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pfm-cracks: A parallel-adaptive framework for phase-field fracture propagation

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ABSTRACT

This paper describes the main features of our parallel-adaptive open-source framework for solving phase-field fracture problems called `pfm-cracks`. Our program allows for dimension-independent programming in two- and three-dimensional settings. A quasi-monolithic formulation for the coupled two-component system of displacements and a phase-field indicator variable is used. The nonlinear problem is solved with a robust, efficient semi-smooth Newton algorithm. A highlight is adaptive predictor–corrector mesh refinement. The code is fully parallelized and scales to 1000 and more MPI ranks. Illustrative tests demonstrate the current capabilities, from which some are parts of benchmark collections.

Code metadata

Current code version	pfm-cracks v1.0
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2020-57
Permanent link to Reproducible Capsule	https://codeocean.com/capsule/1388732/tree/v1
Legal Code License	GNU GPL version 2 or later
Code versioning system used	git
Software code languages, tools, and services used	C++, MPI
Compilation requirements, operating environments & dependencies	deal.II, p4est, Trilinos
If available Link to developer documentation/manual	github.com/tjhei/cracks/
Support email for questions	timo.heister@gmail.com

1. Introduction

In this work, we summarize the main features of `pfm-cracks`, our open-source advanced phase-field fracture framework originally developed in [1] and further extended in [2]. Since 2015, `pfm-cracks` has been used and further extended in mainly five groups in which the authors and close collaborators have worked: Clemson University, UT Austin, Florida State University, Radon Institute for Computational and Applied Mathematics Linz, and Leibniz University Hannover.

The code is hosted at https://github.com/tjhei/cracks and is based on the finite element library deal.II [3,4]. The main features are:

1. Dimension-independent program allowing for 2D and 3D spatial problems [1,5].
2. Quasi-monolithic formulation for a coupled two-component system of displacements and a phase-field indicator variable [1].
3. An extrapolation technique to enforce a convex energy formulation [1]; algorithms for improving the temporal accuracy due to the extrapolation-time-lag are proposed in [6][Chapter 7].
4. A robust and efficient semi-smooth Newton algorithm [1].
5. Adaptive predictor–corrector mesh refinement [1].
6. High performance and parallel implementation demonstrated on up to 2048 cores and 100 million degrees of freedom [2].

The purpose of these developments is to meet the need of today's interest in a robust, efficient, and accurate framework for computing challenging fracture propagation problems using phase-field modeling. Indeed, a simple Google scholar search 'phase-field' reveals 247,000

The code (and data) in this article has been certified as Reproducible by Code Ocean: (https://codeocean.com/). More information on the Reproducibility Badge Initiative is available at https://www.elsevier.com/physical-sciences-and-engineering/computer-science/journals.

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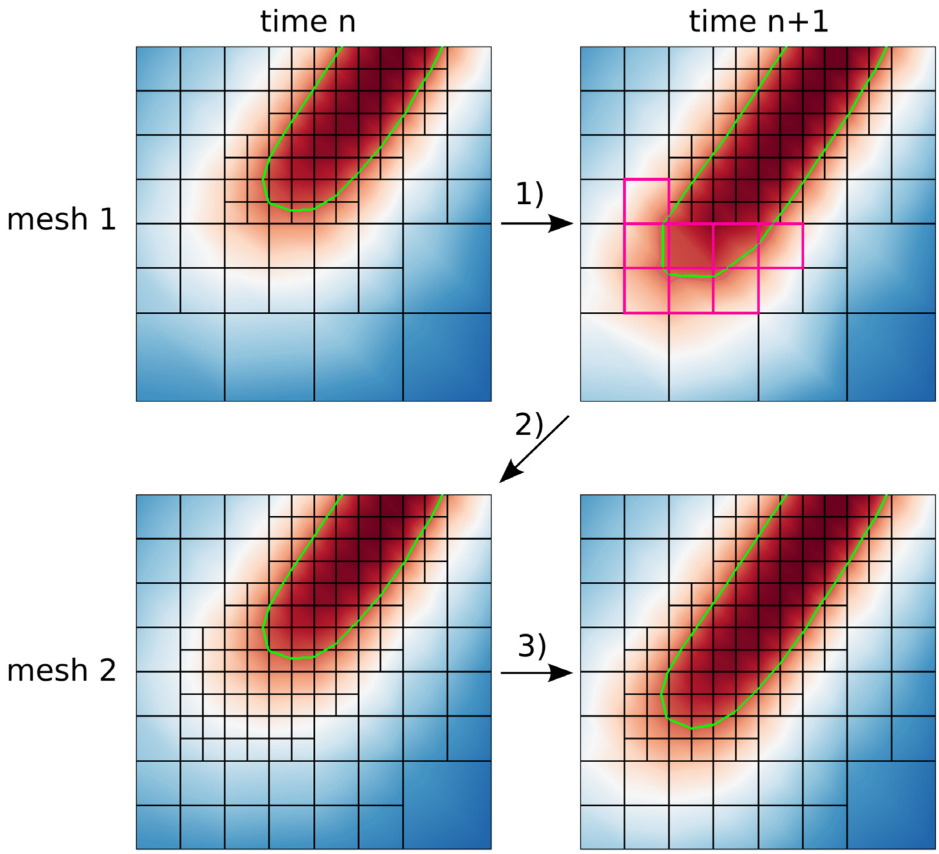

