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Variational phase-field fracture with controlled nucleation

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ABSTRACT

We briefly review the Γ-convergence of phase-field fracture to Griffith fracture, and describe how softening and nucleation occur when implementing phase-field models. An example is given of how this softening and nucleation can be completely stopped, while preserving crack growth and Γ-convergence. We then show how nucleation can locally be turned back on, based on any criterion, such as a stress threshold. Again, these modifications preserve Γ-convergence, and they can be applied to static, quasi-static, and dynamic models. Additionally, we describe why these modifications can be expected to improve the convergence of phase-field models.

1. Introduction

Certain phase-field models for fracture have been shown to converge, in a variational sense, to models for Griffith fracture [1] (see [2]; see also [3] and references therein). These variational phase-field models have a mathematical parameter ε, and the convergence to the Griffith model occurs as ε tends to zero. Computing using these phase-field models has become common, and one aspect we see is that nucleation of cracks is related to the parameter ε. This is considered to be undesirable, since ε is not a physical parameter, but is chosen primarily based on the desired computational cost (related to mesh size, on the scale of ε) and desired accuracy (which improves as ε gets smaller).

Recently, [4] raised the interesting question of modifying the usual phase-field models to include a separate criterion for nucleation. They viewed such a modification as incompatible with a variational, or energy minimizing, formulation, and proposed instead a PDE-based approach. Here, after briefly explaining the variational convergence (Γ-convergence) of the phase-field models and how energy descents can lead to softening and nucleation, we show that both softening and nucleation can be completely turned off while maintaining Γ-convergence, independently of the phase-field surface energy (e.g., using AT1 or AT2). We then describe how the possibility of nucleating can be locally switched back on, based on any local condition desired. We illustrate this using a stress threshold.

A natural question is, if the proposed variational formulations and the original ones both Γ-converge to the same Griffith energy, how can the behavior of solutions be so different? The reason is, in practice, the phase-field energies are not actually minimized, but certain energy descents are performed computationally. It is these descents that can behave very differently with different variational formulations, even if they have the same Γ-limit.

2. Phase-field fracture and Γ-convergence

We now describe the key elements behind the Γ-convergence of Ambrosio–Tortorelli functionals E_ε to the Griffith fracture energy E, proved in [2]. While Γ-convergence is not necessarily the relevant convergence for certain evolution problems, it does give some rigorous connection between the energies E_ε and E. Our main point is that understanding how this convergence works can lead to flexibility in designing phase-field models and algorithms.

For a given Griffith toughness G_c and given domain $\Omega \subset \mathbb{R}^N$, we consider the energy

$$E(u) := \frac{1}{2}\int_\Omega |\nabla u|^2 dx + G_c \mathcal{H}^{N-1}(S_u),$$

defined for $u \in SBV(\Omega)$, a space that allows only smooth and discontinuous variation; S_u is the discontinuity set of u, and $\mathcal{H}^{N-1}(S_u)$ is its $N-1$-dimensional surface area. For simplicity, we consider the elastic energy density $\frac{1}{2}|\nabla u|^2$, which can be replaced with $W(\nabla u)$ for a large class of elastic energy densities W, without significantly changing the analysis. Also, the surface energy $G_c\mathcal{H}^{N-1}(S_u)$ can be replaced when there is a spatially-varying toughness: the new surface energy would be

$$\int_{S_u} G_c(x) d\mathcal{H}^{N-1}(x),$$

but for simplicity here we consider G_c to be constant. For future brevity, we will refer to the first term in E, the elastic potential energy, as $P(u)$ and the second, the surface energy, as $S(u)$.

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Each E_ε is defined on pairs of functions in $H^1(\Omega)$, and is given by

$$E_\varepsilon(u,v) := \frac{1}{2}\int_\Omega (\eta_\varepsilon + v^2)|\nabla u|^2 dx + G_c\left(\frac{1}{4\varepsilon}\int_\Omega (1-v)^2 dx + \varepsilon\int_\Omega |\nabla v|^2 dx\right), \tag{2.1}$$

where η_ε tends to zero faster than ε (the details are explained below). As above, we will refer to the first term in (2.1), the approximate elastic potential energy, as $P_\varepsilon(u,v)$, and the second, the approximate surface energy, as $S_\varepsilon(v)$.

