Interaction and Multiscale Mechanics, Vol. 2, No. 1 (2009) 31-44
DOI: http://dx.doi.org/10.12989/imm.2009.2.1.031

A quasistatic crack propagation model allowing for cohesive forces and crack reversibility

Peter Philip*

Department of Mathematics, Ludwig-Maximilians University (LMU) Munich, Theresienstrasse 39, 80333 Munich, Germany

(Received December 12, 2007, Accepted August 15, 2008)

Abstract. While the classical theory of Griffith is the foundation of modern understanding of brittle fracture, it has a number of significant shortcomings: Griffith theory does not predict crack initiation and path and it suffers from the presence of unphysical stress singularities. In 1998, Francfort and Marigo presented an energy functional minimization method, where the crack (or its absence) as well as its path are part of the problem's solution. The energy functionals act on spaces of functions of bounded variations, where the cracks are related to the discontinuity sets of such functions. The new model presented here uses modified energy functionals to account for molecular interactions in the vicinity of crack tips, resulting in Barenblatt cohesive forces, such that the model becomes free of stress singularities. This is done in a physically consistent way using recently published concepts of Sinclair. Here, for the consistency of the model, it becomes necessary to allow for crack reversibility and to consider local minimizers of the energy functionals. The latter is achieved by introducing different time scales. The model is solved in its global as well as in its local version for a simple one-dimensional example, showing that local minimization is necessary to yield a physically reasonable result.

Keywords: crack propagation; brittle fracture; cohesive forces; reversibility; energy minimization.

1. Introduction

The presented research is aimed at improving the understanding of brittle fracture formation and propagation in materials. While classical applications include construction and machine design, the continuing development of new technologies and new materials keeps expanding the interest in fracture and failure research (de Borst *et al*. 2008, Bradford and Roufegarinejad 2008). New types of ceramics are used in such different areas as aerospace engineering (e.g. vehicle design), power generation (e.g. reactor design), and environmental technologies (e.g. diesel exhaust filters) to mention just a few examples.

The classical theory of Griffith (1921) constitutes the foundation of modern understanding of brittle fracture. However, it still has a number of significant shortcomings: Griffith theory does not predict crack initiation and path and it suffers from the presence of unphysical stress singularities. While the former problem is addressed, e.g., in Francfort and Marigo (1998), Dal Maso *et al*.

* E-mail: philip@math.lmu.de

(2005), and the latter problem is addressed, e.g., in Sinclair *et al.* (2005), this paper is directed at including the ideas of Sinclair *et al.* (2005) for the removal of stress singularities into the framework of Francfort and Marigo (1998), Dal Maso *et al.* (2005).

The approach of Francfort and Marigo (1998), Dal Maso *et al.* (2005) has the advantage that it does not need to prescribe the presence of a crack or its path a priori, but the potential crack as well as its path are part of the problem's solution. It is founded on the global minimization of energy functionals acting on spaces of functions of bounded variations, where the cracks are related to the discontinuity sets of such functions. The idea of Sinclair *et al.* (2005) is to use cohesive forces of Barenblatt-type (1962) to eliminate singularities at crack tips. In Barenblatt (1962), subsequent simplifications provide the same predictions of material failure as Griffith theory, while Sinclair *et al.* (2005) improves on this situation by avoiding such simplifications.

The model of the present article formulates modified energy functionals that account for molecular interactions in the vicinity of crack tips and the cohesive forces in the spirit of Sinclair *et al.* (2005). In contrast to Francfort and Marigo (1998), Dal Maso *et al.* (2005), the model also allows for crack reversibility and considers local minimizers of the energy functionals, employing different time scales. Solving the model for a simple one-dimensional example with a dead load, it is shown that the local energy minimization yields the physically expected result in a situation where the global minimization according to Francfort and Marigo (1998) fails.

The paper is organized as follows: The mathematical framework is described in Sections 2.1 and 2.2, where Sec. 2.1 deals with the static case, whereas Sec. 2.2 considers the time-dependent (quasistatic) case. Boundary conditions are covered in Sec. 2.3. The energy functional allowing for cohesive forces and crack reversibility are formulated in Sec. 2.4. The energy minimization problem is stated in Sec. 2.5, first in its global version, then in its local version. Together with the energy balance, this yields the quasistatic evolution problem in both its global and its local version. Finally, in Sec. 3, the model is solved for a one-dimensional dead load example in both its global and its local version.

2. Formulation of the model

2.1 Description of a strained and cracked body at a fixed time t

2.1.1 Reference configuration

Consider an N-dimensional elastic body, $N \in \{1, 2, 3\}$, and denote its uncracked reference configuration by $\Omega \subseteq \mathbb{R}^N$, where Ω is assumed to be nonempty, bounded, open, connected, with Lipschitz boundary $\partial\Omega$.

2.1.2 Special functions of bounded variation

At each time $t \in [0, T]$, $T > 0$, a strained and cracked configuration of the body is characterized by a displacement field $u : \Omega \to \mathbb{R}^N$ together with a *crack reversibility function* $r : \Omega \to \{0, 1\}$. One has to specify a suitable function space for the displacement field u, and the space of *special functions of bounded variation* $SBV(\Omega, \mathbb{R}^N)$ is often considered to be the appropriate choice. However, to guarantee compactness properties and the existence of minimizers for the energy functionals, one sometimes has to consider larger function spaces: For example, in Dal Maso *et al.* (2005), the space $GSBV(\Omega, \mathbb{R}^N)$ of *generalized special functions of bounded variation* turns out to

be suitable, while, for the example mentioned in the last paragraph of [Sec. 4.6.7 in Ambrosio *et al.* (2000)], $BV(\Omega, \mathbb{R}^N)$ is the appropriate space. To develop a mathematically rigorous existence theory is beyond the scope of the present paper. Thus, for definiteness, the space $SBV(\Omega, \mathbb{R}^N)$ will be used in the following. It is referred to Dal Maso *et al.* (2005) and Ambrosio *et al.* (2000) for the definition of and background material on spaces of functions of bounded variation.

