A PHASE-FIELD APPROACH TO MATERIAL DEGRADATION

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ABSTRACT

One of the major challenges in mechanics is to predict damage, cracks and fragmentation patterns. Besides the high demands on the modeling side, the complicated structure and non-regular behavior of cracks turn numerical simulations of these problems into a difficult task. A promising tool to overcome such difficulties are phase-field methods. The main idea behind it is to mark the material's different states -or *phases*- by continuous order parameter fields, and to let them evolve in space and time. Since the physical properties within the phases are all in all given, the evolving structure is fully described by the position and motion of the phase interfaces. However, an order parameter -or *phase-field*- is by definition a continuous field and thus, the moving boundaries are 'smeared' over a small but finite length, i.e., phase-field models constitute so-called diffuse-interface formulations, see Fig. 1.

Originally derived for diffusion problems, phase-field models are meanwhile used for a variety of interface problems like decomposition, phase transformations or aging of a microstructure. The core of every model is a Landau free energy functional. For two phases and with phase-field s(x,t) it states the potential energy of a body $\mathcal{B} \subset \mathbb{R}^3$

$$E = \int_{\mathcal{B}} \Psi^{\text{con}}(s) + \Psi^{\text{sur}}(\nabla s) \, \mathrm{d}V,\tag{1}$$

where $\Psi^{con}(s)$ denotes a configurational energy density which controls the decomposition of the phases and $\Psi^{sur}(\nabla s)$ is the interfacial or surface free energy density. Additional fields may contribute to the phase evolution but are omitted here for brevity.

Phase-field models of fracture have gained attention only recently. Here, the phase-field indicates the state of the material which may be solid (s = 1) or, if cracked, empty (s = 0). The field s(x,t) is controlled by an additional differential equation which results in a coupled field problem but completely avoids the resolution of discontinuities.

For purpose of illustration let us consider a deforming solid with domain $\mathcal{B} \subset \mathbb{R}^3$ and boundary $\partial \mathcal{B} \equiv \Gamma \subset \mathbb{R}^2$. Crack growth corresponds to the creation of new boundaries $\Gamma(t)$. Hence the total potential energy of a homogenous but cracking solid is composed of its bulk energy with free Helmholtz energy density Ψ^{bulk} and of surface energy contributions from growing crack boundaries.

$$E = \int_{\mathcal{B}} \Psi^{\text{bulk}} \, \mathrm{d}V + \int_{\Gamma(t)} \mathcal{G}_c \, \mathrm{d}S \tag{2}$$

The fracture-energy density \mathcal{G}_c quantifies the material's resistance to cracking, for brittle fracture it corresponds to Griffith's critical energy release rate. However, the energy functional (2) cannot be optimized in general and even an incremental approach is challenging because of the moving boundaries $\Gamma(t)$. Highly sophisticated discretization techniques have been developed to solve such problems, e.g. cohesive zone models, the extended finite element method, eroded finite elements or recently developed eigenfracture strategies. In a phase-field approach to fracture the set of evolving crack boundaries is instead replaced by a surface-density functional $\gamma(t) = \gamma(s(x,t))$ and an approximation of the form

$$\int_{\Gamma(t)} \mathrm{d}S \approx \int_{\mathcal{B}} \gamma(t) \,\mathrm{d}V \;, \tag{3}$$

which allows to re-write the total potential energy of a cracking solid and to formulate the optimization problem locally.

$$E = \int_{\mathcal{B}} \left(\Psi^{\text{bulk}} + \mathcal{G}_c \gamma \right) dV \to \text{ optimum}$$
(4)

In potential (4) the material's energy is again composed of two terms, a bulk energy density Ψ^{bulk} and a surface energy contribution $\mathcal{G}_c \gamma$. By definition γ is only different from zero along cracks.

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Figure 1: The phase-field shows a crack in a 3-point bending test. On the right, the with of the crack zone for different length-scale parameters l_c is illustrated by the decay of phase-field parameter s in the converged state.