Γ-convergence concerns relationships between the energies $E_\varepsilon(u_\varepsilon, v_\varepsilon)$ and $E(u)$ as $\{u_\varepsilon\}$ converges to some u (and $\{v_\varepsilon\}$ converges to 1). In particular, two conditions must be satisfied: first, whenever $u_\varepsilon \to u$ in L^1 and $v_\varepsilon \to 1$ in L^1, it must be that

$$\liminf_{\varepsilon\to 0} E_\varepsilon(u_\varepsilon, v_\varepsilon) \geq E(u). \tag{2.2}$$

Second, for every $u \in SBV(\Omega)$, there must exist $\{u_\varepsilon\}, \{v_\varepsilon\}$ such that $u_\varepsilon \to u$ in L^1 and $v_\varepsilon \to 1$ in L^1, and

$$\limsup_{\varepsilon\to 0} E_\varepsilon(u_\varepsilon, v_\varepsilon) \leq E(u), \tag{2.3}$$

which, with (2.2), implies

$$\lim_{\varepsilon\to 0} E_\varepsilon(u_\varepsilon, v_\varepsilon) = E(u). \tag{2.4}$$

In the above, convergence in L^1 can be replaced by convergence with respect to other norms.

Practically, there are two important issues regarding the convergence of these phase-field models. The first is, is ε small enough that we get a good approximation of minimizers of the limit energy, and of this energy? Here, ε plays at least two roles: it sets the width of the smeared crack approximation, and it needs to be small enough that v is close to 1 except near cracks. Often, this second role is not satisfied, and we see significant softening of the material away from the crack (throughout, by "softening", we mean that v is not close to 1 in some region). Sometimes this softening leads to nucleation, i.e., v continues to decrease until it is close to zero, and sometimes it does not, but still is significant in its effect on the stresses away from the crack, as well as affecting how irreversibility can be implemented.

The second issue comes from the fact that u_ε and v_ε come not from directly minimizing, but from following certain energy descents. As we will see below, this can be a plus, as certain behavior along energy descents seen as undesirable, such as softening, can be blocked without affecting the Γ-convergence.

We also note that the energy convergence (2.4) is merely a possibility, and generally holds only if $u_\varepsilon, v_\varepsilon$ are obtained by minimizing E_ε. As we discuss in more detail below, alternate minimization, or any energy descent, for this phase-field energy E_ε does not necessarily result in energy minimizers.

We now sketch how this convergence of E_ε to E works, so we can see what modifications to E_ε leave the Γ-convergence unchanged.

2.1. *The first term:* $P_\varepsilon(u,v) = \frac{1}{2}\int_\Omega (\eta_\varepsilon + v^2)|\nabla u|^2 dx$

The role of η_ε is explained separately below, and for now we take $\eta_\varepsilon = 0$ for simplicity. We are left with just $\frac{1}{2}v^2|\nabla u|^2$, and the idea is very simple: where $v = 0$, this energy density is zero, and ∇u can concentrate there for free. Where v is close to 1, which is everywhere except for a small set due to the S_ε energy, we just get $\frac{1}{2}|\nabla u|^2$, the elastic energy density, and (2.2) (for P_ε and P) just follows from lower semicontinuity. (2.3) (for P_ε and P) follows by considering $u_\varepsilon = u$ away from the discontinuity set. An important point for later is, where v transitions from near 0 to near 1, the only role $\int v^2|\nabla u|^2$ plays in the Γ-convergence is to be small.

2.2. *The second term:* $S_\varepsilon(v) = G_c\left(\frac{1}{4\varepsilon}\int_\Omega (1-v)^2 dx + \varepsilon\int_\Omega |\nabla v|^2 dx\right)$

The analysis of this term involves two parts. The first is technical, and consists of a slicing argument, showing the problem reduces to the one dimensional case. The second part is treating that one dimensional case, and that is what we focus on here.