Functions in $SBV(\Omega, \mathbb{R}^N)$ have a structure that makes them particularly suitable for fracture modeling. It is recalled that a function $u \in SBV(\Omega, \mathbb{R}^N)$ has a (distributional) derivative Du that can be written as the sum of an ($(N \times N)$-matrix-valued) integrable function ∇u and an ($(N \times N)$-matrix-valued) Dirac δ-distribution concentrated on an $\mathcal{H}^{N-1}$-rectifiable so-called jump set J_u. Technically, this can be stated as (quoting from [Eq. (4.1) in Ambrosio *et al.* (2000)])

$$Du = D^a u + D^j u = \nabla u \mathcal{L}^N + (u^+ - u^-) \otimes \mathbf{n}_{J_u} \mathcal{H}^{N-1} \lfloor_{J_u} \tag{1}$$

i.e., interpreted as an $(N \times N)$-matrix-valued measure, Du is the sum of N-dimensional Lebesgue measure $\mathcal{L}^N$ weighted by the function $\nabla u \in L^1(\Omega, \mathbb{R}^{N^2})$ and the $(N-1)$-dimensional Hausdorff measure $\mathcal{H}^{N-1}$ restricted to the jump set J_u weighted by the $(N \times N)$-matrix-valued function $(u^+ - u^-) \otimes \mathbf{n}_{J_u}$, where u^+ and u^- are the one-sided limits of u with respect to J_u, and $\mathbf{n}_{J_u}$ is the normal vector with respect to J_u. The function u can now be used to describe a strained and cracked body, where the location of the fracture or fractures is related to the discontinuity set J_u.

In Francfort-Marigo theory, e.g., in Francfort and Marigo (1998), Dal Maso *et al.* (2005), the crack is some superset of J_u; it can be strictly larger than J_u due to irreversibility: It can happen that J_u shrinks with time, such that, if cracks are not allowed to shrink, the crack must be allowed to be bigger than J_u. In the model proposed in the following, the crack can be a subset of J_u, it can be a superset of J_u, or it can be neither. However, the crack is still closely related to J_u, and it can be determined from J_u together with the reversibility function r using Eq. (2) below. Let us first look at the reversibility function r in more detail.

The function r is an accounting tool that, for each $x \in \Omega$, records if there is an irreversible crack at x or not: Set $r(x) = 1$ if, and only if, there is an irreversible crack at x. Thus, if $r(x) = 0$, then there is either no crack at x, or there is a reversible crack at x. The crack will always be a superset of $r^{-1}\{1\} := \{x \in \Omega : r(x) = 1\}$. However, $r^{-1}\{1\}$ does not have to be contained in J_u: As in Francfort-Marigo theory, where the crack has become irreversible, J_u can close, but the crack remains open (see Fig. 1 for an illustration of the formation of an irreversible crack Γ and its relation to J_u and r). As described below, irreversibility will be triggered by a crack having opened more than a threshold value a_{th}.

In contrast to Francfort-Marigo theory, here, it seems to make sense to allow situations, where there are parts of J_u that are *not* part of the crack, at least if one wants to consider reversibility and one does not want to restrict oneself to Mode I, i.e., tensile, loading: At a point x, where the crack is still reversible ($r(x) = 0$), the crack should vanish if the *normal distance* of the crack lips has returned to zero, even if $x \in J_u$ with $u^+(x) \neq u^-(x)$ (i.e. if the discontinuity is perpendicular to J_u): Cohesive forces will become active if the normal distance of the crack lips tends to zero, even if there has been a shift parallel to the crack surface (this kind of discontinuity in the displacement field could be interpreted as the presence of *slip dislocations*). Thus, the resulting definition of the crack $\Gamma(u, r)$ is

$$\Gamma(u, r) := r^{-1}\{1\} \cup \{x \in J_u : ([u](x)) \bullet \mathbf{n}_{J_u}(x) > 0\} \tag{2}$$

where $[u]$ is the usual abbreviation for the jump of u:

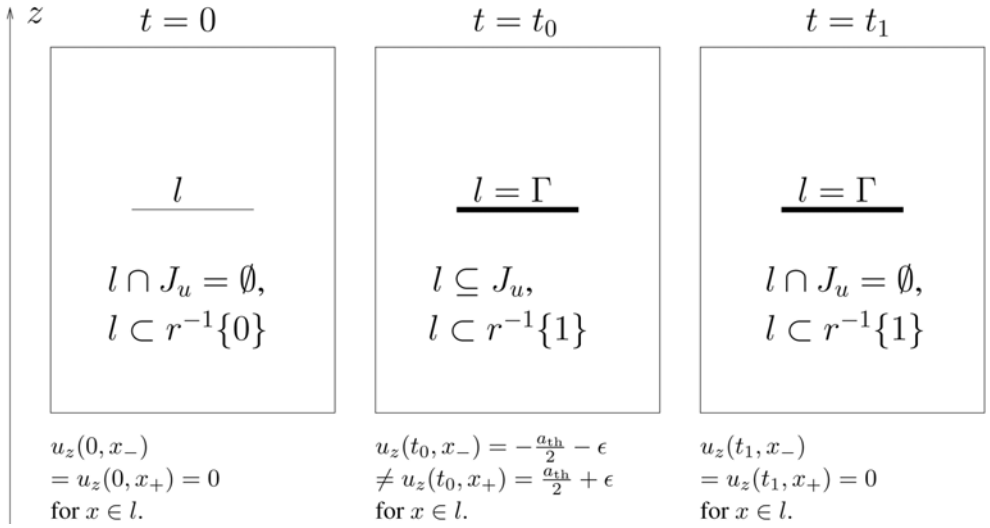

Fig. 1 Formation of an irreversible crack Γ at the location of the set l: At the initial time $t = 0$, there is neither a crack nor a displacement jump at l; at $t = t_0$ there is a vertical displacement jump of size bigger than the threshold value a_{th} at l, i.e., bonds are permanently broken and an irreversible crack has formed; at t_1 the displacement discontinuity at l has vanished, however, the broken bonds do not reform, i.e. the crack persists.

$$[u] : J_u \to \mathbb{R}^N, \; [u](x) := u_+(x) - u_-(x) \tag{3}$$

Note that the crack is determined by u and r, i.e., it does not have to be specified separately as in Francfort-Marigo theory.

2.1.3 Boundedness

From a physical point of view, one would expect the displacement u to be bounded, i.e., $u \in L^\infty(\Omega, \mathbb{R}^N)$, since, otherwise, some parts of the body have been displaced arbitrarily far from the reference configuration. Therefore, it seems reasonable to require that $u \in SBV^\infty(\Omega, \mathbb{R}^N) := SBV(\Omega, \mathbb{R}^N) \cap L^\infty(\Omega, \mathbb{R}^N)$ instead of just $u \in SBV(\Omega, \mathbb{R}^N)$.

2.2 Dependence on time

In the following, to describe time dependence of the displacement field, functions u will be considered that, for each time $t \in [0, T]$, assign a function $u(t) : \Omega \to \mathbb{R}^N$, such that $u(t)$ is the function defined on Ω, describing the displacement at time t. As usual, for such functions, the notation $u(t, x) := u(t)(x)$ will be employed.

