OOP Implementation of Phase-Field Models

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Abstract. The study of fracture mechanisms to prevent the catastrophic collapse of structures is an important research trend. Among the possible approaches, the phase-field modelling, starting from a variational formulation of the Griffith's criterion, allows for a smoothed representation of a sharp crack, without the need for a discrete representation of the sharp crack itself. The phase-field modelling of fracture was recently implemented in INSANE (INteractive Structural ANalysis Environment), an open-source software based on the Object-Oriented Programming paradigm developed by a research group at the Structural Engineering Department of the Federal University of Minas Gerais (UFMG), and currently used in a number of research projects of the group. The results available in the literature and the recent advancements of the group, point out that the phase-field approach is effective for the simulation of cracks nucleation and propagation. In this paper, new results obtained with the phase-field modelling of fracture through the implementation in INSANE will be presented.

Keywords: OOP implementation, Phase-field FEM model, INSANE software

1 Introduction

Nowadays, the phase-field approach have been used as an alternative tool to deal with fracture problems. Phase-field models can detect crack nucleation and, as their main advantage, can describe a sharp crack without worrying with the sharp crack itself. For that, the model introduces a crack density function that is responsible to smooth the crack over the damaged region, and that density is controlled by the phase-field parameter that is 0 where the material is intact and 1 where is completely damaged [1, 2].

The research group of Structures Department of Federal University of Minas Gerais has a large and diverse experience concerning the formulation and implementation of models for crack representation (da Silva et al. [3], Malekan et al. [4], Wolenski et al. [5], Campos et al. [6], Wolff et al. [7], Fonseca et al. [8]), in such way that the study of phase-field approach is a natural consequence of the previous studies of the research group.

The main purpose of this article is to illustrate some details of the implementation of phase-field models done in *INSANE*[1] (INteractive Structural ANalysis Environment), an open source software developed in Java by the research group since 2002, pointing out the advantages of the adopted Object Oriented Programming (OOP) paradigm.

2 INSANE Software

To better present the OOP organization, it is necessary to make a brief introduction about the numerical core of *INSANE*, the software where the implementations were made. As pointed out in Fig. 1, it is composed by the interfaces `Assembler` and `Persistence` and by the abstract classes `Model` and `Solution`. Interface

[1]More information on the project can be found at `https://www.insane.dees.ufmg.br/` and the development code is freely available at the Git repository `http://git.insane.dees.ufmg.br/insane/insane.git`.

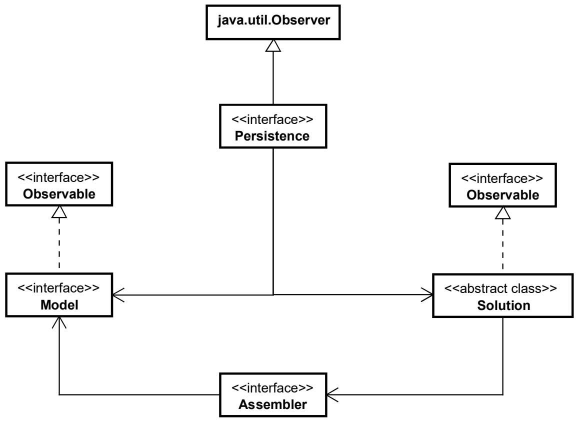


Figure 1. *INSANE* core organization (From Penna [9]).

`Persistence` manages the input/output data, while the interface `Assembler` defines the methods that are necessary for the assembly of the system of equations. The abstract class `Model` allows the representation of a generic discrete model in the numerical core of the software, by storing elements, nodes, loadings, etc. Finally, the abstract class `Solution` provides a set of methods devoted to the solution of different problems.

The classes inheritance was widely used in order to adapt the phase-field model implementation to the OOP generalisation existing in *INSANE*. The following classes and interfaces are of fundamental importance for the development of this work:

- `Material`: Stores the material parameters like the fracture energy, the elasticity modulus, Poisson's ratio, the Energetic Degradation Function and the Geometric Crack Function.
- `ConstitutiveModel`: Responsible to calculate the constitutive material relations and the stress;
- `AnalysisModel`: Has the necessary methods to return all information inherent to the analysis model, for example, the degrees of freedom and the internal variables operator;
- `ProblemDriver`: Calculates the numerical integrals like the element incremental stiffness matrix and the residual vectors;
- `Assembler`: Mounts all vectors and matrices that are necessary to solve system of equations;
- `Step`: Implements the necessary methods to solve each step of a non linear analysis, for example, the Standard Newton Raphson.

