Bridging variational and perturbation approaches in brittle fracture: application to shear crack in heterogeneous media

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Abstract

Modeling three-dimensional crack propagation in perfectly brittle materials is challenging due to the distribution of strong stress concentrations localized in the vicinity of a propagating crack front. In the presence of heterogeneities, crack propagation has been shown to be highly intermittent and to display multi-scale behavior, spanning from the heterogeneity size up to the size of the structure (Bonamy and Bouchaud, Phys. Rep., 2011). The numerical modeling of fracture processes is usually conducted using XFEM (Moës et al., IJNME, 1999) or the phase-field method (Bourdin et al., J. Elast., 2008). Both methods effectively address a wide range of scientific problems: while XFEM helps to handle complex (viscoplastic, hydromechanical, etc.) material behavior using enriched elements around the crack front, the phase-field method provides a variational framework capable of modeling fracture processes, from crack initiation to multiple crack interactions. These methods are computationally intensive, making 3D simulations of composites with numerous heterogeneities impractical without high-performance computing.

The perturbation approach of LEFM, initiated by Rice (J. Appl. Mech., 1985), has proven to be relevant to solving this class of problems because the 3D fracture process is modeled from the meshing of the sole 1D crack front. However, these studies rely on ad-hoc viscous regularization of Griffith's criterion, which may impact the fracture process itself and the apparent fracture behavior (Barés et al., PRL, 2014). In addition, simulations are often conducted for semi-infinite cracks propagating in tensile mode I (Patinet et al., PRL, 2013). Yet, cracks are often of finite size, and they can be loaded in mixed (tensile and shear) modes I+II+III. As a result, the influence of heterogeneities, size effects, and mode mixity on three-dimensional crack is not yet fully understood.

In this work, we consider an isotropic linear elastic body with an initial circular crack embedded within a plane. To model the coplanar propagation of a *sharp* crack, we propose to bridge the variational approach of Francfort and Marigo (JMPS, 1998) and the perturbation theory of Gao (IJSS, 1988) within a unified energetic framework. In this method, equilibrium positions are computed by minimizing the sum of the potential energy of the

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system, which relates to the crack geometry, and the dissipated energy, determined by the (heterogeneous) fracture energy field. Unlike previous approaches based on the resolution of Griffith's criterion through asymptotic estimates of the energy release rate, our energetic method instead builds on the asymptotic estimates of the potential energy of an arbitrarily perturbed configuration. The latter is efficiently computed by meshing only the crack front and using FFT to accelerate calculations. However, the physics of the rupture process imposes three strong constraints on the minimization process: namely (i) crack irreversibility, (ii) the existence of long-range (non-local) elastic forces, and (iii) the inability of the crack to overcome fracture energy barriers larger than its instantaneous energy release rate. To address these constraints, we implemented a (i) *bounded* Newton conjugate gradient method with (ii) *matrix-free* implementation and (iii) *trust region*, using PETSc and its Python wrapper petsc4py. Further speed-up is achieved by *preconditioning* the Hessian matrix with the inverse of the Hessian of a circular penny-shaped crack, propagating in a homogeneous medium, and (ii) leveraging JAX for *automatic differentiation* and *just-in-time compilation*. The final code is benchmarked on simple problems, for which analytical solutions can be derived. It displays remarkable numerical efficiency when applied to randomly heterogeneous problems.

Using our newly developed method, we have conducted 36,000 large-scale simulations of shear crack propagation in several weeks. The largest simulation has been performed on a field with high fracture energy contrast, with a seed crack starting below the heterogeneity scale and extending over three orders of magnitude with a time stepping corresponding to the crack propagation along 1/100 of heterogeneity. It typically requires 8 hours on a single core computer. We demonstrate how modes II+III coupling affects front deformations and apparent fracture energy, depending on heterogeneity properties and Poisson's ratio. Simulations reveal material weakening or strengthening based on disorder intensity and crack size: small heterogeneity contrasts weaken the material, while larger disorder intensities strengthen it, possibly due to front instabilities during crack propagation at higher disorder intensities and larger crack sizes.