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Peridynamics damage model through phase field theory

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ABSTRACT

We attempt a reformulation of the phase field theory in the framework of peridynamics (PD) to arrive at a continuum damage model. This obtains a better criterion for bond breaking in PD, marking a departure from the inherently ad-hoc bond-stretch-based or bond-energy-based conditions and thus allowing for the body to physically break into parts which a phase field model cannot by itself accomplish. Moreover, posed within the PD setup, the integral equation for the phase field eases the smoothness restrictions on the field variable. Taking advantages from both the worlds, the proposed scheme thus offers a better computational approach to problems involving cracks or discontinuities. Starting with Hamilton's principle, an equation of the Ginzburg-Landau type with dissipative correction is arrived at as a model for the phase field evolution. A constitutive correspondence route is followed to incorporate classical constitutive relations within our PD model. Numerical simulations of dynamic crack propagation (including branching) and the Kalthoff-Winkler experiment are also provided. To demonstrate how the model naturally prevents interpenetration, a mode II delamination simulation is presented. A brief discussion on the convergence of PD equations to the classical theory is provided in Appendix I.

1. Introduction

Computational models for fracture prediction and propagation are of current interest in the continuum mechanics of solids. Since material fracture could set off catastrophic effects, importance is naturally accorded to predicting fracture with high precision under various loading conditions. Cracks typically imply material discontinuities and, therefore, problems of crack initiation or propagation do not directly fall under the ambit of continuum formulations without warranting a special treatment. Many theories are however in place to address this problem. One such class of techniques considers cracks as sharp discontinuities in the displacement field or geometry; e.g. extended finite element method (X-FEM) and virtual crack closure technique (VCCT). Cohesive zone modelling (CZM) is another approach that is widely used to numerically simulate damage in the form of cracks or delamination. In all these cases, the crack path has to be defined *a priori*. Simulations of more complex problems such as dynamic crack branching are thus not easy with these methods.

The phase field method, which has of late attracted interest, has the ability to predict spontaneous emergence and propagation of cracks with the added attraction of mathematical simplicity. Here cracks are represented using a supplementary continuous scalar field variable called the phase field (order) parameter, $s \in [0, 1]$ used to distinguish between the damaged and undamaged parts of the material. A sharp crack may be smeared out by a continuous transition of the phase field, considered as a bulk parameter. The evolution equation of the phase field is coupled with the governing momentum balance equations in continuum mechanics. The resulting system of coupled partial differential equations (PDEs) models the problem and is solved to get the displacement, stress and phase field parameter.

Phase field models can be classified according to the viewpoint. There are physically based models which are founded on the Ginzburg-Landau type phase transition theory and the ones based on Griffith's theory [31]. A large body of work is available, including the early attempt by Francfort and Marigo [16], who proposed a variational model for quasi-static crack evolution. Though conceptually close to Griffith's theory of brittle fracture, this model did overcome a major limitation of Griffith's theory: need for a pre-existing crack and a well-defined crack path. Crack regularization in this model was inspired by the work of Ambrosio and Tortorelli [3]. Other related works in the area of brittle fracture based on a phase field are due to Bourdin et al. [6], Hakim and Karma [18], Borden et al. [5], Hofacker and Miehe [19], Kuhn and Müller [23], Verhoosel and Borst [42], Schlüter et al. [30] and Schneider et al. [31]. Bourdin et al. [6] suggest a discrete time model for dynamic fracture based on crack regularization. They establish that phase field models are better than the free discontinuity sets for modelling fracture. Hakim and Karma [18] provide methods to derive the laws of crack motion by a generalization of Eshelby's tensor in the context of phase field models. Miehe et al. [25,26] provide phase field models which are thermodynamically consistent. They derive

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incremental variational principles and use multi-field finite element method for its numerical implementation. In another paper, Miehe et al. [25,26] develop a robust algorithm based on operator splitting for numerical time integration. Kuhn and Müller [23] interpret phase field as an order parameter and propose a Ginzburg-Landau type evolution equation for the phase field. To analyse the dynamic effect on crack growth, Schlüter et al. [30] extend Kuhn and Müller's [23] work to the dynamic case. Starting with Hamilton's principle, they derive a set of coupled Euler-Lagrange equations for displacement and the phase field and numerically solve them using the finite element method. Borden et al. [5] also use Hamilton's principle and extend the quasi-static phase field model to the dynamic case. They present a monolithic and staggered numerical time integration scheme. For spatial integration, they develop a local adaptive refinement strategy based on locally refined T-splines. Hofacker and Miehe [19] propose a computational framework for diffusive fracture in dynamic problems with a view to capturing complex evolving crack topologies and extend the operator split scheme proposed by Miehe et al. [25,26] from quasi-static to dynamic case. All these different variants of the phase field approach involve working with derivatives and thus require adequate smoothness of the field variables.