Optimization of the potentials (1) or (4) leads to evolution equations for the phase-field s(x,t). For a simple ordering type of phase-field, the variation of energy leads the wanted driving force, $\dot{s} = -c\delta_s E$. Herein and below $c, c_1, c_2, \ldots, c_4 \in \mathbb{R}^+$ denote unspecified constants. The corresponding Euler-Lagrange equation is typically named Allen-Cahn equation and has the form of a simple reaction-diffusion equation.

$$\dot{s} = c_1 \phi(s) + c_2 \triangle s \tag{5}$$

In this formulation $\phi(s)$ denotes the reaction term, e.g. $\phi(s) = 2s^3 - s$. If the phase-field variable is a conserved quantity like mass concentration or volume fraction, its evolution has additionally to account for the continuity equation which leads to an evolution equation of Cahn-Hilliard type.

$$\dot{s} = c_3 \triangle \phi(s) - c_4 \triangle \triangle s \tag{6}$$

Obviously, there is no general phase-field evolution equation but instead the specific formulation has to map the physics of the underlying problem. In this contribution we apply different phase-field models to simulate damage in solids of linear-elastic and non-linear materials.

Continuum mechanics

A material point of a solid in its reference configuration \mathcal{B}_0 is labeled by $X = (X_1, X_2, X_3)^T$ and deforms during a time interval $[0, \tilde{t}]$ with a mapping

$$\chi(X,t): \mathcal{B}_0 \times [0,\bar{t}] \to \mathbb{R}^n.$$
(7)

We denote $x = \chi(X,t)$ with the gradient of the deformation $F : \mathcal{B}_0 \times [0, \bar{t}] \to \mathbb{R}^{n \times n}$.

$$F = \nabla_X \chi = \frac{\partial \chi}{\partial X} \tag{8}$$

The elastic boundary value problem follows from the balance of linear momentum,

$$\nabla_{\!X} \cdot P + \bar{B} = \rho_0 \dot{\nu} \qquad \text{in } \mathcal{B}_0 \times [0, \bar{t}], \tag{9}$$

where *P* is the first Piola-Kirchhoff stress tensor; ρ_0 denotes the mass density, \bar{B}, \bar{T} the prescribed body force and traction, and *v* the material velocity. The boundary of the solid is subdivided into displacement and traction boundaries $\partial \mathcal{B}_0^u$, $\partial \mathcal{B}_0^\sigma$ with $\partial \mathcal{B}_0 = \partial \mathcal{B}_0^u \cup \partial \mathcal{B}_0^\sigma$, $\partial \mathcal{B}_0^u = \emptyset$ and

$$x = \bar{x} \text{ on } \partial \mathcal{B}_0^{u} \times [0, \bar{t}] \quad \text{and} \quad PN = \bar{T} \quad \text{on } \partial \mathcal{B}_0^{\sigma}.$$

$$\tag{10}$$

The initial conditions are

$$x(X,0) = x_0$$
 and $v(X,0) = v_0$ in \mathcal{B}_0 . (11)

Let $\Psi^{\text{bulk}}(F, T, s, ...)$ be the local energy density of the bulk material. There may be additional dependencies of Ψ^{bulk} , e.g. on other phase-fields or on internal variables, but we will restrict ourselves here to an isotropic non-linear elastic material with one or two phases. This material will develop damage and/or cracks. From physics we know that fracture requires a local state of tension whereas the compressive part of the deformation does not contribute to crack growth. This requires a split of the bulk energy into compressive and tensional parts, cf. [2; 4; 7].

Phase-field evolution

The evolution equations for both, conservative and non-conservative phase-fields may be re-stated in a general form

$$\dot{s} = -MY(x,s),\tag{12}$$

where *M* denotes a kinematic mobility [1/sec] and Y(x, s) summarizes all (dimensionless) driving forces which typically represent a competition of bulk and surface forces, cf., e.g. [1; 9].

In phase-field fracture such a driving force results from a release of stored elastic energy of the body into the formation of free surfaces. Typically it is derived from an energy potential and we reformulate potential (4) as

$$E = \int_{\mathcal{B}} \frac{\mathcal{G}_c}{l_c} (\underbrace{\Psi^e + l_c \gamma}_{\bar{\Psi}}) \, \mathrm{d}V \qquad \text{with } \bar{\Psi}^e = \frac{l_c \Psi}{\mathcal{G}_c} \,. \tag{13}$$