The basic idea is this: if we consider functions v on $\mathbb{R}$ satisfying $v(0) = 0$, and $v(x) \to 1$ as $|x|$ goes to infinity, a calculation shows that the minimum of $S_\varepsilon(v)$ is G_c. When ε is small, this energy over $\mathbb{R}$ is a good approximation of S_ε on a finite interval. If u_ε is converging to a u with a discontinuity, for $E_\varepsilon(u_\varepsilon, v_\varepsilon)$ to remain bounded, it must be that $v_\varepsilon = 0$ near a discontinuity point, so ∇u_ε can concentrate for free. The cost of this discontinuity comes from $S_\varepsilon(v_\varepsilon)$, and is G_c if v_ε optimally transitions from 1 to 0 back to 1, minimizing S_ε.

It should be noted that the term $(1-v)^2$ in S_ε (often referred to as AT2) can be replaced with other penalties on $|1-v|$, such as $|1-v|$ itself (AT1), with appropriate adjustment of coefficients so the minimum for the new S_ε is also G_c.

2.3. *The role of* η_ε

Without η_ε, E_ε would not have a minimum (which actually does not matter for Γ-convergence). For numerics, η_ε is typically very small, something like 10^{-6}. Exactly how small it needs to be, we will return to shortly. The point of η_ε is to make sure $|\nabla u|^2$ is never multiplied by zero, but it must be small enough that it has a vanishing effect on the energy. A side effect of this term is a limit on how much $|\nabla u|$ concentrates.

Returning to the 1-D case, if ∇u concentrates in an interval I of length h, with $v = 0$ on I, then by convexity the cheapest way to do that is to have $|\nabla u| \propto \frac{1}{h}$ on I. Then $\int_I \eta_\varepsilon |\nabla u|^2 \propto \frac{\eta_\varepsilon}{h}$. This creates an extra contribution to $S_\varepsilon(v)$, namely, $\frac{1}{4\varepsilon}\int_I (1-v)^2 \approx \frac{h}{4\varepsilon}$, since v must be close to zero on I, where ∇u concentrates.

So, both $\frac{\eta_\varepsilon}{h}$ and $\frac{h}{4\varepsilon}$ must go to zero as ε goes to zero. That is, h is small compared to ε, and η_ε is small compared to h. Now, mathematically, only ε and η_ε are specified – h is a result of minimizing E_ε. If $\eta_\varepsilon = o(\varepsilon)$, e.g., $\eta_\varepsilon = \varepsilon^2$, then the h selected by minimization will be such that both $\frac{\eta_\varepsilon}{h}$ and $\frac{h}{4\varepsilon}$ go to zero, such as $h = \varepsilon^{\frac{3}{2}}$.

However, computationally, a lower bound for h is set by the mesh size. This is fine for $\frac{\eta_\varepsilon}{h}$, but typically it means $\frac{h}{\varepsilon}$ is not very small, giving an extra contribution of $G_c\frac{h}{4\varepsilon}$ to the fracture toughness, for an overall toughness of $G_c(1 + \frac{h}{4\varepsilon})$. AT1 has a similar extra contribution.

2.4. *Summary*

The role of v in P_ε is only to provide a place for ∇u to concentrate essentially for free, by v being small on some small set. The price for this concentration is paid only by v in the surface energy S_ε, in the cost of making transitions from 1 to 0, and back to 1.

There are two key points here. First, looking only at P_ε, u_ε can converge to a discontinuous function, with zero cost here. The cost comes completely from S_ε – v_ε must make a transition from being (close to) 1, going down to zero, and then back up to 1. S_ε penalizes this double transition, and the coefficients in S_ε are chosen so that the optimal way of making these transitions has cost 1. These transitions occur on the scale of ε, so in the limit $\varepsilon \to 0$ they, but not their effect, disappear.

