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Evaluation of phase-field models for fracture with an explicit time integration scheme.

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Abstract — We propose different staggered resolution strategies of the variational phase field fracture formulation using a fully explicit time integration scheme. Parabolic or hyperbolic partial differential equations (PDE) are two alternatives governing the damage evolution and compatible with explicit solvers. We have implemented these models and compared with the standard elliptic damage formulation. The results show globally similar qualitative behavior, but highlight the challenge in the interpretation of additional physical parameters introduced in the damage PDE of the phase field models.
Keywords — Phase field model, fast crack propagation, explicit time integration scheme, hyperbolic and parabolic PDE.

Introduction

Phase field models are originally used in computational mechanics to simulate continuous phase transfer reactions *e.g.* material solidification processes. Toward the end of the twentieth century, advanced numerical models in fracture mechanics have been proposed using variational phase-field modeling. Among them, the one of Francfort and Marigo [1] have presented an energetic variational approach based on Griffith's theory to handle quasi-static brittle failure mechanisms. Bourdin et al. [2] reviewed the related numerical methods. The model has known an increasing interest in the field computional damage mechanics. Since then, many improvements have been brought in phase-field numerical strategies especially for the quasi-static regime. Considering transient loads leads to an extension of the phase-field models into a dynamic framework. Because of phase-field formulations nonlinear features, implicit time integration schemes are mainly used in numerical resolution strategies contrary to explicit time integration schemes which are less considered, although they are among the most common strategies to solve fast transient dynamic phenomenologies.

1 Phase-field modelling for fracture in dynamics

1.1 Context and approach

Phase-field models involve a minimization of a regularized two-field energy functional. The free discontinuity problem is approximated by the evolution of continuous displacement and damage fields governed by a unique coupled system of equations. In a dynamic framework, the energy functional, commonly named the Lagrangian L^{dyn} (Eq. 1) , is composed of the kinetic, elastic, and fracture energies. The fracture energy is the product of a the critical energy released rate G_c and the integral of a crack surface density function γ. This density is introduced by an approximation proposed by Bourdin et al. [2] based on the Mumford-Shad potential and depends of the damage gradient $\underline{\nabla} d$, a characteristic internal length l_c and a potential function $w(d)$, allowing to control the damage spatial diffusion.

$$L^{dyn}(t,\underline{u},\underline{\dot{u}},d,\dot{d}) = \int_\Omega \frac{\rho_u}{2}\underline{\dot{u}}^2 dx - \left(\int_\Omega \Psi\left(\underline{\underline{\varepsilon}}(\underline{u}),d\right)dx + \int_\Omega G_c\gamma(d,\underline{\nabla} d)\,dx - P_{ext}(\underline{u})\right) \tag{1}$$

The system of equations of the phase field fracture problem is derived from Euler-Lagrange equations (Eq. 2). It leads to the classical hyperbolic form of the displacement governing equation and a standard elliptic one for the damage equation. In the equation (Eq. 2b), the term $-g'(d)H(\underline{u})$ represents the driving force and it is defined as the product of a degradation function g and an history variable H introduced by Miehe et al. [3] to ensure the irreversibility condition of the damage evolution. This constraint is a method among many others.

$$\rho_u \ddot{\underline{u}} = \underline{\mathrm{div}}(\underline{\underline{\sigma}}) + \underline{b} \quad \text{on} \quad \Omega_u, \quad -\underline{\underline{\sigma}} \cdot \underline{n}_s + \underline{t} = \underline{0} \quad \text{on} \quad \partial\Omega_u \tag{2a}$$

$$g'(d)H(\underline{u}) + G_c\left(\frac{w'(d)}{c_w l_c} - 2l_c \underline{\nabla}^2 d\right) = 0 \quad \text{on} \quad \Omega_d, \quad \frac{\partial\gamma}{\partial\underline{\nabla} d}\cdot\underline{n}_d = 0 \quad \text{on} \quad \partial\Omega_d \tag{2b}$$

The elliptic form of the damage equation is mainly solved using iterative methods. Although implicit methods are unconditionally stable, the use of linear system solvers can make the resolution cumbersome for large problems. To overcome these cost issues, explicit time integration schemes is another alternative. These approaches allow the use of lumping techniques operated on the mass matrix related to the second order term. It's diagonalization shrinks the resolution to a single, vector/vector Hadamard product, hence a reduction of computational costs.
Since the elliptic form is not adapted for it, it is necessary to update the damage formulation to a direct time-dependent model *i.e.* one involving a parabolic [3, 4, 5] or an hyperbolic [6, 7] partial differential equation. The use of a dissipative process in the Lagrangian allows three different damage formulations of the phase field model. (a) The elliptic one without direct time dependency of the damage field (Eq. 2b). (b) The parabolic one, introducing a damage rate $\dot{d}$ and a viscous regularization η in the governing equation (Eq. 3) with $\rho_d = 0$. A damping term $\left(\frac{\eta}{2}\dot{d}^2\right)$ is incorporated in the energy functionnal and turns the system into a non-consertative one. (c) And finally the hyperbolic one (Eq. 3), including a damage inertia ρ_d related to the damage field. This form is derived from a Lagrangian function including a new kinetic energy associated to a damage inertial effect $\frac{\rho_d}{2}\dot{d}^2$.