According to Sec. 2.1, one is seeking functions $u : [0, T] \to SBV^\infty(\Omega, \mathbb{R}^N)$ and $r : [0, T] \times \Omega \to \{0, 1\}$. A crack becoming irreversible once $r(t, x) = 1$ means that, for each $x \in \Omega$, the function $r(\cdot, x)$ has to be nondecreasing. Given u and the threshold distance $a_{\text{th}} > 0$, one can actually define $r = r_u$ in terms of u:

$$r_u(t, x) = \begin{cases} 0 & \text{if } ([u](t, x)) \bullet \mathbf{n}_{J_{u(t)}}(x) < a_{\text{th}} \text{ for all } s \le t \\ 1 & \text{otherwise} \end{cases} \tag{4}$$

Thus, r_u can be seen as a *memory* function for u: The energy at time t does not only depend on $u(t)$, but also on $r_u(t)$, i.e., on the history of u.

2.3 Boundary conditions

Consider a decomposition of the boundary of Ω into a Dirichlet boundary $\partial_{\mathrm{D}}\Omega$ and a Neumann boundary $\partial_{\mathrm{N}}\Omega$:

$$\partial\Omega = \overline{\partial_{\mathrm{D}}\Omega} \cup \overline{\partial_{\mathrm{N}}\Omega}, \qquad \partial_{\mathrm{D}}\Omega \cap \partial_{\mathrm{N}}\Omega = \varnothing \tag{5}$$

where $\partial_{\mathrm{D}}\Omega$ and $\partial_{\mathrm{N}}\Omega$ are relatively open subsets of $\partial\Omega$, and the closures in Eq. (5) are meant with respect to the relative topology.

A Dirichlet boundary condition is assumed on $\partial_{\mathrm{D}}\Omega$: The deformation u is prescribed on $\partial_{\mathrm{D}}\Omega$ according to a given function $u_{\mathrm{D}} : [0, T] \to L^{\infty}(\partial_{\mathrm{D}}\Omega)$, that means, for each $t \in [0, T]$, $u_{\mathrm{D}}(t)$ should be the trace of $u(t)$ on $\partial_{\mathrm{D}}\Omega$:

$$u_{\mathrm{D}}(t) = \mathrm{tr}_{\partial_{\mathrm{D}}\Omega}\ u(t) \tag{6}$$

Surface forces are assumed to be given on the Neumann boundary $\partial_{\mathrm{N}}\Omega$. The surface forces are assumed to be represented by a sufficiently regular function $G : [0, T] \times (\partial_{\mathrm{N}}\Omega) \times \mathbb{R}^N \to \mathbb{R}$ (see Sec. 2.4.4 below).

2.4 Energy functionals

For each time t, the goal is to determine the energy of the strained and cracked configuration $(u(t), r(t))$. The total energy $\mathcal{E}(t)$ consists of several contributions which are considered in the following.

2.4.1 Energy of the crack

The energy $\mathcal{E}_{\mathrm{cr}}$ of the crack is defined by

$$\mathcal{E}_{\mathrm{cr}}(u, r) := \int_{\Gamma(u, r)} \kappa(x, \mathbf{n}_{\Gamma}(x), [u](x), r(x))\mathrm{d}\mathcal{H}^{N-1}(x) \tag{7}$$

where

$$\kappa : \Omega \times \mathbb{S}^{N-1} \times \mathbb{R}^N \times \{0, 1\} \to \mathbb{R}_0^+ \cup \{\infty\} \tag{8}$$

$\mathbb{S}^{N-1}$ denoting the $(N-1)$-dimensional unit sphere, is a function that will have to satisfy various regularity properties (typically something like lower semicontinuity) as part of a rigorous mathematical existence theory. As mentioned before, this path will not be pursued in the present article. The dependence of κ on x and $\mathbf{n}_{\Gamma}(x)$ describes the location- and direction-dependent toughness of the material. The dependence of κ on its third variable allows to account for Barenblatt-type energies corresponding to cohesive forces depending on the normal distance of the crack lips. Permitting κ to depend on the entire jump $[u](x)$ instead of just on the jump in the normal direction allows to include energy barriers for slip dislocations (jumps of u parallel to the crack). The dependence on $r(x)$ allows to account for crack reversibility: The idea is to use this as a switch for the dependence of κ on its third variable: As cohesive forces should play no role once the crack has become irreversible, κ should depend nontrivially on the third variable if, and only if,

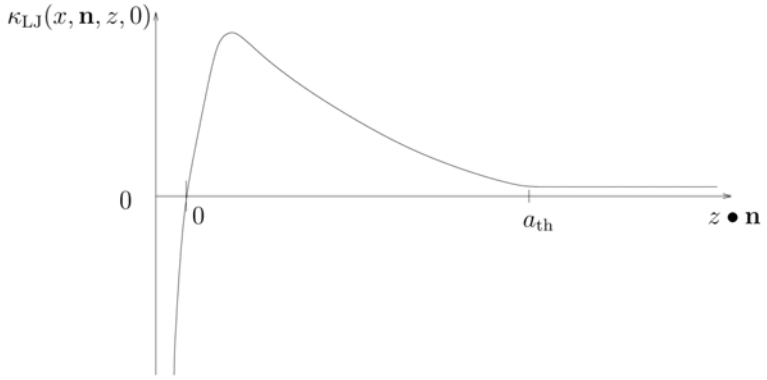

Fig. 2 Qualitative picture of the dependence of the function κ_{LJ} defined in Eq. (11a) on the normal separation $z \bullet \mathbf{n}$.

the fourth variable is 0. An example will be given shortly.

To prevent crack lip interpenetration, one might want to assume

$$\kappa(x, \mathbf{n}, z, r) = \infty \text{ whenever } z \bullet \mathrm{n} < 0 \tag{9}$$

i.e., such configurations would have infinite energy and, thereby, be excluded. From a multiscale point of view, it does not seem unreasonable to allow a small amount of interpenetration, which can be interpreted as a compression of interatomic bonds on the microscale. This has the advantage of avoiding a discontinuity of κ at $z \bullet \mathrm{n} = 0$. As an example consider

$$\kappa(x, \mathbf{n}, z, r) = |\kappa_{LJ}(x, \mathbf{n}, z, r)| + \kappa_{slip}(x, \mathbf{n}, z, r) \tag{10}$$

where κ_{LJ} is a Lennard-Jones-type function, e.g. (see Fig. 2)

$$\kappa_{LJ}(x, \mathbf{n}, z, 0) := \begin{cases} -\infty & \text{for } z \bullet \mathbf{n} \le -a_{th} \\ \left(\left(\dfrac{a_{th}}{a_{th} + z \bullet \mathbf{n}}\right)^6 - \left(\dfrac{a_{th}}{a_{th} + z \bullet \mathbf{n}}\right)^{12}\right) & \text{for } -a_{th} < z \bullet \mathbf{n} \le a_{th} \\ 2^{-6} - 2^{-12} \approx 0.0154 & \text{for } a_{th} \le z \bullet \mathbf{n} \end{cases} \tag{11a}$$

$$\kappa_{LJ}(x, \mathbf{n}, z, 1) := 2^{-6} - 2^{-12} \approx 0.0154 \tag{11b}$$

and κ_{slip} is a periodic function providing a potential barrier for the occurrence of slip dislocations.