Again, our main observation is the following: the role of v in the first term in E_ε is to be very small somewhere, providing a place for u to concentrate its gradient *at no cost.* The cost is paid only by v in S_ε, for providing such a location for ∇u to concentrate. Here is the key: where v makes the transition from near 0 to near 1, the term $v^2|\nabla u|^2$ plays no important role in the Γ-convergence. In fact, it is unnecessary to even consider $v^2|\nabla u|^2$ in this region. Yet this product, in this region, is what produces both softening and nucleation. Any modification of P_ε that removes the interaction between v and u where v is not very small *has no effect* on the Γ-convergence, but it will stop softening and nucleation.

3. Energy descents: softening and nucleation

In practice, the energies E_ε are not actually minimized. For static and quasi-static fracture, alternate minimization of E_ε is used (subject to some irreversibility condition), repeatedly minimizing in u and then v until some criterion is met. E_ε is not convex, but it is separately convex, that is, if u is fixed, the map $v \mapsto E_\varepsilon(u,v)$ is convex, and if v is fixed, $u \mapsto E_\varepsilon(u,v)$ is convex. So the natural way to attempt to minimize E_ε is alternate minimization: fix, say, an initial u_0, minimize $v \mapsto E_\varepsilon(u_0,v)$, obtaining v_0. Then minimize $u \mapsto E_\varepsilon(u,v_0)$, obtaining u_1, etc. We can at most expect this to converge to something stationary (see, e.g., [5,6]).

In dynamics, $v \mapsto E_\varepsilon(u,v)$ is minimized at each time step, and updates to u come from elastodynamics, with stiffness $\eta_\varepsilon + v^2$. Therefore, there is no alternate minimization — there is one minimization in v, and one time step in u. Much of the modifications we discuss below apply equally to dynamics.

3.1. Static and quasi-static evolution: energy descents

The interaction between u and v in E_ε is only in the product $v^2|\nabla u|^2$ in the first part of the energy, $P_\varepsilon(u,v)$. Since this is minimized over v, as $|\nabla u|$ gets large, v will decrease to lower this product (no matter how u is evolving). $|\nabla u|$ will then tend to increase where v has decreased, thus driving v to decrease even more. This is behind both nucleation of fracture and softening.

Our main point is that this interaction is actually unnecessary for (and even unrelated to) the Γ-convergence. The product $v^2|\nabla u|^2$ matters for Γ-convergence only where v is very small, allowing u to vary essentially for free there, and v pays the price in the other term, $S_\varepsilon(v)$. But the softening caused by this interaction can be significant, both by altering the distribution of $|\nabla u|$, increasing it where the material has softened, and therefore tending to decrease its concentration at crack tips, resulting in v decreasing less at crack tips, which means the crack does not grow as fast.

On the other hand, the interaction term $v^2|\nabla u|^2$ is important for energy descents leading to crack growth. Near crack tips, $|\nabla u|$ will be large because of the geometry of the domain near the crack tip. On top of that, it will be even larger where v is less than 1 near the tip. If these effects combine to drive v to zero in front of a pre-existing crack tip, the crack grows. Note that this should only happen if the decrease in the interaction term, i.e., the elastic energy $\frac{1}{2}\int_\Omega(\eta_\varepsilon + v^2)|\nabla u|^2$, is enough to offset the increase in S_ε, i.e., G_c times the length of the crack increment, measured in S_ε by the energy of cross-sections of v across this crack increment. We return to these descents in more detail later, but we note for now that these energy descents at crack tips are desirable for allowing crack growth at crack tips.