Fig. 1. Illustration of the predictor–corrector mesh refinement algorithm: (1) Advance in time, crack leaves fine mesh (cells violating the refinement condition are marked in purple). (2) Refine and go back in time (interpolate old solution). (3) Advance in time again on new mesh. Repeat until mesh does not change anymore. Refinement is triggered for $\phi < C = 0.2$ (green contour line) here. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
Source: This figure is a modified version from [1] used with permission from Elsevier.

entries and 'phase-field fracture' yields 23,700 entries by end of October 2020. Phase-field modeling is used for approximating interfaces in multiphase flow, solidification problems, microstructure evolutions, damage and fracture propagation. Therefore, this code may be adapted to address problems other than fracture mechanics.

In the following, we briefly describe the physical system and the principal algorithms and give some illustrative examples. After that, we outline the impact of this work to date.

2. High-level functionality and purpose of pfm-cracks

2.1. Basic mathematical model

Let B be a domain with the boundary $\partial B := \partial\Omega_{ND} \cup \partial\Omega_{HN}$. The unknown solution variables are: vector-valued displacements $u := u(x,t) : B \times (0,T) \to \mathbb{R}^d$, where d is the spatial dimension; a smoothed scalar-valued indicator phase-field function $\varphi := \varphi(x,t) : B \times (0,T) \to [0,1]$. The latter one describes the crack path in a smeared fashion. Specifically: $\varphi = 0$ denotes the crack region; $\varphi = 1$ characterizes the unbroken material; and $0 < \varphi < 1$ are intermediate values constituting a smooth transition zone dependent on the regularization parameter $\varepsilon > 0$.

We impose $\partial_t \varphi \leq 0$ to achieve crack irreversibility (the crack cannot heal). The prototype problem reads as follows. Find a displacement function $u : B \times (0,T) \to \mathbb{R}^d$ and a phase-field indicator function $\varphi : B \times (0,T) \to [0,1]$, such that

$$-\nabla \cdot (g(\varphi)\sigma(u)) = f \quad \text{in } B \times (0,T), \tag{1}$$

$$(1-\kappa)\varphi\sigma(u) : e(u) - \varepsilon\Delta\varphi - \frac{1}{\varepsilon}(1-\varphi) \leq 0 \quad \text{in } B \times (0,T), \tag{2}$$

$$\partial_t \varphi \leq 0 \quad \text{in } B \times (0,T), \tag{3}$$

$$\left[(1-\kappa)\varphi\sigma(u) : e(u) - \varepsilon\Delta\varphi - \frac{1}{\varepsilon}(1-\varphi)\right] \cdot \partial_t\varphi = 0 \quad \text{in } B \times (0,T), \tag{4}$$

where ε, κ are small positive phase-field regularization parameters, and the linear strain $e(u) = \frac{1}{2}(\nabla u + \nabla u^T)$ and the stress tensor $\sigma(u) = 2\mu e(u) + \lambda tr(e(u))I$, where I is the unit second-order tensor, and μ, λ the Lamé coefficients.