More information on the *INSANE* numerical core organisation can be found in some papers produced by the research group with the authors belong to [10–14].

3 OOP Implementation

To implement the phase-field models, the entire process was designed in order to reduce the intervention in the code. In the UML diagrams presented throughout this section, the modified classes will be depicted in yellow, the new classes in green and the non modified classes in white.

The modification in the *INSANE* code started by the implementation of some functions that are key for phase-field modelling. They are the Energetic Degradation Function, that represents the degradation of the initially-elastic strain energy density, and the Geometric Crack Function, which determines how the phase-field will be distributed. As it can be observed in Fig. 2, the functions that were implemented are the ones defined in the papers by Alessi et al. [15], Bourdin et al. [16], Karma et al. [17], Pham et al. [18], Kuhn et al. [19].

The Energetic Degradation Function and the Geometric Crack Function directly affect the material behaviour. In this way the class `PhaseFieldMaterial` that extends the superclass `Material` was created. That class is responsible to store those functions and the parameters previously defined, like the elasticity modulus, Poisson's ratio, the fracture energy and the length scale parameter used in phase-field formulations (Fig. 3). The `PhaseFieldMaterial` class also implements the methods that return the matrices with the material properties.

The OOP implementation of the constitutive model is illustrated in Fig. 4. In this work 4 constitutive models were implemented: the isotropic model and the anisotropic constitutive models of Lancioni and Royer-Carfagni [20], Amor et al. [21] and Miehe et al. [22]. There are two approaches to solving phase-field modelling, the monolithic and the staggered solvers and it is important to emphasise that, due to the peculiarities of each solver,

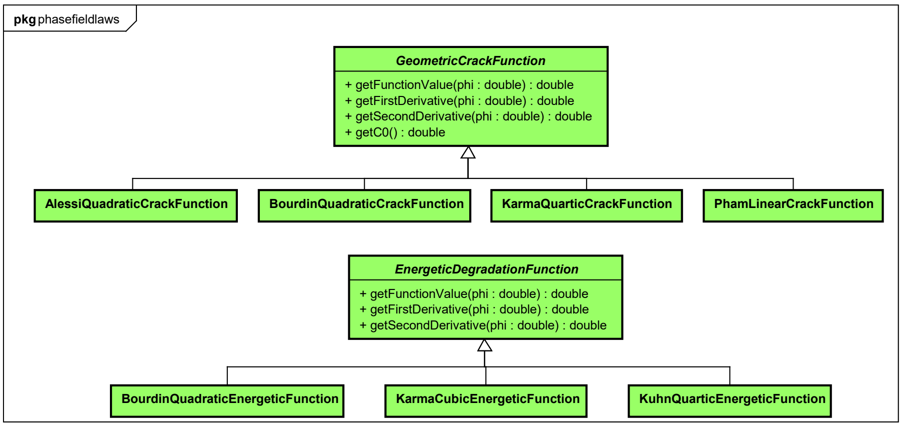


Figure 2. Package with crack geometric functions and energetic degradation functions.

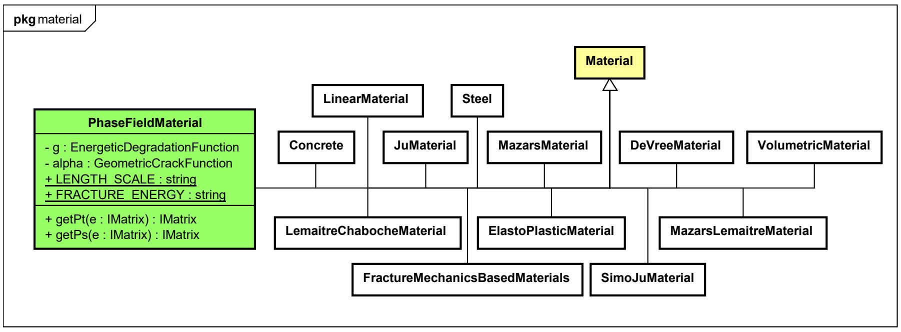


Figure 3. Package with phase-field material.