$$\rho_d \ddot{d} + \eta\dot{d} + g'(d)H(\underline{u}) + G_c\left(\frac{w'(d)}{c_w l_c} - 2l_c \underline{\nabla}^2 d\right) = 0 \quad \text{on} \quad \Omega_d, \tag{3}$$

For an explicit time integration scheme a critical time step exists above which the stability cannot be ensured. In the general case, the time step of hyperbolic PDEs evolves linearly with the smallest mesh size h compared to a quadratic evolution h^2 for parabolic formulations. The time step resulting from the damage equation of the phase field models shows a dependence on material and energetic parameters such as the positive elastic energy density, $\Psi^+\left(\underline{\underline{\varepsilon}}(\underline{u}), d\right)$. This point can be a drawback in the resolution because it drastically reduces the critical time step at the crack initiation and during crack propagation. Some studies of the literature based on a fully explicit resolution proposed approximated expressions of the critical time step. The time steps used in their resolution are small enough to satisfy the stability, although they don't follow a rigorous analysis on the critical time step.

The physical evolution induced by parabolic and hyperbolic formulation is another aspect often unclear in damage fracture modelling. Although the parabolic and hyperbolic PDE enable to control time evolution of crack propagation, they are generally used to model different phenomena. Indeed, the parabolic one describes a diffusive behavior with a damage velocity weighted by viscous parameters. Whereas the hyperbolic one describes wave propagation mechanisms featured by a viscosity and an inertia related to damage field. An interesting comparison has been initiated by Kamensky [7] between the elliptic and the hyperbolic formulations. He proposed some guidelines in the choice of the parameters in the hyperbolic form of the equation. The difficulty remaining today is to bring physical interpretation of these choices.

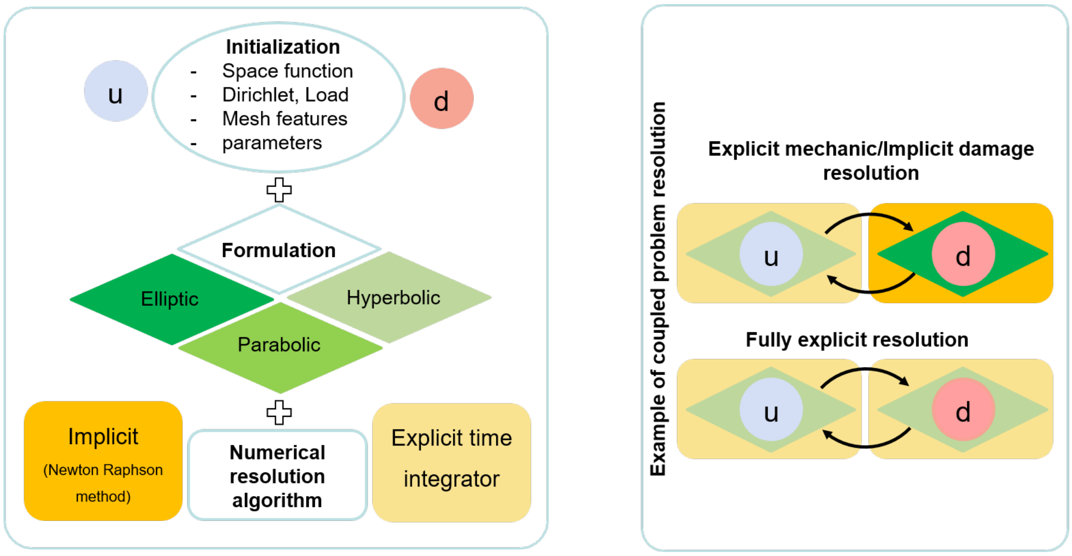
To deal with these issues, one of the objectives of the present work is to provide first indicators in the use of parabolic and hyperbolic governing equations solved with explicit time integration schemes. Meanwhile, the first results will help to determine to what extent the approximated critical time steps are sufficient to ensure the stability condition of the explicit resolution schemes.