This system is complemented by the following boundary and initial conditions:

$$u(x,t) = u_D(x,t) \quad \text{on } \partial\Omega_{ND} \times (0,T),$$
$$\varphi^2 \nabla u \cdot n = 0 \quad \text{on } \partial\Omega_{HN} \times (0,T),$$
$$\varepsilon\partial_n\varphi = 0 \quad \text{on } \partial B \times (0,T),$$
$$\varphi(x,0) = \varphi_0 \quad \text{on } B \times \{0\},$$

with an initial fracture φ_0.

2.2. Pressurized fractures and stress splitting

In the previous system, we have not shown a stress-splitting of $\sigma(u)$ according to [7,8], which distinguishes fracture propagation according to tensile and compressive forces. Moreover, a given pressure $p : \Omega \times (0,T) \to \mathbb{R}$ can be added according to model developed in [9,10]. Details of these modifications and algorithmic realizations can be found in our original paper [1].

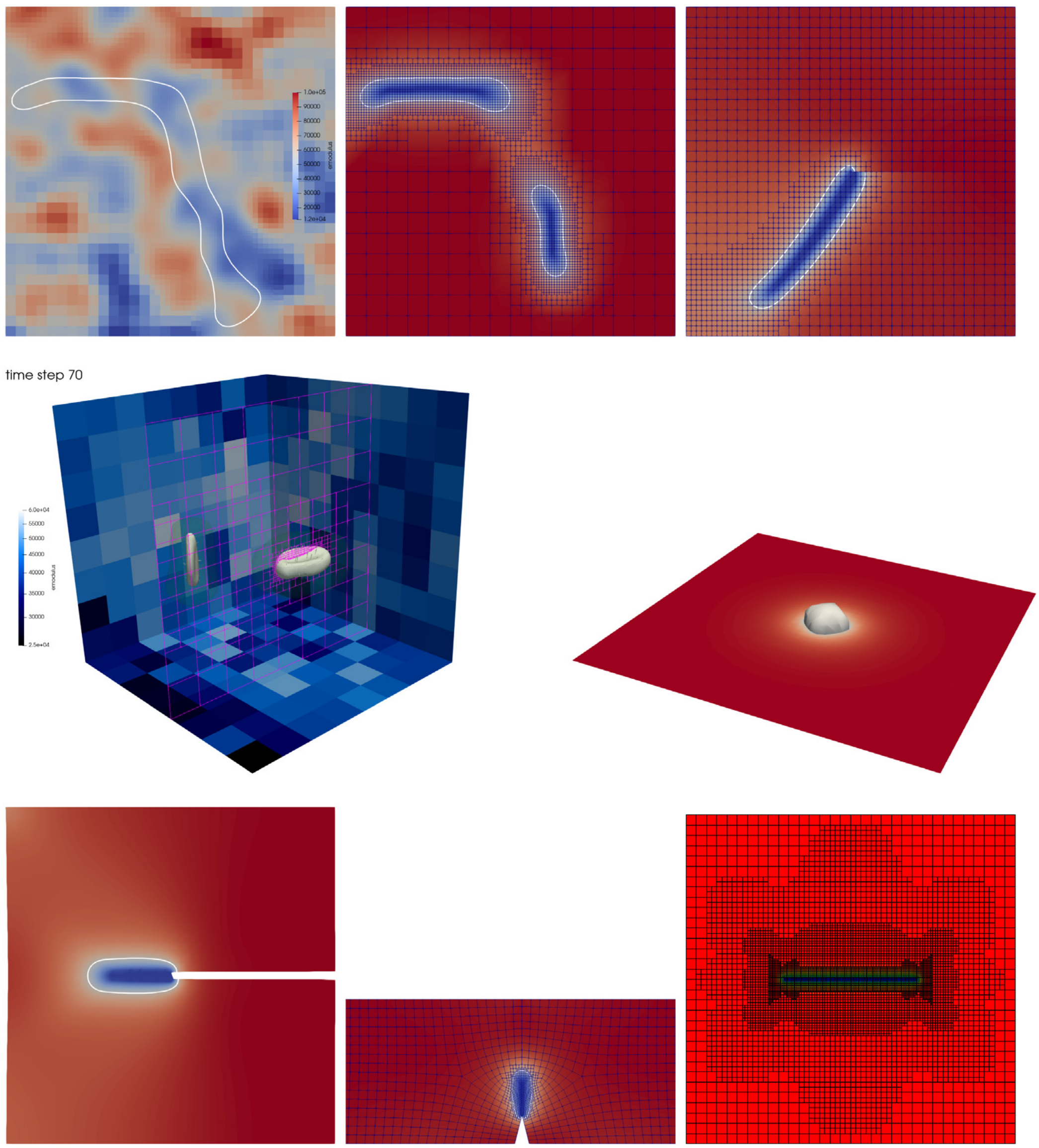

Fig. 2. Illustrative Examples from left to right, top to bottom (name to run the example in parenthesis): Multiple cracks in a heterogeneous medium (`hetero`), Multiple cracks in a homogeneous medium (`homo`), Shear test (`miehe_shear`), 3D test with two fractures (see also Fig. 3), 3D Sneddon test (`sneddon_3d`), Tension test (`miehe_tension`), Three-point bending test (`threepoint`), Coin-shaped pressurized crack in 2d (`sneddon_2d`).

2.3. Discretization, solution algorithms, and parallel framework

