

# MAFELAP 2019 abstracts for the mini-symposium Numerical Methods for Phase Field Fracture Problems

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# A PARALLEL, ADAPTIVE PHASE-FIELD FRACTURE CODE

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We present an open source, finite element code to simulate crack propagation using a quasi-static fracture model. The cracks are discretized using a phase-field approach, which allows merging and joining of cracks.

We employ an efficient numerical scheme based on an active set strategy formulated as a semi-smooth Newton method. We propose a strategy for adaptive mesh refinement that saves computational time and offers a convergent scheme.

To confirm these claims, we show benchmark results that show convergence of our adaptive scheme under mesh refinement and phase field parameter. Finally, we show the parallel scalability of the algorithm on thousands of processors.

- T. Heister, T. Wick:  
Parallel solution, adaptivity, computational convergence, and open-source code of 2d and 3d pressurized phase-field fracture problems.  
Proc. Appl. Math. Mech., 2018. doi:10.1002/pamm.201800353
- T. Heister, M. Wheeler, T. Wick:  
A primal-dual active set method and predictor-corrector mesh adaptivity for computing fracture propagation using a phase-field approach  
CMAME, Volume 290, 15 June 2015, Pages 466-495. doi:10.1016/j.cma.2015.03.009

# MATRIX-FREE MULTIGRID FOR PHASE-FIELD FRACTURE PROBLEMS

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Standard matrix-based FEM requires huge amounts of memory as the number of elements increases. This non neglectable drawback can be overcome by using matrix-free methods. Such methods do not require building and storing huge linear systems, instead they compute the necessary information on the fly. Hence, such approaches need far less memory than classical methods, which makes them the method of choice for very large problems. Without the matrix at hands, the number of available solvers is very limited, i.e., direct solvers and algebraic multigrid methods are no longer possible. A class of solvers that is very suitable in this case are geometric multigrid methods. These methods do not require explicit knowledge about the matrix entries and, thus, can be applied in a matrix-free fashion. In this talk, we present a framework for the matrix-free solution to a monolithic quasi-static phase-field fracture model. The equations of interest are nonlinear and need to satisfy a variational inequality. This imposes several challenges for the implementation, which will be discussed throughout the talk. Finally, several numerical examples are presented to show the applicability and parallel scalability of the matrix-free geometric multigrid solver.

# PHASE FIELD FRACTURE MODELLING OF HYDROGEN EMBRITTLEMENT

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Hydrogen embrittlement is arguably one of the most challenging problems in traditional solid mechanics. Hydrogen is ubiquitous, diffuses rapidly through the crystal lattice, and drastically reduces the ductility and fracture toughness of metals. The sensitivity to hydrogen damage increases with the yield strength and hydrogen related failures are now pervasive in the energy, defence, transport, and construction sectors. The prevention and modelling of hydrogen-induced fracture requires capturing multiple micro-mechanical and chemical phenomena across a wide range of scales. We take advantage of recent developments in variational methods for fracture to develop a novel phase field formulation for hydrogen assisted cracking. The model builds upon a coupled mechanical and hydrogen diffusion response, driven by chemical potential gradients, and a hydrogen-dependent fracture energy degradation law grounded on first principles calculations. The coupled problem is solved in an implicit time integration scheme, where displacements, phase field order parameter and hydrogen concentration are the primary variables. We showcase the capabilities of the model by addressing engineering case studies with complex loading conditions and crack trajectories. It is found that phase field formulations for fracture are particularly suitable to capture material degradation due to hydrogen. The finite element code developed can be downloaded from [www.empaneda.com/codes](http://www.empaneda.com/codes).

# A PRIORI ERROR ESTIMATES FOR A FRACTURE CONTROL PROBLEM

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An optimal control problem governed by a time-discrete fracture propagation process is considered. The nonlinear fracture model is treated once as a linearized one, while the original nonlinear model is dealt with afterwards. The discretization of the problem in both cases is done using a conforming finite element method. Regarding the linearized case, in contrast to many works on discretization of PDE constrained optimization problems, the particular setting has to cope with the fact that the linearized fracture equation is not necessarily coercive. A quasi-best approximation result will be shown in the case of an invertible, though not necessarily coercive, fracture equation. Based on this, a priori error estimates for the control, state, and adjoint variables will be derived. The discretized nonlinear fracture model will be analyzed as well, which leads to a quantitative error estimate, while we avoid unrealistic regularity assumptions.