Summarizing, the toughness function κ should, at least, have the following properties:

(a) $\kappa(x, \mathbf{n}, z, r) < \infty$ for each $(x, \mathbf{n}, z, r) \in \Omega \times \mathbb{S}^{N-1} \times \mathbb{R}^N \times \{0, 1\}$ such that $z \bullet \mathbf{n} \ge 0$.

(b) $\kappa(x, \mathbf{n}, z_1, 1) = \kappa(x, \mathbf{n}, z_2, 1)$ for each $(x, \mathbf{n}, z_1, z_2) \in \Omega \times \mathbb{S}^{N-1} \times \mathbb{R}^N \times \mathbb{R}^N$ such that $z_1 \bullet \mathbf{n} \ge 0$ and $z_2 \bullet \mathbf{n} \ge 0$.

(c) For each $(x, \mathbf{n}) \in \Omega \times \mathbb{S}^{N-1}$, the function $z \mapsto \kappa(x, \mathbf{n}, z, 0)$ is continuous on the set $\{z \in \mathbb{R}^N : 0 \le z \bullet \mathbf{n} \le a_{th}\}$.

(d) $\kappa(x, \mathbf{n}, z, 0) = \kappa(x, \mathbf{n}, z, 1)$ for each $(x, \mathbf{n}, z) \in \Omega \times \mathbb{S}^{N-1} \times \mathbb{R}^N$ such that $z \bullet \mathbf{n} = a_{th}$.

2.4.2 Strain energy of the bulk

The strain energy $\mathcal{E}_b$ of the bulk is defined by

$$\mathcal{E}_b(u) := \int_\Omega W(x, \nabla u(x))\mathrm{d}x \text{ with a suitable function } W : \Omega \times \mathbb{R}^{N^2} \to \mathbb{R}_0^+ \tag{12}$$

Again, for the mathematical existence theory, W will have to satisfy suitable regularity properties. At least, for each $\xi \in \mathbb{R}^{N^2}$, $W(\cdot, \xi)$ should be measurable, and, for each $x \in \Omega$, $W(x, \cdot)$ should be continuous.

2.4.3 Energy of the body forces

The body forces are assumed to be represented by a function $F : [0, T] \times \Omega \times \mathbb{R}^N \to \mathbb{R}$ such that the energy of the body forces can be computed as $\mathcal{F}(t, u) := \int_\Omega F(t, x, u(x))\mathrm{d}x$. In particular, it is assumed that, for each $(t, z) \in [0, T] \times \mathbb{R}^N$, $F(t, \cdot, z)$ is measurable, and, for each $(t, x) \in [0, T] \times \Omega$, $F(t, x, \cdot)$ is continuous. Further regularity conditions on F will have to be imposed in a rigorous existence theory.

2.4.4 Energy of the surface forces

The energy due to the surface forces G (cf. Sec. 2.3 above) can be computed as $\mathcal{G}(t, u) := \int_{\partial_N\Omega} G(t, x, u(x))\mathrm{d}x$. In particular, it is assumed that, for each $(t, z) \in [0, T] \times \mathbb{R}^N$, $G(t, \cdot, z)$ is measurable, and, for each $(t, x) \in [0, T] \times \partial_N\Omega$, $G(t, x, \cdot)$ is continuous. And, once again, further regularity conditions on G will have to be imposed in a rigorous existence theory.

2.4.5 Total energy

Given (u, r), the auxiliary total energy $\mathcal{E}_{aux}(t)$ at time t is determined by the energy of the crack, the bulk energy, the energy of the body forces, and the energy of the surface forces:

$$\mathcal{E}_{aux}(t)(u, r) := \mathcal{E}_{cr}(u, r) + \mathcal{E}_b(u) - \mathcal{F}(t, u) - \mathcal{G}(t, u) \tag{13}$$

Recall from Sec. 2.2 that, given $u : [0, T] \to SBV^\infty(\Omega, \mathbb{R}^N)$, the reversibility function r_u corresponding to u is defined by Eq. (4). Thus, at time $t \in [0, T]$, the total energy $\mathcal{E}(t)$ of the time-dependent displacement $u : [0, T] \to SBV^\infty(\Omega, \mathbb{R}^N)$ is defined by

$$\mathcal{E}(t)(u) := \mathcal{E}_{aux}(t)(u(t), r_u(t)) \tag{14}$$

2.5 Energy minimization

2.5.1 Admissible displacement fields

An admissible displacement field u at time $t \in [0, T]$ is a function $u \in SBV^\infty(\Omega, \mathbb{R}^N)$ that respects the Dirichlet boundary condition Eq. (6) on $\partial_D\Omega$. That means, the set AD(t) of admissible displacement fields at time t is defined by

$$\mathrm{AD}(t) := \{u \in SBV^\infty(\Omega, \mathbb{R}^N) : u_D(t) = \mathrm{tr}_{\partial_D\Omega}\, u\} \tag{15}$$

As the trace operator $\mathrm{tr}_{\partial_D} : SBV(\Omega, \mathbb{R}^N) \to L^1(\partial_D\Omega, \mathbb{R}^N)$ is surjective and positive (cf. [Th. 3.87 in Ambrosio *et al.* (2000)] and its following paragraph), AD(t) is nonempty if, and only if, $u_D(t) \in L^\infty(\partial_D\Omega, \mathbb{R}^N)$.