1.2 Implementation

To solve the variational phase-field problems, three staggered strategies have been implemented, depending on the damage governing equation used. Staggered methods allow to propose different resolution schemes for each equation of the coupled problem. For the all the resolution, an explicit, central difference time intergration scheme is used to solve the hyperbolic mechanics PDE. Regarding the damage evolution, three alternatives are studied:

- An elliptic damage evolution. To provide generic programming, a standard Newton-Raphson method is chosen, although the current form is linear.
- A parabolic evolution. The forward Euler time integration methods is used. A lumped "damping" matrix is used in the resolution.
- A hyperbolic evolution. A verlet time integration scheme is applied with a lumped damage inertia matrix.

Since the study considers different PDE involving different time integration methods, a versatile numerical toolbox has been implemented. Figure 1 illustrates some strategies of resolution for a coupled system of equations. The simulation are carried out on *FEniCSx* [8], a set of open-source C++ libraries interfaced with python which provides an efficient framework to solve variational problems.
The integration of the constitutive laws is handled by a code generator named *MFront* [9]. This library enables to achieve to a more portable code.



(a) A python workflow module for solving coupled problem.

(b) Python module application of coupled problem resolution.

Figure 1: Toolbox implementation interfaced with *FEniCSx* for solving different phase field fracture coupled equations. (1a) Initialization of the displacement and damage fields, formulation of the gouverning equations and resolution of these formulations with two possible time integrator. (1b) Two instances of resolution strategies. The first one proposes an explicit central difference scheme to solve the mechanical equation and a Newton-Raphson method for the standard elliptic equation of the damage field. The second one illustrates the resolution of two hyperbolic coupled formulations with explicit time integration scheme for each equation.

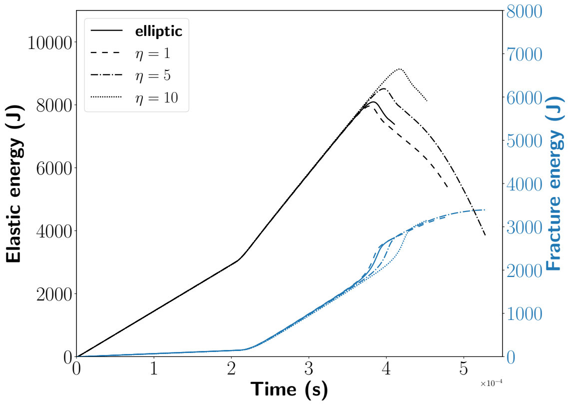
Aside the development of the toolbox, an analytical analysis was performed on the parabolic and hyperbolic PDE to assess the damage critical time step. The resulting time steps show a dependence on material and energetic parameters. Although most of the work in the literature succeed in using approximate time stepping, the knowledge of rigorous time step is important in case of stability issue encountered during the simulation.

2 Simulations and results

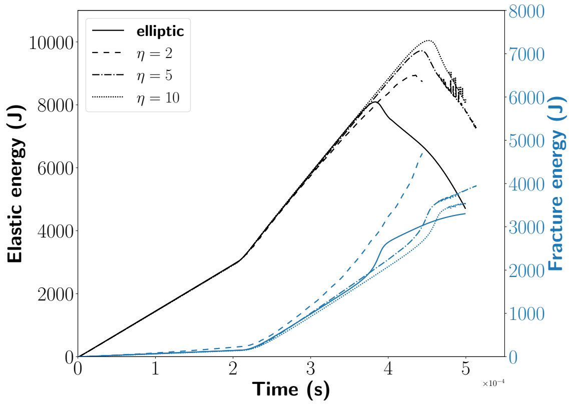
2.1 Tensile testing of a bar

Simulations of a tensile test on a bar have been carried out to better understand the influence of the model parameters in the damage formulations. We consider a fixed damage inertia ρ_d in the hyperbolic model according to an expression proposed in the literature [7]. As shown in Figure 2, hyperbolic and parabolic models introduce a delay effect in the crack onset compared to the ellitpic solution. In terms of energy, an increase of the viscious η parameter induces more stored energy and slows down the fracture dissipative process. With a hyperbolic model in figure (2b), a higher value of this η parameter is required to reduce the oscillating behaviour induced by the wave-propagation inevitably induced by the formulation itself. Indeed, we need to satisfy a overdamped condition to prevent from causing a nonphysical reversibility of the damage evolution.