To solve the previous system, we first derive a weak formulation and then apply Galerkin finite elements in space on quadrilaterals/hexahedra, respectively. This coupled variational inequality system is then treated in a monolithic fashion with a semi-smooth Newton method `newton_active_set()` that was developed for phase-field fracture in [1] and combines two Newton methods: solving the nonlinear problem and treating the irreversibility constraint.

The code is fully parallelized using MPI by building on the deal.II finite element library [4]. The adaptive meshes are handled by p4est [11] and the linear algebra is built on Trilinos [12]. This parallel software framework is discussed in [13]. From our original work [1], we extended the active set strategy with a method to detect and constrain alternating active set indices to avoid cycles of the method similar to [14].

2.4. Adaptive mesh refinement

The code supports various refinement strategies in the function `refine_mesh ()`. The most prominent is a predictor–corrector strategy as displayed in Fig. 1 to enforce sufficient refinement in the crack region to resolve the crack. Combinations with other strategies such as a jump estimator for the displacements are available as well.

2.5. Evaluation of quantities of interest and benchmarking

The solution can be postprocessed by visualizing with the standard VTK (visualization toolkit) format. Moreover, various quantities of interest are evaluated such as point value evaluations, stress computations over boundaries, crack opening displacements, total crack volumes, and elastic/crack energies. The code was used for the Sneddon 2D benchmark [15] and Sneddon 2D/3D [2] in which several of these quantities of interest are computed.