2.5.2 Global energy minimization

Global energy minimization in the spirit of the condition of *global stability* in [Sec. 3.9 in Dal Maso *et al*. (2005)] means that, for each $t \in [0, T]$, $u(t)$ needs to be a minimizer of the total energy $\mathcal{E}(t)$ among all admissible $v \in \mathrm{AD}(t)$. For the precise formulation of this statement, one has to use some care due to the presence of the reversibility function r. For a fixed time $t \in [0, T]$, the goal is to formulate the minimality condition that $u(t)$ needs to satisfy. Due to the presence of the reversibility function, to be able to formulate the condition at time t, one has to make use of the function u already defined for times smaller than t:

Let $v \in \mathrm{AD}(t)$ be an admissible displacement field at time t, and let $u : [0, t[\to SBV^\infty(\Omega, \mathbb{R}^N)$ be given. Then u can be extended to time t by v:

$$u_v : [0, t] \to SBV^\infty(\Omega, \mathbb{R}^N), \qquad u_v(s) := \begin{cases} u(s) & \text{for } s < t \\ v & \text{for } s = t \end{cases} \tag{16}$$

Thereby, v also gives rise to a reversibility function r^v by letting

$$r^v : [0, t] \to \{0, 1\}, \; r^v := r_{u_v} \tag{17}$$

With these preparations in place, one is in a position to state the global minimality condition at time t: $u(t)$ needs to satisfy

$$u(t) \in \mathrm{AD}(t) \text{ and } \mathcal{E}(t)(u_{u(t)}) \le \mathcal{E}(t)(u_v) \text{ for each } v \in \mathrm{AD}(t) \tag{18}$$

2.5.3 Local energy minimization

The condition for a global energetic minimum of the previous section has the advantage of being conceptionally fairly simple: Under the assumption that quasistatic modeling is at all reasonable and minimizers $u(t)$ satisfying Eq. (18) exist for all t, the idea is, that, for each t, the system settles into the global energetic minimum given by Eq. (18) according to some dynamics taking place on a faster time scale. However, it might not be physically realistic that the system can always settle into the *global* energetic minimum given by Eq. (18), since this global minimum might be barred from "previous" states by an energy barrier, i.e. there is no "admissible path" to the global minimum.

The arising conceptional problems are the following: It is not obvious what exactly one would mean by "previous" states given a continuous, but *quasistatic* time variable. Likewise, it is not obvious what a "path" in the space of admissible displacement fields should be. Here, by a "path", one would usually mean a continuous function $p : [0, 1] \to SBV^\infty(\Omega, \mathbb{R}^N)$; but continuous with respect to which metric or topology on $SBV^\infty(\Omega, \mathbb{R}^N)$?

A physically reasonable distance function d on $SBV^\infty(\Omega, \mathbb{R}^N)$ should be such that, for small $d(u, v)$, the difference of the energies of u and v is likewise small. More precisely, if $p : [0, 1] \to SBV^\infty(\Omega, \mathbb{R}^N)$ is a continuous path with respect to d, then $a \mapsto \mathrm{Energy}(p(a))$ should also be a continuous function (the energy should change continuously along paths in $SBV^\infty(\Omega, \mathbb{R}^N)$). Note that one would need an exception to this assumption if one were to allow the energy to change discontinuously to ∞ at $[u] \bullet \mathbf{n} = 0$ to avoid crack lip interpenetration.

Given the continuous dependence of κ on $[u](x)$ according to condition (c) at the end of Sec. 2.4.1, the continuous dependence of W on $\nabla u(x)$, the continuous dependence of F on $u(x)$, and the continuous dependence of G on $u(x)$, a suitable distance function on $SBV^\infty(\Omega, \mathbb{R}^N)$ might be proposed by the norm $||\cdot||_{\infty,1}$ on $SBV^\infty(\Omega, \mathbb{R}^N)$ defined by

$$||u||_{\infty,1} := ||u||_\infty + ||\nabla u||_1 \tag{19}$$

where ∇u is meant in the same sense as in Eq. (1).

To be able to define the set of admissible paths between states v_1 and v_2 at time t, $(v_1, v_2) \in \mathrm{AD}(t)$, one needs to make use of the function u already defined for times $s < t$. As for the global energy minimization in the previous section, this is due to the energy at time t depending on the history of u via the reversibility function r.

Using the notation introduced in Eq. (16) and Eq. (17) in the previous section, for a fixed time $t \in [0, T]$, given $u : [0, t[\to SBV^\infty(\Omega, \mathbb{R}^N)$, define the set $P_t(v_1, v_2)$ of *admissible paths* between states v_1 and v_2, $(v_1, v_2) \in \mathrm{AD}(t) \times \mathrm{AD}(t)$, as the set of maps $p : [0, 1] \to \mathrm{AD}(t)$ continuous with respect to $||\cdot||_{\infty,1}$ (note $\mathrm{AD}(t) \subseteq SBV^\infty(\Omega, \mathbb{R}^N)$), such that $p(0) = v_1$, $p(1) = v_2$, and such that the map $a \mapsto \mathcal{E}(t)(u_{p(a)})$ is nonincreasing on $[0, 1]$.

In analogy with the global minimality condition Eq. (18) above, at time t, the local minimality condition is stated as follows:

$u(t) \in \mathrm{AD}(t)$ and there is $\varepsilon > 0$ such that: $\mathcal{E}(t)(u_{u(t)}) \le \mathcal{E}(t)(u_v)$

for each $v \in \mathrm{AD}(t)$ satisfying $||u(t) - v||_{\infty,1} < \varepsilon$ (20)

Now, condition Eq. (20) needs to be combined with the concept of quasistatic evolution. The idea for doing that is to consider different scales for the time dependence:

A function $u : [0, T] \to SBV^\infty(\Omega, \mathbb{R}^N)$ will be called *energetically admissible* if, and only if, u satisfies the following conditions (i) and (ii):

(i) $u(t)$ satisfies (20) for each $t \in [0, T]$.

(ii) There exists a finite sequence of times $0 = t_0 < \cdots < t_n = T$ such that u is continuous with respect to the $||\cdot||_{\infty,1}$-norm on each interval $[t_{\nu-1}, t_\nu[$, $\nu \in \{1, \ldots, n\}$, and, for each $\nu \in \{1, \ldots, n\}$, there is $v_\nu \in \mathrm{AD}(t_\nu)$ such that the map

$$u_\nu : [t_{\nu-1}, t_\nu] \to SBV^\infty(\Omega, \mathbb{R}^N), \qquad u_\nu(t) := \begin{cases} u(t) & \text{for } t < t_\nu \\ v_\nu & \text{for } t = t_\nu \end{cases}$$

is continuous with respect to the $||\cdot||_{\infty,1}$-norm on the entire closed interval $[t_{\nu-1}, t_\nu]$, and such that there is an admissible path $p_\nu \in P_{t_\nu}(v_\nu, u(t_\nu))$connecting v_ν and $u(t_\nu)$.

