet-type PF boundary conditions, an initial strain history term, and through physical discontinuities in the mesh. The comparison is made using the load-displacement responses for a common tensile benchmark fracture problem.

Key words: *fracture; phase field; finite element method*

1 Introduction

Phase field (PF) models are an example of a diffused approach to fracture simulation, which have gained popularity in recent years. This method is made possible by Francfort and Marigo [1] revisiting Griffith's energy-based fracture theory [2] and reforming it as an energy minimisation problem. The subsequent regularisation of this approach by [3] and [4] has allowed for the development of PF models for brittle fracture which allow fracture problems to be solved numerically, typically using the finite element method (FEM), with accurate models for crack propagation, nucleation and branching.

Much of PF research has focused on practical applications and reducing the computational expense of such simulations. In literature, benchmark problems presented often include initial cracks which then propagate during the simulation. In order to prescribe the initial cracks in these problems, different approaches have been used. Some prescribe a PF value at the crack, some use an initial strain history field to represent the crack, and others prescribe the crack through the geometry of the mesh [4, 5]. While these methods exist, there is little discussion in the literature as to the impact of the methods on the accuracy and efficiency of simulations. In this paper, an investigation into the effect of the different methods of prescribing initial cracks is presented.

2 Phase Field (PF) Fracture

An arbitrary domain $\Omega \subset \mathbb{R}^n$ where $n \in \{1,2,3\}$ with the boundary $\partial\Omega$ is considered, on which a coupled elasticity and fracture problem is solved. This section focuses only on the solution to the fracture problem. The boundary is subject to Neumann or Dirichlet boundary conditions on $\partial\Omega_N$ and $\partial\Omega_D$ respectively, where $\partial\Omega_N \cup \partial\Omega_D = \partial\Omega$ and $\partial\Omega_N \cap \partial\Omega_D = \emptyset$. The fracture surface can be considered an internal discontinuity boundary Γ.

In Griffith's theory [2], for a quasi-static brittle fracture process, the elastic strain energy released during fracture growth must be balanced by the energy required to generate new fracture surfaces. Following

the work of Francfort and Marigo [1], this can be stated in variational form

$$\Pi = \int_\Omega \psi(\boldsymbol{\varepsilon})\, dV + \int_\Gamma G_c\, d\Gamma \tag{1}$$

where Π is the total potential energy functional of the body, which should be minimised to solve for the fracture path. $\psi(\boldsymbol{\varepsilon})$ is the elastic strain energy density, $\boldsymbol{\varepsilon}$ the strain tensor and G_c is the rate of energy required per incremental increase in crack surface area. It is however challenging to minimise the functional Π in its current state due to the difficulty in tracking and integrating over the evolving fracture surface Γ. A scalar phase field variable ϕ is therefore introduced to diffuse the discrete crack over an approximate volume, where $\phi = 0$ represents intact material, and $\phi = 1$ for fully cracked material.

A monotonically decreasing function $g(\phi) = (1-\phi)^2$ is used to degrade the material's stiffness as in [4]. The energy functional is therefore reformed as

$$\Pi_l = \int_\Omega (1-\phi)^2\, \psi(\boldsymbol{\varepsilon})\, dV + G_c \int_\Omega \frac{1}{2l}\phi^2 + \frac{l}{2}|\nabla\phi|^2\, dV \tag{2}$$

where l is the length scale which influences the regularisation of the crack surface and $\nabla\phi$ corresponds to the spatial gradient of the PF value.

Following the approach of [6], differences in fracture propagation in tensile and compressive loading are accounted for by decomposing the strain energy density into tensile $\psi^+(\boldsymbol{\varepsilon})$ and compressive $\psi^-(\boldsymbol{\varepsilon})$ components through spectral decomposition of the strain tensor. To ensure damage irreversibility a strain history term $\mathcal{H}$ is introduced which tracks the maximum tensile strain energy density over time or quasi-time t such that $\mathcal{H} = \max_{t\in T}(\psi_t^+(\boldsymbol{\varepsilon}))$ where T denotes the total time domain. Substituting $\mathcal{H}$ for $\psi^+(\boldsymbol{\varepsilon})$ in (2), the Euler-Lagrange equations are used to obtain the strong form equations for the PF

$$\begin{aligned} \left(2\mathcal{H} + \tfrac{G_c}{l}\right)\phi - G_c l \Delta\phi = 2\mathcal{H} \qquad & \text{in } \Omega \\ \nabla\phi \cdot \mathbf{n} = 0 \qquad & \text{on } \partial\Omega_N \\ \phi = g_D \qquad & \text{on } \partial\Omega_D \end{aligned} \tag{3}$$

where $\mathbf{n}$ is the outward normal to the boundary $\partial\Omega$, g_D is the imposed PF value on the Dirichlet boundary and $\Delta\phi$ is the Laplacian of the PF. The discretised weak form of these equations and the coupled elasticity equations are solved using standard FEM with a staggered scheme as in [6].

3 Prescribing Initial Cracks

The three methods that have been used in literature to prescribe initial cracks in PF problems are described in this section. The first option is through imposed Dirichlet-type boundary conditions for the PF along the initial crack surface, as described in [4]. Here, a value of $\phi = 1$ is imposed along Γ.

