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PHASE-FIELD MODELING FOR BRITTLE FRACTURE DUE TO RESIDUAL STRESS

Turbino, D. R., Aguiar, T. B., Guerra, G. M., Duda, F. P.

Diego R. D. Turbino
Thiago B. de Aguiar
Fernando P. Duda
Programa de Engenharia Mecânica, Universidade Federal do Rio de Janeiro - COPPE/UFRJ,, Brazil
diego.turbino@gmail.com, thiagoaguiar@poli.ufrj.br, duda@mecanica.ufrj.br

Gabriel M. Guerra
Departamento de Engenharia Mecânica, Universidade Federal Fluminense - UFF, Brazil
gguerra@id.uff.br

Abstract. *In this paper, we present the formulation and numerical implementation of a continuum theory for brittle fracture in elastic solids under small strains. In order to describe fracture, an extra independent kinematical descriptor, the phase or damage field, is introduced along with the corresponding balanced force system. The salient feature of this theory relies on the regularized treatment of the classical condition of damage irreversibility achieved by selecting an appropriate rate-dependent constitutive damage response. For the numerical implementation, which employs the finite-element method for spatial discretization and a backward Euler scheme for the time integration, a Python code using FEniCS is written. To illustrate its potential utility, we apply the model to simulate numerically a problem that mimics the crack nucleation and growth in a residually-stressed elastic solid from a random initial condition for the damage field which characterizes a body with heterogeneities.*

Keywords: *Phase-field, Fracture, Crack propagation, Residual stress, Finite elements*

INTRODUCTION

We consider an elastic body $\mathcal{B}$ under residual stress, which is treated via the prescription of a stress-free strain field, and capable of undergoing brittle fracture. We aim at the formulation of a theory for the behavior of $\mathcal{B}$ that provides a systematic way to describe the interplay between elastic deformation, residual stress and fracture. We select a version of theory to numerically study crack nucleation and growth in a residually-stressed elastic solid from a random initial condition for the damage field. This work builds upon Duda *et al.* (2018) where the general description of fracture is made by means of phase field and considering stress-free strains. But contrary to the mentioned work, we consider that the damage irreversibility conditions are not treated as a constraint but rather are imposed in a regularized fashion by selecting an appropriate rate-dependent damage response. Further, the stress-free strain is given rather than calculated. For a review on the of the phase -approach to brittle fracture in the presence of residual stress, we refer the reader to Salvati (2021), da Silva *et al.* (2013), Aranson *et al.* (2000) and references cited therein.

PHASE-FIELD MODEL FOR BRITTLE FRACTURE

From the standpoint of kinematics, we consider that $\mathcal{B}$ is described by the two independent fields, namely the displacement field $\mathbf{u}$ and the phase field φ, which may be interpreted as the fraction of broken bonds and takes values on the interval $[0;1]$. Then, we invoke the principle of virtual power to derive the local forms of the basic balances of the theory, namely the standard force balance and the microforce balance:

$$\mathrm{Div}\,\mathbf{S} + \mathbf{b} = 0; \quad \mathrm{Div}\,\xi + \pi + \gamma = 0. \tag{1}$$

Here and henceforth, “Div" is the divergence operator, $\mathbf{S}$, the stress tensor, $\mathbf{b}$ the body force density, ξ the microstress vector, and π and γ the internal and external microforces densities. In addition to these balances, we impose the first and second laws of thermodynamics via a free-energy imbalance, which in local form is given by:

$$\dot{\psi} - \mathbf{S}\cdot\dot{\mathbf{E}} + \pi\dot{\varphi} - \xi\cdot\nabla\dot{\varphi} \le 0, \tag{2}$$

where ψ is the free-energy density, $\mathbf{E} = \frac{1}{2}\left[\nabla\mathbf{u} + \nabla\mathbf{u}^{\top}\right]$ the infinitesimal strain tensor, and ∇ the gradient operator.