The explanation for condition (ii) is as follows: First, assume that the local minima in Eq. (20) are strict. Then, the macro time scale is active as long as $u(t)$ "naturally" sits in a local minimum for the energy according to Eq. (20). This is the case inside each interval $[t_{\nu-1}, t_\nu[$. The energy of $u(t)$ can actually increase with t, but, at each t, it is smaller than for any state in some $||\cdot||_{\infty,1}$-neighborhood of $u(t)$. Since $\mathcal{E}(t)$ changes with time, so does the energy landscape. At the times t_ν, $\nu \in \{1, \ldots, n\}$, it has changed so much that what used to be a strict local minimum is no longer a strict local minimum, and there exists an admissible path in $\mathrm{AD}(t_\nu)$ to some state of lower energy. The assumption of quasistatic evolution means that the system follows such a path on the micro time scale, finding a new local energetic minimum. This happens instantaneously on the macro time scale, namely at time t_ν.

The consideration of nonstrict, plateau-type local minima is somewhat more subtle (depending on the energy functionals such plateaus might or might not exist). As condition (ii) is formulated, given plateaus, it allows multiple solutions. The system can remain in each point of the plateau, but it can

also explore the plateau to find admissible paths to even lower energies. Depending on the (micro) time needed to explore such plateaus, it might be reasonable to revise condition (ii) to require the system to move out of plateaus toward lower energies whenever an admissible path exists. This would, in general, dramatically reduce the number of solutions. However, uniqueness could still not be expected, as there can be multiple wells leading out of a given plateau.

Moreover, it could happen that $\mathcal{E}(t)$ changes in such a way that it has a plateau for each $t \in [t_{\nu-1}, t_\nu]$, but not for *any* $t > t_\nu$. For example, assume that m_1 and m_2 are the only local minima for $t > t_\nu$. Then the system would have to be in either m_1 or m_2 for $t > t_\nu$, and, by continuity, also for $t = t_\nu$. So, in this situation, quasistatic modeling requires that the system would have to move to m_1 or m_2 for some $t \leq t_\nu$ *in anticipation* of the change of $\mathcal{E}(t)$ at t_ν. In reality, this would occur within a short (micro) time after t_ν. The anticipation seems to be the price one pays for not resolving the microtime in this case.

It is remarked that, a priori, it is not clear if, and under what conditions, there exists $u(t)$ satisfying Eq. (20). And even if there does exist $u(t)$ satisfying Eq. (20) for each $t \in [0, T]$, then it is still not clear if, and under what conditions, there is $u : [0, T] \to SBV^\infty(\Omega, \mathbb{R}^N)$ that is energetically admissible in the sense defined above. This question remains to be investigated in future research.

2.5.4 Energy balance

In analogy with [Eq. (3.50) and Rem. 3.12 in Dal Maso *et al.* (2005)], for each time interval, the increment in stored energy plus the energy spent in crack increase (or recovered by crack closure) needs to equal the work W_{ext} of the external forces:

$$W_{\text{ext}}(t)(u) - W_{\text{ext}}(s)(u) = \mathcal{E}(t)(u) - \mathcal{E}(s)(u) \text{ for each } (s, t) \in [0, T]^2,\ s < t \tag{21}$$

As described in [Sec. 1 in Dal Maso *et al.* (2005)], there are three contributions to the work of the external forces:

$$W_{\text{ext}}(t)(u) = W_{\text{D}}(t)(u) + W_F(t)(u) + W_G(t)(u) \tag{22}$$

where W_{D} is the work arising from the prescribed deformation on the Dirichlet boundary $\partial_{\text{D}}\Omega$, W_F is the external work of the body forces, and W_G is the external work of the surface forces. According to the formula in Dal Maso *et al.* (2005) before [Eq. (1.1) in Dal Maso *et al.* (2005)]:

$$W_{\text{D}}(t)(u) = \int_{\partial_{\text{D}}\Omega} \partial_2 W(x, \nabla u(t, x))\mathbf{n}_{\partial\Omega}\, \partial_1 u_{\text{D}}(t, x)\, \mathrm{d}\mathcal{H}^{N-1}(x) \tag{23}$$

In the absence of sufficient regularity, Eq. (23) has to be interpreted in a suitable weak sense as described in Dal Maso *et al.* (2005) after [Eq. (3.46) in Dal Maso *et al.* (2005)]. Next, according to [Sec. 3.9 in Dal Maso *et al.* (2005)], one has

$$W_F(t)(u) = -\int_0^t \int_\Omega \partial_1 F(\tau, x, u(\tau, x))\mathrm{d}x\, \mathrm{d}\tau, \qquad W_G(t)(u) = -\int_0^t \int_{\partial_{\text{N}}\Omega} \partial_1 G(\tau, x, u(\tau, x))\mathrm{d}x\, \mathrm{d}\tau \tag{24}$$

2.5.5 Quasistatic evolution problem: global version

A *quasistatic evolution of globally minimizing energy configurations* (*QEGMEC*) is a function $u : [0, T] \to SBV^\infty(\Omega, \mathbb{R}^N)$ satisfying the following conditions:

(a) For each $t \in [0, T]$: $u(t) \in \mathrm{AD}(t)$.

(b) For each $t \in [0, T]$: $\mathcal{E}(t)(u_{u(t)}) \leq \mathcal{E}(t)(u_v)$ for every $v \in \mathrm{AD}(t)$.

(c) $W_{\text{ext}}(t)(u) - W_{\text{ext}}(s)(u) = \mathcal{E}(t)(u) - \mathcal{E}(s)(u)$ for each $(s, t) \in [0, T]^2$, $s < t$.

2.5.6 Quasistatic evolution problem: local version

A *quasistatic evolution of locally minimizing energy configurations* (*QELMEC*) is a function u : $[0, T] \to SBV^{\infty}(t)$ satisfying the following conditions:

(a) For each $t \in [0, T]$: $u(t) \in \mathrm{AD}(t)$.

(b) For each $t \in [0, T]$, there is $\varepsilon > 0$ such that $\mathcal{E}(t)(u_{u(t)}) \leq \mathcal{E}(t)(u_v)$ for each $v \in \mathrm{AD}(t)$ satisfying $||u(t) - v||_{\infty,1} < \varepsilon$.

(c) There exists a finite sequence of times $0 = t_0 < \cdots < t_n = T$ such that u is continuous with respect to the $||\cdot||_{\infty,1}$-norm on each interval $[t_{\nu-1}, t_\nu[$, $\nu \in \{1, ..., n\}$, and, for each $\nu \in \{1, ..., n\}$, there is $v_\nu \in \mathrm{AD}(t_\nu)$ such that the map

$$u_\nu : [t_{\nu-1}, t_\nu] \to SBV^{\infty}(\Omega, \mathbb{R}^N),\ u_\nu(t) := \begin{cases} u(t) & \text{for } t < t_\nu \\ v_\nu & \text{for } t = t_\nu \end{cases}$$

is continuous with respect to the $||\cdot||_{\infty,1}$-norm on the entire closed interval $[t_{\nu-1}, t_\nu]$, and such that there is an admissible path $p_\nu \in P_{t_\nu}(v_\nu, u(t_\nu))$connecting v_ν and $u(t_\nu)$.