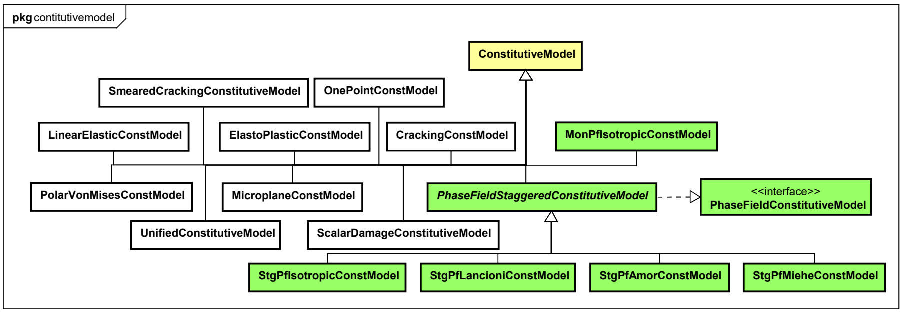


Figure 4. Constitutive model package.

the same constitutive model was implemented separately for each one. The constitutive model classes has the necessary methods to mount the tangent and secant constitutive matrices and to calculate the stress at the element integration points.

The analysis model has to be implemented separately for each type of solver due to the same reason as the constitutive model. In this work just the plane stress and plane strain analysis models were implemented as illustrated in the UML diagram of Fig. 5. The analysis model implements the methods that return the state and internal variables matrices and that mounts the constitutive matrix consistent with the considered analysis model. It is important to emphasize here that the constitutive model and the analysis model are independents.

When using the monolithic solver, the existing implementation of the classes `ProblemDriver`, `Assembler` and `Step` was enough to deal with the phase-field analysis. When using the staggered solver, on the other hand, new classes that inherit the already existent ones had to be created to deal with the decoupled equations that characterise the staggered solver. The `ProblemDriver` calculates the decoupled phase-field element stiffness matrix, the Assembler mounts the decoupled vectors and matrices regarding to Phase-Field variables and the Step calculates, in staggered iterations, the results for displacement and phase-field [23].

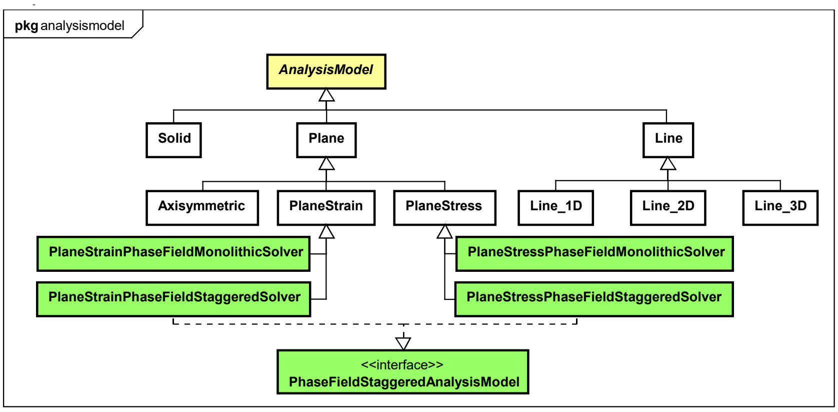


Figure 5. Analysis model package.

4 Numerical examples

In this section some numerical examples to highlight the generality of the presentation will be presented. It is made a comparison between the monolithic and staggered solvers and between the implemented constitutive models. Later, the ability of phase-field to detect crack nucleation is performed.

4.1 Comparison between monolithic and staggered solver

The setting depicted in Fig. 6.a is used to compare the monolithic and staggered solver. The model is subjected