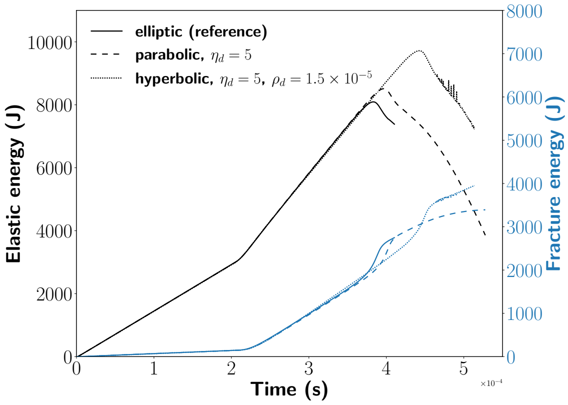
In the parabolic case, figure (2a), a decreasing viscosity induces a behavior that tends to the reference solution. However, the critical time step is expressed as a linear function of this parameter. Therefore, the viscosity η must not be set too small to avoid a small time step and thus a slow computational resolution (2d).



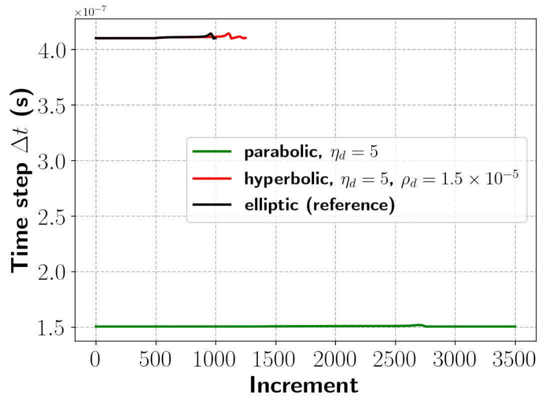
(a) Damage viscosity effect on the phase field model with a parabolic damage formulation



(b) Damping effect of the η parameter on the phase field model with a hyperbolic damage model



(c) Comparison of elliptic, parabolic, and hyperbolic model at fixed η and ρ_d model parameters



(d) Time step evolution for an elliptic, a parabolic and hyperbolic damage PDE

Figure 2: Energy balance comparison of the tensile testing of a bar for different phase field models and influence of the damage η parameter on the physical behavior of the model and on the time computational cost.

2.2 Kalthoff and Winkler test

The three implemented models have been also tested on the Kalthoff and Winkler test [10]. One half of the plate is modeled due to the assumption of symmetrical behavior and is descretized with $\approx$ 1M elements. We take into account in the material law an asymmetric fracture behavior in traction and compression. This results in strain energy density split based on an orthogonal decomposition [11]. This decomposition not only preserves the variational formalism of the phase field fracture model but also allows to extend the analysis to anisotropic materials. The viscous parameter η is set to 10 Pa.s in both hyperbolic and parabolic cases. The simulation results of the three damage governing equations show qualitatively similar crack orientations and are in good agreement with the experiments.

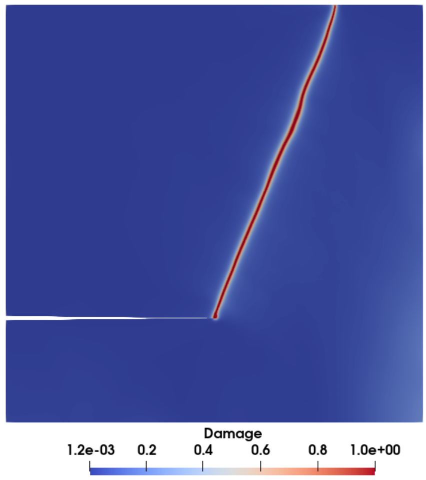


Figure 3: Kalthoff et al. test with hyperbolic damage formulation

3 Conclusion and discussion

These studies aim to propose a robust and an efficient resolution of a varitional phase field fracture formulation with an explicit time integration scheme. So far, several fully explicit strategies have been implemented and we show that each of them comes with many issues : (a) the parameter setting and (b) the time step to use.

This paper shows first results in the use of these different models, solved with explicit methods. In terms of the physical model, all PDE's seem to show globally similar qualitative results. Nonetheless, for hyperbolic PDE, the wave propagation behavior needs to be closely monitored. Indeed, the crack initiation and his propagation seems to be delayed by the features of this formulation but it is compensated by the used of a higher time step. In comparison with the parabolic model, the damage can evolve faster by the decrease of the viscious parameter but it is to the detriment of a slower computational time to satisfy the stability of the resolution scheme.

A comprehensive post-processing based on a crack velocity analysis is currently under development in order to bring more rigorous conclusions between the two parabolic and hyperbolic damage formulations both solved with an explicit time integration scheme. Indeed, the crack velocity seems to be a key element to help in the development of a criteria on the damage viscosity η and damage inertia ρ_d parameters.

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