3.2. Dynamics

The Ambrosio–Tortorelli approximation can also be used for dynamic fracture, as shown in [7]. Here, v follows the same minimization as above, namely, at each time t, $v(t)$ minimizes $E_\varepsilon(u(t),\cdot)$ (subject to some irreversibility condition). Instead of being obtained by minimization, u is obtained by solving

$$u_{tt} - \mathrm{div}([\eta_\varepsilon + v^2]\nabla u) = 0.$$

Here, softening and nucleation are more subtle than for pure minimization problems. As before, if $|\nabla u|$ gets large somewhere, v will decrease, which means the material gets softer. Then two things occur: the wave speed decreases in this region, and $|\nabla u|$ tends to increase. This last feature can be temporary, since it might be that a wave travels through this region, and afterwords the displacement is close to constant there. Of course, this also depends on how irreversibility is implemented. We just note that softening is problematic here too, just as it is in static and quasi-static settings.

3.3. Softening and the approximate surface energy

The approximate surface energy

$$S_\varepsilon(v) = G_c\left(\frac{1}{4\varepsilon}\int_\Omega (1-v)^2 dx + \varepsilon\int_\Omega |\nabla v|^2 dx\right)$$

approximates the limit surface energy

$$G_c\mathcal{H}^{N-1}(S_u)$$

only when v minimizes S_ε, subject to v being close to zero where u wants to jump, and v being close to 1 away from that set. That is, v needs to make the optimal transition, in the sense of minimizing S_ε, between the sets where v is close to zero, and where it is close to 1. To the extent the term $v^2|\nabla u|^2$ in P_ε is neither close to zero (where v is very close to zero) nor close to $|\nabla u|^2$ (where v is close to 1), it interferes with v minimizing S_ε, and artificially adds to the surface energy S_ε. This holds also for other surface energies, such as AT1.

4. Modifications preventing softening and nucleation: stopping and controlling certain energy descents

4.1. Stopping softening and nucleation

We describe one simple modification based on preserving Γ-convergence while altering softening and nucleation. We leave S_ε unchanged, and alter only the function that multiplies $|\nabla u|^2$ in P_ε: replace E_ε with

$$E_\varepsilon^\beta(u,v) := \frac{1}{2}\int_\Omega(\eta_\varepsilon + v_\beta^2)|\nabla u|^2 dx + G_c\left(\frac{1}{4\varepsilon}\int_\Omega(1-v)^2 dx + \varepsilon\int_\Omega|\nabla v|^2 dx\right),$$

where $\beta \in (0,1)$ is fixed and

$$v_\beta(x) := \begin{cases} 1 & \text{if } v(x) \geq \beta \\ v(x) & \text{if } v(x) < \beta. \end{cases}$$

There are two points to introducing this β. First, if β is small, only small values of v interact with ∇u in the $v_\beta^2|\nabla u|^2$ term, which is all that is necessary for the Γ-convergence. The profile of v is therefore relatively unaffected when it makes the transitions between 0 and 1, since it is essentially just trying to minimize S_ε, and so the cost is closer to the minimum of S_ε, which is G_c. Second, perturbing v a little below 1 does not affect v_β, and therefore does not affect $v_\beta^2|\nabla u|^2$, so that

$$\frac{\partial}{\partial v}\left(\frac{1}{2}(\eta_\varepsilon + v_\beta^2)|\nabla u|^2\right) = 0$$

wherever v is 1 (and where it is more than β). These perturbations only cause an increase in the surface energy S_ε, and so they will not occur in energy descents. Softening and nucleation are thereby prevented for any numerical scheme based on the gradient of the energy, and even for methods that consider discrete but small changes in v.

4.2. Locally switching nucleation back on

Further modifications are possible for models intended to allow nucleation, for example if nucleation occurs if $u(x), v(x)$ satisfy some condition $C(u(x),v(x))$. At such points, we want to return to the original formulation that allows softening and nucleation. One possibility is to have the β above be a function of x (and, we will see, possibly t), for example, for a static problem,

$$v_\beta(x) := \begin{cases} 1 & \text{if } v(x) \geq \beta(x) \\ v(x) & \text{if } v(x) < \beta(x), \end{cases}$$

where

$$\beta(x) := \begin{cases} 1 & \text{if } C(u(x),v(x)) \text{ holds} \\ \gamma & \text{otherwise.} \end{cases}$$

The idea is, γ somewhat plays the role of β before, and if after minimizing E_ε^β in u the condition $C(u(x),v(x))$ is nowhere satisfied, then there can be no softening or nucleation (if $\gamma < 1$), and $v(x) = 1$ (approximately) everywhere away from the crack.