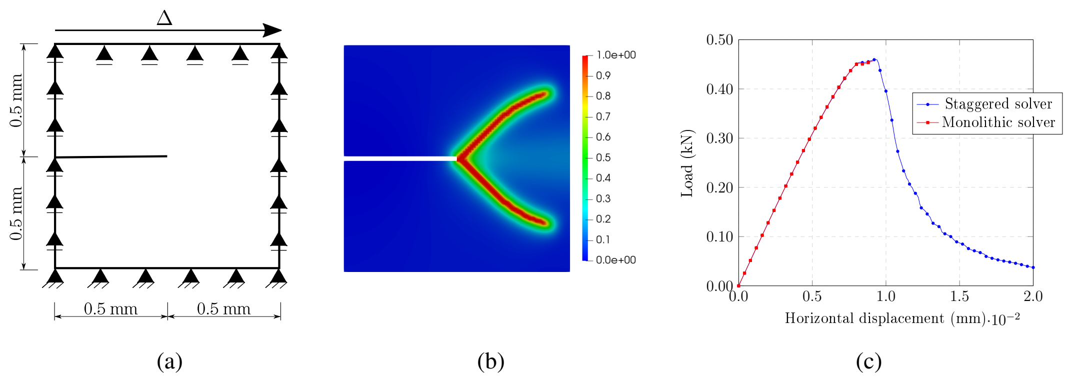


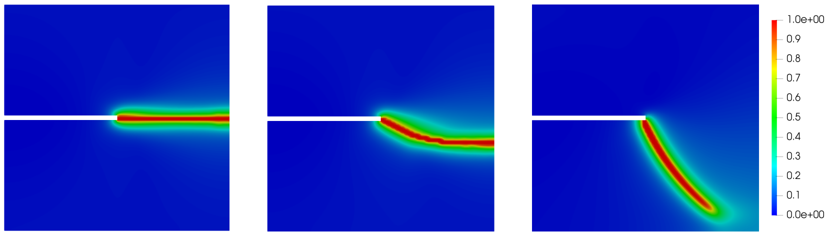
Figure 6. Shear test. (a) Problem setting, (b) Phase-field contour plot for staggered solver at the lest step, (c) Load-displacement curve.

to a plane strain state with the a fixed bottom edge and the other edges restrained in the vertical direction. A constant horizontal displacement is imposed at all nodes of the top edge. The mesh is composed by four nodes quadrilateral elements with size of $0.01\ \mathrm{mm}$. The isotropic constitutive model was considered with the following material parameters: elasticity modulus $E_0 = 210\ \mathrm{kN/mm^2}$, Poisson's ration $\nu = 0.2$, fracture energy $G_c = 0.0027\ \mathrm{kN/mm}$ and length scale $l_0 = 0.02\ \mathrm{mm}$.

The results presented in Fig. 6.c show that the monolithic solver loses convergence as soon as the crack starts to propagate. On the other hand, the staggered solver is able to continue the analysis until it reaches the defined step limit.

4.2 Comparison between constitutive models

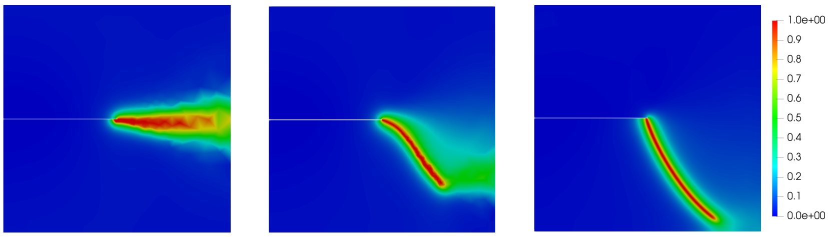
In order to compare the constitutive models two different meshes were considered, one of them the same as in section 4.1 and another that will be described later. Considering the analyses obtained with the quadrilateral mesh, the resulted crack paths are shown in Fig. 7, and they are are different from the already existent in the literature. Thus, a new mesh, refined in the crack region was considered. That new mesh was composed by triangular



(a) (b) (c)

Figure 7. Phase-field profile for shear test, using quadrilateral elements, and the constitutive models of (a) Lancioni and Royer-Carfagni [20], (b) Amor et al. [21], (c) Miehe et al. [1].

elements (T3) with nodal mean distance of 0.1 mm in unrefined region and 0.002 mm in the refined region. The obtained results are shown in Fig. 8. It can be noted that Lancioni and Royer-Carfagni [20] constitutive model is



(a) (b) (c)

Figure 8. Phase-field profile for shear test, using refined mesh, and the constitutive models of (a) Lancioni and Royer-Carfagni [20], (b) Amor et al. [21], (c) Miehe et al. [1].

very unstable and mesh dependent. It would be good to repeat the analysis considering the constitutive model of [20] and a refined mesh in all domain, but that is computationally expensive in such way that is impossible with the hardware utilized in this work. The constitutive model of Amor et al. [21] has presented a little instability but, after the refinement, the results agree with already existent in literature, and the constitutive model of Miehe et al. [1] was the most stable for this test. More informations about this analysis can be found in Leão [23].