We now turn to the constitute equation. Guided by the free-energy inequality, we consider response functions for ψ, $\mathbf{S}$, $\mathbf{xi}$, and π in terms of $(\mathbf{E}, \varphi, \nabla\varphi, \dot{\varphi})$, obeying Eq. (2) in every admissible process. In this case, it can be shown that the free-energy can not depend on $\dot{\varphi}$ and the following relations must hold:

$$\mathbf{S} = \frac{\partial\psi(\mathbf{E},\varphi,\nabla\varphi)}{\partial\mathbf{E}}; \quad \xi = \frac{\partial\psi(\mathbf{E},\varphi,\nabla\varphi)}{\partial\nabla\varphi}; \quad \pi = -\frac{\partial\psi(\mathbf{E},\varphi,\nabla\varphi)}{\partial\varphi} - \beta(\mathbf{E},\varphi,\nabla\varphi,\dot{\varphi})\dot{\varphi}, \tag{3}$$

with $\beta(\mathbf{E},\varphi,\nabla\varphi,\dot{\varphi}) \geq 0$. Thus, from the constitutive point of view the theory is defined by two scalar response functions, one for the free energy ψ and other for the kinetic modulus β. Here, we focus our attention on the response function

$$\psi(\mathbf{E},\varphi,\nabla\varphi) = \frac{(1-\varphi)^2}{2}\left(\lambda(\mathrm{tr}\,(\mathbf{E}-\mathbf{E}_0))^2 + 2\mathrm{G}|\mathbf{E}-\mathbf{E}_0|^2\right) + \frac{g_f}{2l}\left(\varphi^2 + l^2(\nabla\varphi)^2\right) \tag{4}$$

for the free energy. Here, λ and G are the Lamé moduli, $\mathbf{E}_0$ the stress-free strain, g_f the fracture energy, and l a characteristic length. As for the response for the kinetic modulus, we assume that

$$\beta(\dot{\varphi}) = \frac{\beta^+ + \beta^-}{2} + \left(\frac{\beta^+ - \beta^-}{2}\right)\tanh(\kappa\dot{\varphi}). \tag{5}$$

for the free energy and kinetic modulus, where β^+, β^- and κ are positive parameters. See Fig. 1.

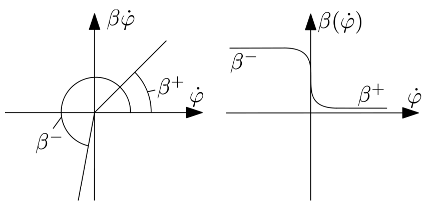

Figure 1. Penalization of the kinetic coefficient β for irreversibility hypothesis.

A standard hypothesis for fracture modeling is that $\dot{\varphi} \geq 0$, in this case the damage at each point of the body is irreversible in time. In this paper, we incorporate this condition in a regularized manner by choosing β^- high enough.

NUMERICAL APPLICATION AND RESULTS

It is sought to verify the numerical behavior of the exposed phase field model by applying residual stresses under the formulation of a two-dimensional problem, namely a plane-strain state. For this, consider the scheme shown in Fig. 2 where item (a) demonstrates a two-dimensional body governed by Eqs.(1), whose constitutive equations follows the Eqs.(3), (4) and (5). Some considerations are important to be defined to solve this problem: the first one is the term $\Delta\mathrm{T}$ which indicates a residual stress modeling that will be imposed on the model, equivalent to a problem of a cooling metal specimen being constrained whose deformation follows the additive decomposition of a elastic and a thermal part, in which α and $\Delta\mathrm{T}$ will be the only parameters with the analogous idea to a coefficient of thermal expansion and the variation of temperature in relation to the state without thermal stresses: $\mathbf{E} = \mathbf{E}_e + \mathbf{E}_0$; $\mathbf{E}_0 = (\alpha\Delta\mathrm{T})\mathbf{I}$

The second consideration of the problem is the periodic boundary conditions that characterize a numerical model of a sufficiently extensive domain that ignores edge effects, that is, the values of the two variables of the problem in a contour are equal to the one of the opposite contour, as defined in Eq. $(6)_{1,2}$. The third consideration refers to the initial condition of the problem: once a stress concentrator is needed to the nucleation of a crack, a hypothesis to approximate the modeling of a body with imperfections is to consider that each point of the mesh has an initial random damage ($0 \leq \varphi \leq 0.5$), according to item (b) of Fig. 2 and the Eq. $(6)_3$.