(d) $W_{\mathrm{ext}}(t)(u) - W_{\mathrm{ext}}(s)(u) = \mathcal{E}(t)(u) - \mathcal{E}(s)(u)$ for each $(s, t) \in [0, T]^2$, $s < t$.

In short, a QELMEC is an energetically admissible function in the sense of Sec. 2.5.3 that satisfies the energy balance.

3 Example: dead load via a constant body force

3.1 General setting

In the following, a dead load example of the type [Sec. 5.2 in Francfort and Marigo (1998)] is considered. The issue discussed in [Sec. 5.2 in Francfort and Marigo (1998)] is basically that the energy minimization yields an unphysical result, namely failure for an arbitrarily small nonzero load. This problem is due to the global energy minimization, and the following example shows that introducing reversibility and cohesive forces does nothing to change the situation (see Sec. 3.2). However, the local version of the energy minimization considered in Sec. 3.3 yields the physically expected result that failure occurs only once the load surpasses a critical value.

Consider the following one-dimensional problem (see Fig. 3), letting

$$\Omega := \{x \in \mathbb{R} : 0 < x < 2\},\ \partial_{\mathrm{D}}\Omega := \{2\},\ \partial_{\mathrm{N}}\Omega := \{0\},$$

$$u_{\mathrm{D}} : [0, T] \to L^{\infty}(\partial_{\mathrm{D}}\Omega, \mathbb{R}),\ u_{\mathrm{D}}(t)(2) := 0,\ G : [0, T] \times (\partial_{\mathrm{N}}\Omega) \times \mathbb{R} \to \mathbb{R}, \qquad G(t, 2, z) := 0,$$

$$W : \Omega \times \mathbb{R} \to \mathbb{R}_0^+, \qquad W(x, \xi) := \xi^2 / 2,\ F : [0, T] \times \Omega \times \mathbb{R} \to \mathbb{R}, \qquad F(t, x, z) := -t\, z,$$

$$a_{\mathrm{th}} := 1, \qquad \kappa : \Omega \times \mathbb{S}^{N-1} \times \mathbb{R}^N \times \{0, 1\} \to \mathbb{R}_0^+ \cup \{\infty\}, \qquad \kappa(x, \mathbf{n}, z, r) := |\kappa_{\mathrm{LJ}}(x, \mathbf{n}, z, r)|,$$

where $\kappa_{\mathrm{LJ}}(x, \mathbf{n}, z, r)$ is according to Eq. (11).

From these functions, one can compute the total energy:

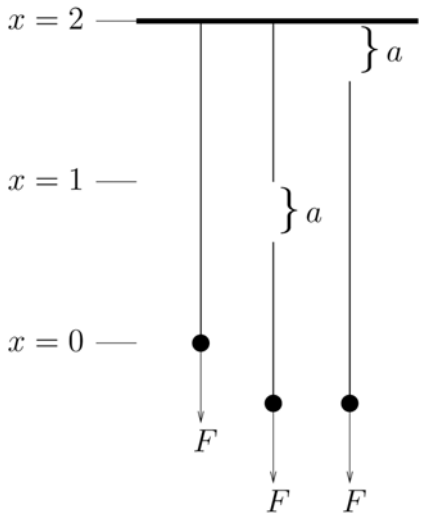

Fig. 3 Illustration of the dead load example considered in Sec. 3: Global energy minimization (Sec. 3.2) predicts the unphysical result that a crack must appear for any nonzero load F (it can appear at the location depicted in the middle drawing or at any other location). However, local energy minimization (Sec. 3.3) predicts the physically reasonable result that no crack appears for small loading F, and a crack appears at the top (as indicated in the right-hand drawing) once F surpasses a critical value.

$$\begin{aligned}\mathcal{E}_{\text{aux}}(t)(u,\,r) &= \int_{\Gamma(u,\,r)} \kappa(x,\,\mathbf{n}_{\Gamma(u,r)}(x),\,[u](x),\,r(x))\mathrm{d}\mathcal{H}^{N-1}(x)\\ &+ \int_\Omega W(x,\,\nabla u(x))\mathrm{d}x - \int_\Omega F\,(t,\,x,\,u(x))\mathrm{d}x - \int_{\partial_{\mathrm{N}}\Omega} G(t,\,x,\,u(x))\mathrm{d}x\\ &= \int_{\Gamma(u,\,r)} |\kappa_{\mathrm{LJ}}\,(x,\,\mathbf{n}_{\Gamma(u,\,r)}(x),\,[u](x),\,r(x))|\;\mathrm{d}\mathcal{H}^{N-1}(x)\\ &\quad + \int_0^2 \frac{1}{2}\,(\nabla u(x))^2\;\mathrm{d}x + \int_0^2 t\,u(x)\;\mathrm{d}x \end{aligned} \tag{25}$$

$$\begin{aligned}\mathcal{E}\,(t)(u) &= \mathcal{E}_{\text{aux}}(t)(u(t),\,r_u(t))\\ &= \int_{\Gamma(u(t),\,r_u(t))} |\kappa_{\mathrm{LJ}}(x,\,\mathbf{n}_{\Gamma(u(t),\,r_a(t))}(x),\,[u(t)](x),\,r_u(t,\,x))|\;\mathrm{d}\mathcal{H}^{N-1}(x)\\ &\quad + \int_\Omega \frac{1}{2}\,(\nabla u(t,\,x))\bullet(\nabla u(t,\,x))\;\mathrm{d}x + \int_\Omega t u(t,\,x)\;\mathrm{d}x \end{aligned} \tag{26}$$

3.2 Global minimization

The following shows that the situation described in [Sec. 5.2 in Francfort and Marigo (1998)] persists for the current model in the global version of the minimization problem. The interpretation given in [Sec. 5.2 in Francfort and Marigo (1998)] is that the model unphysically predicts an arbitrarily small force to break the body into at least two pieces, sending off one of the pieces to infinity. In the setting of the present example, there is no $t \in]0,\,T]$ such that the minimization (b) of the global version (see Sec. 2.5.5) has a solution.