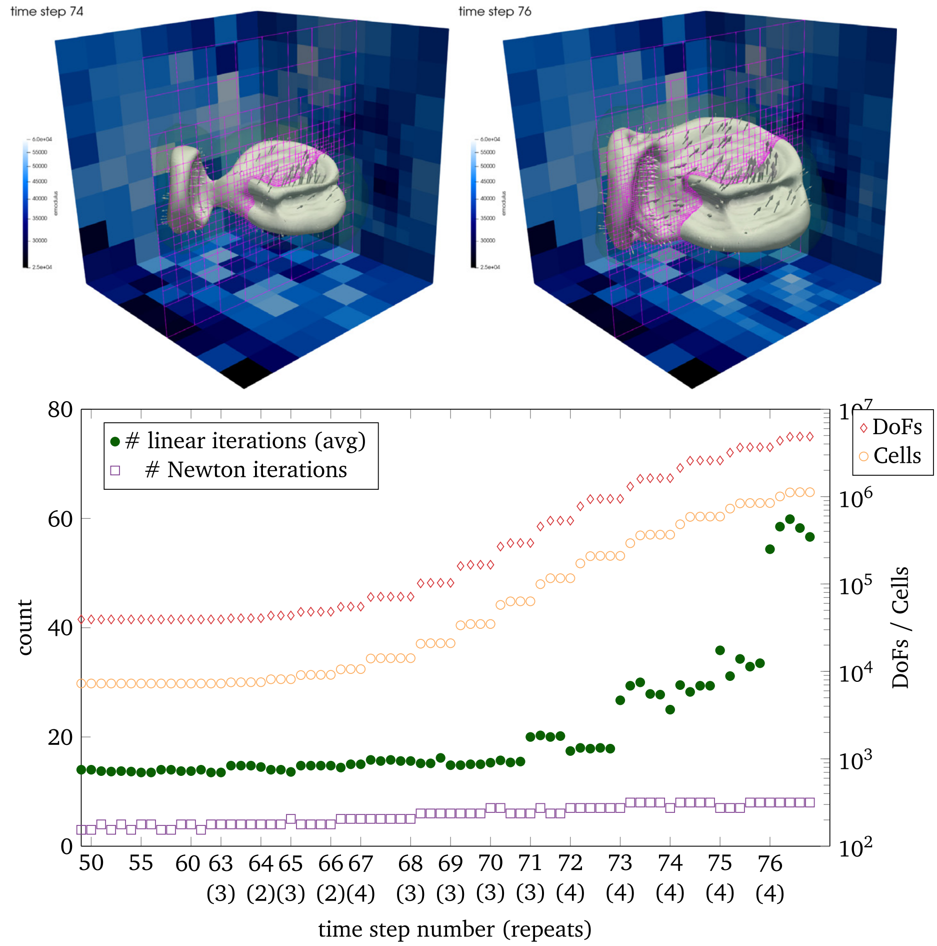

Fig. 3. Heterogeneous 3d example with two initial cracks growing based on an increasing applied pressure in the crack region. Top: solutions at different time steps. Isosurface of $\phi = 0.5$ in white. Blue colors denote the local material property. Purple lines show the computational mesh on a slice in the middle of the domain. Bottom: Statistics (number of linear and nonlinear iterations, number of degrees of freedom and cells) by computational step. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

2.6. Illustrative examples

The software includes a collection of test problems and benchmarks; see Fig. 2 for a gallery of some of the numerical solutions. In addition, we include a new computation for a heterogeneous three dimensional pressurized fracture. Here, two small initial cracks (for that, see Fig. 2) have an increasing pressure applied over time, so the cracks grow until they finally merge. We plot various statistics and the solutions in Fig. 3.

3. Impact

Since its first publication on github accompanied to the paper [1], `pfm-cracks` allowed us to address new scientific questions in both engineering and numerical mathematics. According to Google scholar, our software is cited by 180 documents; scopus: 126 citations; mathscinet 55 citations. All indices were measured in October 2020. Moreover, Google scholar reports (referencing our first work [1]) that the code is known in the United States, Europe, and Asia.

3.1. Research impact

The code is currently used and further developed at Center for Subsurface Modeling UT Austin [16], Florida State University [16–18], RICAM Linz [19,20], China University of Petroleum Beijing [21], Clemson University [1,2,22], and Leibniz University Hannover.

Our own publications using this code (in part) or direct extensions include our own key publications [1,2]. Moreover, the code plays an important role in the recent monograph [6].

In addition, the further impact can be summarized as follows. A crucial point in phase-field modeling is the relationship between the model regularization parameters and the discretization. With our code very fine ε studies and crack-oriented mesh refinement could be carried out by us as shown in [1,2,5,16,17,23,24]. Extensions to large-scale 3D simulations were done in [2,5,25] and comparison with matrix-free multigrid solutions were undertaken in [19,20]. Challenging engineering applications were addressed in [5,16,18,25–30]. New research questions have been enabled for fracture in incompressible solids [31] (doctoral researcher Katrin Mang in collaboration with the authors), and efficient multiphysics phase-field fracture simulations [5,16,29]. Potential future work is in experimental verifications and validations (very little work known to date), for instance several examples in elasticity are provided in [32] from which we have computed some in [1]. Finally, the predictor–corrector methodology inspired an adaptive non-intrusive global–local approach developed in [33,34].