$$\begin{cases} \varphi(x,0,t) = \varphi(x,1,t);\ \mathbf{u}(x,0,t) = \mathbf{u}(x,1,t) & \text{at} \quad \Gamma_{P_x}, \\ \varphi(0,y,t) = \varphi(1,y,t);\ \mathbf{u}(0,y,t) = \mathbf{u}(1,y,t) & \text{at} \quad \Gamma_{P_y}, \\ \varphi(x,y,0) = \varphi_0 & \text{at} \quad t = 0s \end{cases} \tag{6}$$

In Eq. (6), is defined: $\Gamma_{P_x} = \{(0,y) \cup (1,y) \subset \partial\Omega\}$, $\Gamma_{P_y} = \{(x,0) \cup (x,1) \subset \partial\Omega\}$ and $\varphi_0 = \{\varphi_0 \in \mathbb{R} \mid \varphi_0 \in (0, 0.5)\}$. The parameters used, inspired by the simulations of Miehe *et al.* (2010) and Kuhn and Müller (2010), follow Tab. 1, the generated mesh is structured and has 20.000 triangular elements, necessary refinement to have numerical convergence in the propagation interface described by the characteristic parameter l. For the spatial discretization of the elements, we consider for the calculation of the variable of the displacement vector $\mathbf{u}$ triangular quadratic elements and for the calculation of the damage φ triangular linear. For the temporal discretization, for reasons of simplicity and stability, the implicit Euler method was used. The computational simulation code was all developed in Python using the *FEniCS*

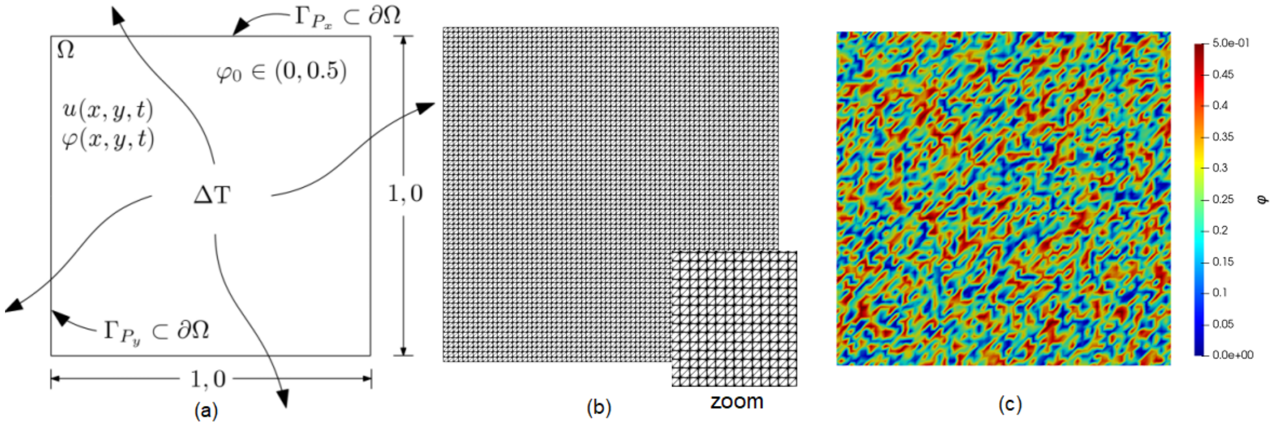

Figure 2. (a) Body under residual stresses with boundary and initial conditions. (b) Structured triangular mesh (c) Random initial damage condition at t=0s.

Table 1. Elastic, fracture and numerical parameters of the computational simulation.