For normalization we introduce here a potential $\overline{\Psi}$ which summarizes elastic and fracture energy contributions, $\overline{\Psi} = \overline{\Psi}^e + l_c \gamma$, and a characteristic length l_c which corresponds to half of the diffuse 'crack width', i.e. the transition zone between intact and broken material. The surface-density functional γ may be understood as a wavenumber of the moving disturbance; it characterizes the shape of the diffuse zone. By definition, function γ has a small support and is symmetric to the 'real' crack path. In general it is defined as a function of the phase-field parameter *s* solely, $\gamma = 1/l_c f(s)$. Then, an ansatz of the form

$$f(s) = c_0 |1 - s|^2 + c_1 l_c^2 |\nabla s|^2 + c_2 l_c^4 |\Delta s|^2 + c_3 l_c^6 |\nabla^3 s|^2 + \dots$$
(14)

can be made. Inserting it into (3) and minimizing the corresponding potential (13) analytically, leads for the simplest uniaxial case to an exponential solution of the form $s = 1 - \exp(-|x|/l_c)$. Now we determine the constants $c_0, c_1, c_2, c_3, \ldots$ in such a way, that this disturbance is approximated properly. In consequence we obtain for the surface-density function a second order approximation of the form

$$\gamma = \frac{1}{2l_c} \left((1-s)^2 + l_c^2 (\nabla s)^2 \right).$$
(15)



Figure 2: Model with loading conditions and computed phase-field distribution for mode I, mode II and mode III fracture.

The consideration of higher order terms gives an overall continuous analytical solution. Approximating the corresponding disturbance $s = 1 - \exp(-|x|/l_c) \cdot (1 + |x|/l_c)$, the fourth order crack-density functional reads

$$\gamma = \frac{1}{4l_c} \left((1-s)^2 + 2l_c^2 (\nabla s)^2 + l_c^4 (\Delta s)^2 \right) \,. \tag{16}$$

Note that an approximation (14) with the first term only describes a sharp transition and would result in the typical difficulties of moving discontinuities. The gradient term $(\nabla s)^2$ regularizes the crack zone and renders the method non-local. The additional Laplacian in (16) affects the curvature of the diffuse interface approximation and smoothes the transition. We would like to emphasize that gradient terms are known from continuum damage mechanics. However, in opposite to a damage variable here the material's state is well defined only for phase-field parameter s = 1 (intact) and s = 0(broken). The transition zone is a consequence of the regularized model and an intermediate value 0 < s < 1 state has no physical meaning.

In a variational approach the driving force of equation (12) is derived from the potential energy of the cracked body (4) or its normalized energy density in (13), i.e.,

$$Y = \delta_s \bar{\Psi} = \delta_s \left(\bar{\Psi}^e + l_c \gamma \right) = Y^e + l_c \delta_s \gamma \tag{17}$$

where Y^e summarizes the normalized crack driving force and $l_c \delta_s \gamma$ represents a kinematic fracture resistance. It evolves for the second order crack-density approximation (15) and for the fourth order crack-density approximation (16) to

$$l_c \delta_s \gamma = -(1-s) - l_c^2 \bigtriangleup s \quad \text{and} \quad l_c \delta_s \gamma = -\frac{1}{2}(1-s) - l_c^2 \bigtriangleup s - \frac{1}{2} l_c^4 \bigtriangleup \bigtriangleup s, \tag{18}$$

respectively. The dependence of the elastic energy term $\bar{\Psi}^e(F,T,s)$ on the phase-field *s* can be modeled in different ways. In the simplest case, a linear-elastic bulk energy, i.e. $\bar{\Psi}^e_0 = \frac{1}{2}\varepsilon : \bar{\mathbb{C}}\varepsilon$ with normalized elasticity tensor $\bar{\mathbb{C}} = l_c / \mathcal{G}_c \mathbb{C}(T)$, is multiplied with a degradation function,

$$\bar{\Psi}^e = g(s)\bar{\Psi}^e_0. \tag{19}$$

This function g(s) is such that in regions where the material is broken (s = 0), the contribution to the elastic energy is zero, while in the intact regions the elastic energy contribution recovers the one prescribed by the material's energy density.

A variational functional with quadratic degradation function was first introduced by Francfort, Marigo [5] and with slight modifications this ansatz has become very popular since, see, e.g., Miehe et al. [8] and Borden et al. [3]. Here the local energy function is of the form

$$Y = \delta_s \bar{\Psi} \quad \text{with } \bar{\Psi} = s^2 \bar{\Psi}_0^e + \frac{1}{2l_c} (1-s)^2 + \frac{l_c}{2} |\nabla s|^2,$$
(20)

which corresponds to (17) with a second order crack-density approximation (15).

A derivation of the driving force from an energy potential, however, is not necessary for a phase-field approach to fracture. Likewise the driving force can directly be modeled by a classical failure criterion. In general, the phase-field fracture approach offers many new opportunities in fracture simulations

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