3.2. Educational impact

We decided to keep the same structure as a typical deal.II tutorial step. Therefore, it is simple to learn as we have seen from the work by current and past Ph.D. students Katrin Mang, Daniel Jodlbauer, Nima Noii, and Meng Fan. Consequently, with basic training in deal.II, `pfm-cracks` is relatively easy to use to address challenging phase-field fracture applications. The code has also been used in education in the lecture "Numerical methods for contact problems: application to variational phase-field fracture propagation" (German winter semester 2018/2019, see also the lecture notes [35]).

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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References

[1] T. Heister, M.F. Wheeler, T. Wick, A primal-dual active set method and predictor-corrector mesh adaptivity for computing fracture propagation using a phase-field approach, Comput. Methods Appl. Mech. Engrg. 290 (2015) 466–495.

[2] 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. 18 (1) (2018) e201800353, http://dx.doi.org/10.1002/pamm.201800353, arXiv:https://onlinelibrary.wiley.com/doi/pdf/10.1002/pamm.201800353, URL https://onlinelibrary.wiley.com/doi/abs/10.1002/pamm.201800353.

[3] D. Arndt, W. Bangerth, D. Davydov, T. Heister, L. Heltai, M. Kronbichler, M. Maier, J.-P. Pelteret, B. Turcksin, D. Wells, The deal.II finite element library: Design, features, and insights, Comput. Math. Appl. (2020) http://dx.doi.org/10.1016/j.camwa.2020.02.022.

[4] D. Arndt, W. Bangerth, B. Blais, T.C. Clevenger, M. Fehling, A.V. Grayver, T. Heister, L. Heltai, M. Kronbichler, M. Maier, P. Munch, J.-P. Pelteret, R. Rastak, I. Thomas, B. Turcksin, Z. Wang, D. Wells, The `deal.II` library, version 9.2, J. Numer. Math. 28 (3) (2020) 131–146, http://dx.doi.org/10.1515/jnma-2020-0043, URL https://dealii.org/deal92-preprint.pdf.

[5] S. Lee, M.F. Wheeler, T. Wick, Pressure and fluid-driven fracture propagation in porous media using an adaptive finite element phase field model, Comput. Methods Appl. Mech. Engrg. 305 (2016) 111–132.

[6] T. Wick, Multiphysics Phase-Field Fracture: Modeling, Adaptive Discretizations, and Solvers, De Gruyter, Berlin, Boston, 2020, http://dx.doi.org/10.1515/9783110497397, URL https://www.degruyter.com/view/title/523232.

[7] C. Miehe, F. Welschinger, M. Hofacker, Thermodynamically consistent phase-field models of fracture: variational principles and multi-field FE implementations, Int. J. Numer. Methods Engrg. 83 (2010) 1273–1311.

[8] C. Miehe, M. Hofacker, F. Welschinger, A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits, Comput. Methods Appl. Mech. Engrg. 199 (2010) 2765–2778.

[9] A. Mikelić, M. Wheeler, T. Wick, A Phase-Field Approach to the Fluid Filled Fracture Surrounded by a Poroelastic Medium, iCES Report 13–15, 2013.

[10] A. Mikelić, M.F. Wheeler, T. Wick, Phase-field modeling through iterative splitting of hydraulic fractures in a poroelastic medium, GEM Int. J. Geomath. 10 (1) (2019).

[11] C. Burstedde, L.C. Wilcox, O. Ghattas, P4Est: Scalable algorithms for parallel adaptive mesh refinement on forests of octrees, SIAM J. Sci. Comput. 33 (3) (2011) 1103–1133, http://dx.doi.org/10.1137/100791634.

[12] M.A. Heroux, R.A. Bartlett, V.E. Howle, R.J. Hoekstra, J.J. Hu, T.G. Kolda, R.B. Lehoucq, K.R. Long, R.P. Pawlowski, E.T. Phipps, A.G. Salinger, H.K. Thornquist, R.S. Tuminaro, J.M. Willenbring, A. Williams, K.S. Stanley, An overview of the Trilinos project, ACM Trans. Math. Software 31 (3) (2005) 397–423.

[13] W. Bangerth, C. Burstedde, T. Heister, M. Kronbichler, Algorithms and data structures for massively parallel generic adaptive finite element codes, ACM Trans. Math. Software 38 (2) (2012).