The second method uses an initial strain history field $\mathcal{H}_0$ to model initial cracks as described in [5]. Taking L to represent the line of the discrete initial crack, the function $d(\mathbf{x}, L)$ represents the distance from $\mathbf{x}$ to L, where $\mathbf{x}$ represents a position in the domain Ω. Through substitution of $\Delta\phi = 0$ and $\phi \approx 1$ into equation $(3)_1$ and considering the history term to linearly decay with distance from the crack, $\mathcal{H}_0$ is obtained.

$$\mathcal{H}_0 = C \begin{cases} \frac{G_c}{2l}\left(1 - \frac{d(\mathbf{x},L)}{l}\right) & d(\mathbf{x},L) \le l \\ 0 & d(\mathbf{x},L) > l \end{cases} \tag{4}$$

The constant $C = (\frac{1}{\phi} - 1)^{-1}$. ϕ must be chosen as close to, but not equal to 1 to avoid division by 0. In this paper it is chosen that $\phi = 0.999$.

The final option is to prescribe initial cracks through a physical crack or discontinuity in the mesh.

4 Results and Discussion

The three methods described above are applied to a benchmark problem of a unit square specimen with an initial single edge crack as in Figure 1, based on the test in [4, 6]. The specimen is tested subject to tensile loading with the upper side displaced by $u = 6 \times 10^{-3}$mm over 1500 load steps, where the first 500 load steps apply displacement increments of $\Delta u = 1 \times 10^{-5}$mm and in the subsequent load steps $\Delta u = 1 \times 10^{-6}$mm. Linear triangular elements are used to mesh the domain, with an element size of $h = 0.01$mm. The length scale is set as $l = 0.02$mm, satisfying the condition $h \leq l/2$ as in [4]. The load-displacement response of the specimens with the three methods is shown in Figure 2.

The load-displacement responses are significantly different across the three methods. The PF boundary condition produces a response which is initially too stiff, as although $\phi = 1$ at the crack, the Gauss points adjacent to the crack are not fully damaged, resulting in incomplete degradation of the material stiffness. Once the Gauss points become fully damaged as load is applied, a drop in stiffness occurs. This effect is highly dependent on the length scale relative to the mesh size - length scales much larger than the mesh size are required to eliminate the erroneously high initial stiffness. This either reduces the accuracy or increases the computational expense, depending on if the length scale is increased or the mesh size reduced. The method also requires the initial crack to coincide with the mesh nodes, and is therefore more difficult to implement with complex crack geometries.

The initial history field and mesh discontinuity methods produce more realistic results. However, the mesh discontinuity method produces a stiffer response and one that more closely matches the reference solution for this problem in [6]. This is due to the fact that the initial history field method smoothes the initial crack, thus producing what is effectively a wider notch in the material. To approach a discrete crack with close to zero thickness, this method therefore requires a smaller length scale and hence a finer mesh, increasing computational expense. The advantage of the initial history field over the mesh method is, however, that this allows initial cracks to be specified without reference to the mesh, meaning complex crack geometries can be specified more easily.

5 Conclusions

A comparison of the impact of using different methods for prescribing initial cracks for a simple PF problem has been presented. Given the same mesh size and length scale, prescribing cracks through physical discontinuities in the mesh gives the most accurate result. Using an initial history field to model pre-existing cracks gives reasonable results and has the advantage of being the most straightforward to implement with complex crack geometries. However, it requires finer meshes and smaller length scales to give the same accuracy as the mesh discontinuity method, and therefore comes at greater computational expense. Using a Dirichlet-type boundary condition for the PF value performs poorly and is difficult to implement with complex crack geometries.

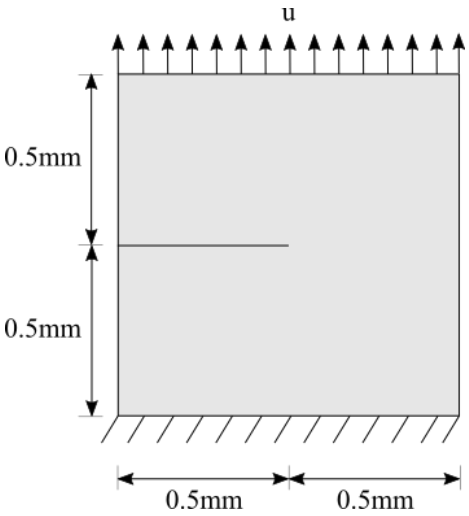

Figure 1: Geometry and boundary conditions for single edge notched tension test.

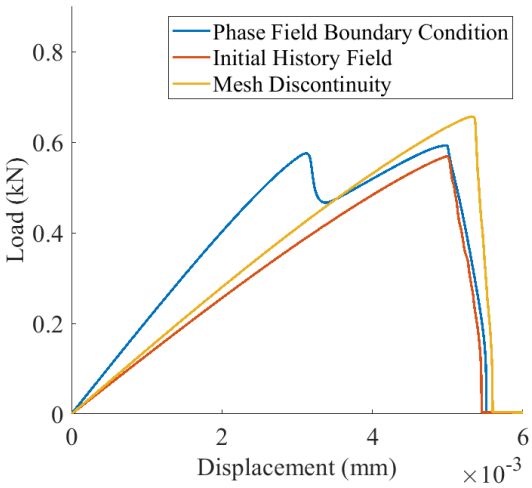

Figure 2: Load-displacement responses of single edge notched tension test.

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