On the other hand, if when first minimizing E_ε^β in u it happens that $C(u(x), v(x))$ is satisfied on some set S, then $v_\beta = v$ on S, and alternate minimization will allow v to decrease there, allowing softening and nucleation. This would initiate in S, but could end up outside S at the end of alternate minimization.

An example of such a condition is if nucleation occurs if the stress exceeds some specified value c_r. We then have

$$v_\beta(x) := \begin{cases} 1 & \text{if } v(x) \geq \beta(x) \\ v(x) & \text{if } v(x) < \beta(x), \end{cases}$$

where

$$\beta(x) := \begin{cases} 1 & \text{if } v(x)^2|\nabla u|(x) > c_r \\ \gamma & \text{otherwise.} \end{cases}$$

Put another way,

$$v_\beta(x) := \begin{cases} v(x) & \text{if } v(x) < \gamma \text{ or } v(x)^2|\nabla u|(x) > c_r \\ 1 & \text{otherwise.} \end{cases}$$

For time evolutions, either quasi-static or dynamic, we would have $u(x,t)$ and $v(x,t)$. We could consider

$$v_\beta(x,t) := \begin{cases} 1 & \text{if } v(x,t) \geq \beta(x,t) \\ v(x,t) & \text{if } v(x,t) < \beta(x,t), \end{cases}$$

where

$$\beta(x,t) := \begin{cases} \gamma & \text{if } v(x)^2|\nabla u|(x,t) \leq c_r \\ 1 & \text{otherwise.} \end{cases}$$

Another option is to have a model such that once the c_r threshold is crossed, the material is permanently open to softening and nucleation there. A corresponding β would be

$$\beta(x,t) := \begin{cases} \gamma & \text{if } v(x)^2|\nabla u|(x,\tau) \leq c_r \text{ for all } \tau \leq t \\ 1 & \text{otherwise.} \end{cases}$$

4.3. *Effect on crack growth*

v is less than 1 near the crack tip generally for two reasons. First, because it is zero in the crack, and must make a continuous transition to 1 away from the crack. Second, because $|\nabla u|$ is large there, and so the term $v^2|\nabla u|^2$ prefers v to be small. It is this second reason that is also behind crack growth, as discussed above.

If we imagine largely removing this interaction, e.g., the interaction term $v^2|\nabla u|^2$ is restricted to where v is very small:

$$E_\varepsilon^\beta(u,v) := \int_\Omega (\eta_\varepsilon + v_\beta^2)|\nabla u|^2 dx + G_c \left(\frac{1}{4\varepsilon} \int_\Omega (1-v)^2 dx + \varepsilon \int_\Omega |\nabla v|^2 dx \right),$$

$$v_\beta(x) := \begin{cases} 1 & \text{if } v(x) \geq \beta \\ v(x) & \text{if } v(x) < \beta \end{cases}$$

where now $\beta \ll 1$, then the benefit of reducing v is very small and can only occur in a small region. Nevertheless, it seems plausible that crack growth could still occur, unless β is so close to 0 that v cannot effectively decrease where it is already less than β.

Potentially depending on exactly how gradient descents are implemented, any $\beta < 1$ should be enough to prevent softening and nucleation away from the crack. However, because v will necessarily be below 1 close to the crack, there is potential for unwanted softening there, too. Numerical experiments are needed to determine values of β that sufficiently restrict softening, while allowing crack growth.

Finally, it is important when implementing phase-field models to numerically calculate the surface energy $S_\varepsilon(v)$, and compare it with estimates of the computed crack length. Softening will tend to create errors in the surface energy, artificially increasing it, and we predict that with the modifications described here, the surface energy approximations will improve.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Christopher Larsen reports financial support was provided by National Science Foundation.

Data availability

No data was used for the research described in the article.

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