Define

$$\Omega_{\text{high}} := \{x \in \mathbb{R} : 1 < x < 2\},\ \Omega_{\text{low}} := \{x \in \mathbb{R} : 0 < x < 1\} \tag{27}$$

and, for each $a \in]a_{\text{th}}, \infty[$, consider

$$u_a : [0, T] \to SBV^{\infty}(\Omega, \mathbb{R}),\ u_a := \begin{cases} u_a(t, x) := 0 & \text{for}(t, x) \in [0, T] \times \Omega_{\text{high}} \\ u_a(t, x) := -a & \text{for}(t, x) \in [0, T] \times \Omega_{\text{low}} \end{cases} \tag{28}$$

(this situation is depicted in the middle of Fig. 3). Then, since $\text{tr}_{\partial_D \Omega}\, u_a(t) = u_D$, it is $u_a(t) \in \text{AD}(t)$ for each $t \in [0, T]$. The total energy amounts to

$$\mathcal{E}(t)(u_a) = \int_{\overline{\Omega}_{\text{low}} \cap \overline{\Omega}_{\text{high}}} \kappa_{\text{LJ}}(x, 1, a, 1)|\, \mathrm{d}\mathcal{H}^{N-1}(x) - \int_{\Omega_{\text{low}}} t\, a\, \mathrm{d}x = 2^{-6} - 2^{-12} - t\, a \tag{29}$$

Thus, for $t > 0$, $\mathcal{E}(t)(u_a) \to -\infty$ for $a \to \infty$, showing that the minimization (b) of the global version has no solution.

3.3 Local minimization

For each $t \in [0, T]$, let $u_e(t)$, $u_e(t) : \Omega \to \mathbb{R}$, $u_e(t) \le 0$, be the solution for the "perfectly elastic" limit of the material, i.e. $u_e(t)$ is the (global) minimizer of

$$\mathcal{E}_e(t)(f) := \int_\Omega \frac{1}{2} (\nabla u(x)) \bullet (\nabla u(x)) \mathrm{d}x + \int_\Omega t\, u(x)\, \mathrm{d}x \tag{30}$$

Now, the idea is to introduce a crack at $y \in \Omega$. For each step function $\phi_{a, b, y} := -a\, 1_{[0, y[} + b\, 1_{]y, 2]}$, $(a, b) \in \mathbb{R}^2$, one can investigate if the energy of $u_e(t) + \phi_{a, b, y}$ is more or less than the energy of $u_e(t)$. First, note that $b = 0$, as, in order for $u_e(t) + \phi_{a, b, y}$ to satisfy the Dirichlet condition, $0 = u_e(t)(2) + \phi_{a, b, y}(2) = 0 + b = b$. Let $\phi_{a, y} := \phi_{a, 0, y}$. As $\nabla \phi_{a, y} = 0$, one has $\nabla (u_e(t) + \phi_{a, y}) = \nabla (u_e(t))$. Thus, the energy of $u_e(t) + \phi_{a, y}$ is

$$\begin{aligned} \mathcal{E}(t)(u_e(t) + \phi_{a, y}) &= \kappa_j(a) + \int_\Omega \frac{1}{2} (\nabla u_e(t, x)) \bullet (\nabla u_e(t, x)) \mathrm{d}x + \int_\Omega t\, (u_e(t, x) + \phi_{a, y}(x)) \mathrm{d}x \\ &= \mathcal{E}_e(t)(u_e(t)) + \kappa_j(a) - t\, a\, y \end{aligned} \tag{31}$$

where $\kappa_j :]a_{\text{th}}, \infty[\to \mathbb{R}_0^+$, $\kappa_j(a) := |\kappa_{\text{LJ}}(1, 1, a, 0)|$ (cf. (11a)). Thus, $\mathcal{E}(t)(u_e(t))$ is a local minimum if, and only if, $a \mapsto \kappa_j(a) - tay$ has a local minimum at 0. This is clearly the case for small positive t, and the solution is crack-free. Then, at a critical $t > 0$, a crack will appear at $x = 2$ (see the right-hand drawing of of Fig. 3), which is the physically expected result.

4. Conclusions

We have described a new quasistatic model for the formation and propagation of brittle fracture using the energy functional minimization method. New terms in the energy functional allow for the molecular interactions occurring at crack tips to avoid stress singularities. The model was

formulated in two versions, one requiring global energy minimization, the other requiring local energy minimization. For the local version, it was necessary to introduce a second, faster time scale into the quasistatic model. It was demonstrated for a simple example that it is necessary to use the local energy minimization version of the model to arrive at the physically expected result. While the global energy minimization has a nonsensical result, predicting failure under any nonzero load, the local minimization correctly predicts failure under a critical positive load. It also correctly predicts the location of crack formation.

Acknowledgements

This work has been supported by the DFG Research Center MATHEON - "Mathematics for key technologies" (FZT 86) in Berlin, by the Institute for Mathematics and its Applications (IMA) in Minneapolis, and by Corning Incorporated, Corning, NY.

References

Ambrosio, L., Fusco, N. and Pallara, D. (2000), *Functions of Bounded Variation and Free Discontinuity Problems*, Oxford Mathematical Monographs, Oxford University Press, Oxford, UK.

Barenblatt, G.I. (1962), "The mathematical theory of equilibrium cracks in brittle fracture", *Advan. Appl. Mech.*, **7**, 55-129.

de Borst, R., Rethore, J. and Abellan, M.-A. (2008), "Two-scale approaches for fracture in fluidsaturated porous media", *Interaction Multiscale Mech., An Int. J.*, **1**, 83-101.

Bradford, M.A. and Roufegarinejad, A. (2008), "Elastic local buckling of thin-walled elliptical tubes containing elastic infill material", *Interaction Multiscale Mech., An Int. J.*, **1**, 143-156.

Dal Maso, G., Francfort, G.A. and Toader, R. (2005), "Quasistatic crack growth in nonlinear elasticity", *Arch. Ration. Mech. Anal.*, **176**, 165-225.

Francfort, G.A. and Marigo, J.-J. (1998), "Revisiting brittle fracture as an energy minimization problem", *J. Mech. Phys. Solids*, **46**, 1319-1342.

Griffith, A.A. (1921), "The phenomenon of rupture and flow in solids", *Phil. Trans. Roy. Soc. London. Ser. A*, **221**, 163-198.

Sinclair, G.B., Meda, G. and Smallwood, B.S. (2005), *On the stresses at a Griffith crack*. Report No. ME-MA1-05, Dep. Mechanical Engineering, LSU, Baton Rouge, LA, 2005. Available in pdf-format at http://appl003.lsu.edu/mech/mechweb.nsf/$Content/MA+Technical+Reports/$file/ME_MA1_05.pdf.