On the other hand, the peridynamics (PD) - a nonlocal continuum theory proposed by Silling [35] - by design involves no spatial derivatives of field variables and is thus a powerful tool to study emergence and propagation of cracks. The governing equations are of the integro-differential type (and not PDEs), an aspect that allows for an easy tracking of discontinuities. The PD considers finite-distance interaction among material particles and is therefore a nonlocal theory. The finite neighbourhood in which the interaction remains restricted is referred to as the horizon. There are a couple of variants of the PD theory, viz. bond based and state based. State based PD can be of ordinary or non-ordinary type. In bond based PD, force in a bond connecting two interacting particles depends only on the deformation of that bond and acts along the bond. For linear isotropic elastic solids, this results in restrictive Poisson's ratios of 1/4 and 1/3 respectively for plane strain and plane stress cases. Ordinary state based PD offers a generalization by allowing the force in a bond to depend on the collective deformation of all the bonds in the horizon. Here again, the direction of the force vector in a bond is the same as the bond direction. Non-ordinary state based PD is a generalization of ordinary state based PD wherein the direction of the force vector is not restricted along the bond direction. Unavailability of PD based constitutive equations is however a more serious issue that may limit the usefulness of the PD almost to that of a mesh-free discretization scheme [33]. In the absence of such constitutive models, a method of constitutive correspondence for incorporating classically known constitutive equations within the PD has been suggested by Silling et al. [37].

The aim of this work is to reframe the phase field theory within a PD-based setup, considered ideal in the numerical simulation of material fragmentation. Incorporating the phase field to describe damage evolution (using integro-differential equations characteristic of a PD model) provides for a rational basis for 'bond breaking' (or bond snapping) and does away with the ad hocism in a criterion based on bond stretch or bond energy [11,36,7]. Indeed, a phase field typically represents a bulk measure of damage with a crack or discontinuity regularized through a smooth field and, on its own, it cannot display physical discontinuities. Moreover, gradient/divergence terms in the usual evolution laws of a phase field model could be a source of inconsistency with the onset of material discontinuity. We may therefore anticipate that the notion of phase field embedded within the PD should ameliorate these limitations inherent in the stand-alone versions of the PD and the phase field theory. Starting with a Hamilton's principle, we write the Lagrange density in the PD framework and thus derive the governing equations of the PD phase field by incorporating a dissipative relaxation term. In the absence of PD constitutive equations, we adopt constitutive correspondence to exploit classical constitutive equations in the PD. We assess the performance of our proposal by the numerical simulation of a dynamic crack propagation/branching problem and of the Kalthoff-Winkler experiment. The simulation results correlate well with experimental observations reported in the literature. For further illustration on the capability of our approach, we consider a mode II delamination problem where a major challenge is to prevent matter interpenetration. Presently, this problem is handled in PD by ad-hoc short range forces (see [36]) and also through nonlocal Seth-Hill measures of strain, which being nonlinear makes the computation complicated whilst being unsuited to the incorporation of different types of classical constitutive equations in non-ordinary state based PD. Our approach in contrast provides for a computationally simpler alternative to prevent interpenetration by its very construction.

The rest of the article is arranged as follows. In Section 2, recaps of the phase field and non-ordinary state based PD theories are presented. Section 3 reformulates the phase field equation in the framework of PD. A criterion is suggested for bond breaking in Section 4. The issue of the prevention of matter interpenetration is taken up in Section 5. Numerical simulations are given in Section 6 for a dynamic crack branching problem and for the well-known Kalthoff-Winkler experiment. For demonstrating prevention of matter interpenetration, simulation of a mode II delamination problem is presented next. The work is concluded in Section 7. A brief discussion on the convergence of PD equations to classical theory is included in Appendix A.

2. Phase field theory and non-ordinary state based PD

A brief review of the phase field theory including equations of motion, boundary conditions and constitutive relations are furnished below (see [19,30]). Non-ordinary state based PD following Silling et al. [37] is also briefly recapitulated.

2.1. Phase field theory

The phase field model introduces a regularized, diffusive representation of a sharp crack topology [25,26]. Consider a reference configuration $\Omega \subset \mathbb{R}^n$, surface $\partial\Omega \subset \mathbb{R}^{n-1}$ and time interval $T \subset \mathbb{R}$, with n either 2 or 3 depending on the spatial dimension of the body (see Fig. 1). To characterize the state of the body, we introduce the displacement vector field $(\mathbf{u}(\mathbf{x}, t))$ and a phase field or an order parameter scalar field $(s(\mathbf{x}, t) \in [0, 1])$. The value of s is 1 in the undamaged material and 0 in the fully damaged material.

Crack surface is approximated by a crack functional (Kuhn and Muller [23])

$$\Gamma \approx \int_\Omega \left[\frac{(1-s)^2}{4l} + l\,|\nabla s|^2 \right] dV \tag{1}$$

Here l is a length scale parameter associated with the gradient of the phase field. (see Fig. 1). Assuming the critical energy release rate (G_c) to be independent of the crack velocity, fracture energy may be approximated as:

$$\int_\Gamma G_c\, dA \approx \int_\Omega G_c \left[\frac{(1-s)^2}{4l} + l\,|\nabla s|^2 \right] dV \tag{2}$$

Assuming displacement gradients to be small, the small strain tensor is written as:

$$\boldsymbol{\varepsilon} = \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^T}{2}. \tag{3}$$

The Lagrange density per unit volume is given by:

$$\mathcal{L} = \psi_k - \psi_e - \psi_s \tag{4}$$

where the kinetic energy density (ψ_k), strain energy density (ψ_e) and fracture energy (ψ_s) are defined as follows.