E (kN/mm^2)	ν	g_f (kN/mm)	Δt (s)	l (mm)	β^+ (kN.s/mm^2)	β^- (kN.s/mm^2)	κ	$\alpha\Delta$T
1.0	0.3	0.001	1.0	0.02	0.1	1500.0	10.0	1.0

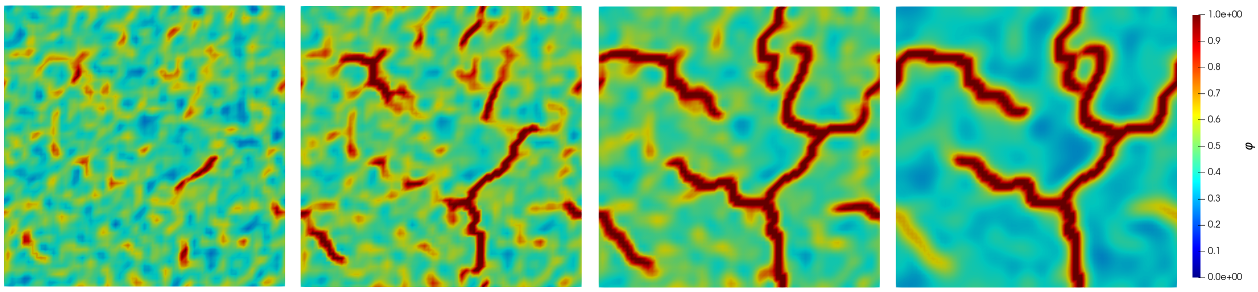

Figure 3. Damage evolution in t=2000s, t=2500s, t=3000s and the equilibrium state at t=5000s.

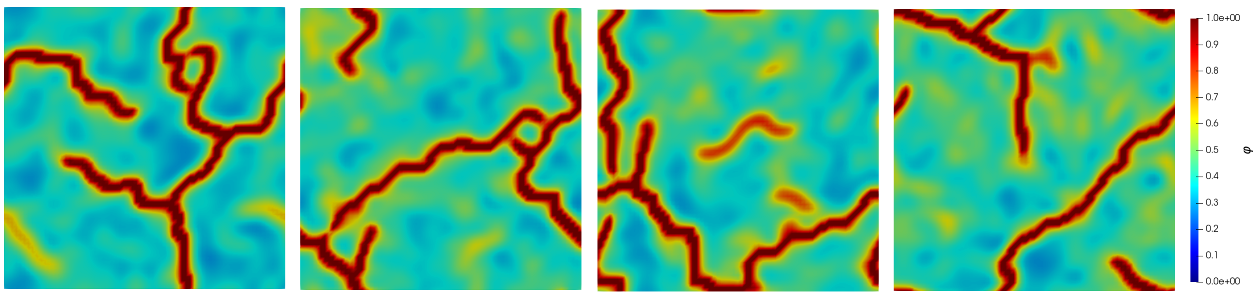

Figure 4. Equilibrium state of four simulations with different random initial conditions at t=5000s.

finite element library for solving partial differential equations. The jobs were run in parallel mode using four cores of a intel i7 computer with 8GB of RAM taking about four hours of wll-time to reach the final equilibrium state in which the cracks stop propagating. The results were post-processed through the open-platform Paraview tool.

In Fig. 3 is shown the evolution of damage over time in the body in which the nucleation of the first few cracks occurs around $t = 2000s$ followed by its propagations at $t = 2500s$ and $t = 3000s$. Finally, at $t = 5000s$ is shown the state of equilibrium, in which there is no further damage evolution, the cracks do not propagate anymore and there are no more new nucleation points, only a tiny regeneration rate already penalized by the developed formulation.

In Fig. 4, due to the random initial conditions of each of them, four states of different equilibria are shown at $t = 5000s$ The fact that they reach equilibrium at similar times shows that the magnitude of the residual stresses is the main factor responsible for the evolution of the fracture process, and further analysis is necessary to study this phenomena.

CONCLUSION

The paper presented a phase-field model for brittle fracture accounting for the presence of residual stresses, wherein damage irreversibility was imposed by penalizing damage healing. A solver suitable to linear and isotropic elastic solids was developed using the finite element method and implemented in Python with the aid of *Fenics* library. As an illustrative example, we considered the nucleation and propagation of crack patterns due to thermal-induced residual stresses. When considering random initial conditions, we observed the expected variability of the crack patterns, with the corresponding steady-states reached at similar times. As a subsequent step, we will investigate how the model parameters impact the predictive power and numerical performance of proposed phase-field model.

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