4.3 Ability to detect crack nucleation

This section presents the problem depicted in Fig. 9, adapted from Simão [24], in order to verify the ability of the phase-field modelling to detect crack nucleation. Two different tests were performed with the constitutive model of Miehe et al. [1]. For each of them the value of x and the material parameters are related in Table 1.

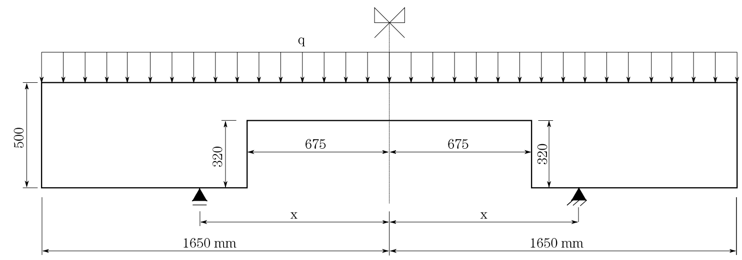
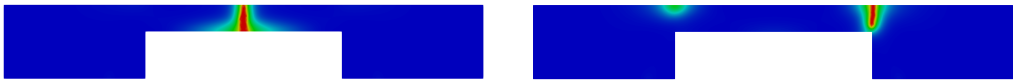


Figure 9. Two failure modes of a beam without initial crack. Thickness of 120 mm.

Table 1. Considered values for each test.

	$E_0(\text{kN/mm}^2)$	$G_c(\text{kN/mm})$	$l_0(\text{mm})$	x (mm)
Test 1	25	35×10^{-6}	67.6	928.60
Test 2	18	41×10^{-6}	67.6	859.50

The structure was subjected to a plane stress state and it was discretised with three nodes triangular elements with mean nodal distance of 15 mm across the domain. The reference load was defined as $q = 1$ kN/m. Fig. 10 presents the phase-field contour plot after crack propagation. The difference in the failure mode observed in both



(a) (b)

Figure 10. Phase-field contour plot. (a) For Test 1, (b) For Test 2.

cases is due to the changing of the support position, that changes the location where the highest tensile stress, responsible for crack growing, occurs. It also important to emphasise that in Test 2 the solution had localised and the crack just grows in the right side, but that could occur in the left side, or both, depending on the mesh.

5 Conclusions

The main objective of this work was to describe the OOP implementation of phase-field models. This implementation was done in the software *INSANE* and it was very clear that this software is very robust and has a great potential to include different kinds of models, due to its Object-Oriented Programming design. The legacy of the *INSANE* source code was crucial to ease all the implementation tasks required by this work, especially the existent resources for constitutive modelling and for solution of nonlinear equations.

When comparing the monolithic and staggered solvers it was observed that the monolithic solver, that solves both equations in same iteration, has presented convergence issues, stopping the incremental-iterative process when the external loads started to decrease. The staggered solver, that uncouples the problem, results in a more robust process, and was able to continue the analysis in the fracture propagation phase. The comparative study of the constitutive models showed that the model proposed by Lancioni and Royer-Carfagni [20] is very unstable and mesh dependent. The model proposed by Amor et al. [21] showed a great advance when compared to that proposed by Lancioni and Royer-Carfagni [20] but, it was the model proposed by Miehe et al. [1] that exhibited the best results, in terms of stability and mesh dependency.

The ability of phase-field to detect crack nucleation was also tested. In the tests performed the analysis was able to start the crack and continue its path, without any previous indication where the nucleation should occur. More information about phase-field modelling and the presented analysis can be found in Leão [23].

Acknowledgements. The authors gratefully acknowledge the support from the Brazilian research agencies CAPES (*Coordenação de Aperfeiçoamento de Pessoal de Nível Superior*), FAPEMIG (*Fundação de Amparo à Pesquisa do Estado de Minas Gerais*; Grant PPM-00747-18) and CNPq (Conselho Nacional de Desenvolvimento Científco e Tecnológico; Grant 309515/2017-3).

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