[14] F.E. Curtis, Z. Han, D.P. Robinson, A globally convergent primal-dual active-set framework for large-scale convex quadratic optimization, Comput. Optim. Appl. 60 (2) (2015) 311–341, http://dx.doi.org/10.1007/s10589-014-9681-9.

[15] J. Schröder, T. Wick, S. Reese, P. Wriggers, R. Müller, S. Kollmannsberger, M. Kästner, A. Schwarz, M. Igelbüscher, N. Viebahn, H.R. Bayat, S. Wulfinghoff, K. Mang, E. Rank, T. Bog, D. d'Angella, M. Elhaddad, P. Hennig, A. Düster, W. Garhuom, S. Hubrich, M. Walloth, W. Wollner, C. Kuhn, T. Heister, A selection of benchmark problems in solid mechanics and applied mathematics, Arch. Computat. Methods Eng. (2020) URL https://doi.org/10.1007/s11831-020-09477-3.

[16] M.F. Wheeler, T. Wick, S. Lee, IPACS: Integrated Phase-Field Advanced Crack Propagation Simulator. An adaptive, parallel, physics-based-discretization phase-field framework for fracture propagation in porous media, Comput. Methods Appl. Mech. Engrg. 367 (2020) 113124, http://dx.doi.org/10.1016/j.cma.2020.113124, URL http://www.sciencedirect.com/science/article/pii/S0045782520303091.

[17] S. Lee, B. Min, M.F. Wheeler, Optimal hydraulic fracturing design using the phase field model coupled with global-objective genetic algorithm, Comput. Geosci. 22 (3) (2018).

[18] S. Lee, M. Wheeler, Modeling interactions of natural and two-phase fluid-filled fracture propagation in porous media, Comput. Geosci. (2020).

[19] D. Jodlbauer, U. Langer, T. Wick, Matrix-free multigrid solvers for phase-field fracture problems, Comput. Methods Appl. Mech. Engrg. 372 (2020) 113431, http://dx.doi.org/10.1016/j.cma.2020.113431, URL http://www.sciencedirect.com/science/article/pii/S0045782520306162.

[20] D. Jodlbauer, U. Langer, T. Wick, Parallel matrix-free higher-order finite element solvers for phase-field fracture problems, Math. Comput. Appl. 25 (3) (2020) 40.

[21] M. Fan, Y. Jin, T. Wick, A Phase-Field Model for Mixed-Mode Fracture, Institutionelles Repositorium der Leibniz Universität Hannover, Hannover, 2019, http://dx.doi.org/10.15488/5369.

[22] E. Cinatl, Finite Element Discretizations for Linear Elasticity (Master's thesis), Clemson University, 2018, URL https://tigerprints.clemson.edu/all_theses/2977/.

[23] S. Lee, A. Mikelić, M.F. Wheeler, T. Wick, Phase-field modeling of proppant-filled fractures in a poroelastic medium, Comput. Methods Appl. Mech. Engrg. 312 (2016) 509–541, Phase Field Approaches to Fracture.

[24] S. Lee, M.F. Wheeler, T. Wick, Iterative coupling of flow, geomechanics and adaptive phase-field fracture including level-set crack width approaches, J. Comput. Appl. Math. 314 (2017) 40–60, http://dx.doi.org/10.1016/j.cam.2016.10.022, URL http://www.sciencedirect.com/science/article/pii/S0377042716305118.

[25] T. Wick, S. Lee, M. Wheeler, 3D phase-field for pressurized fracture propagation in heterogeneous media, 2015, ECCOMAS and IACM Coupled Problems Proc., May 2015 at San Servolo, Venice, Italy, URL http://congress.cimne.com/coupled2015/frontal/default.asp.

[26] T. Almani, S. Lee, M. Wheeler, T. Wick, Multirate coupling for flow and geomechanics applied to hydraulic fracturing using an adaptive phase-field technique, 2017, SPE RSC 182610-MS, Feb. 2017, Montgomery, Texas, USA.

[27] S. Lee, J.E. Reber, N.W. Hayman, M.F. Wheeler, Investigation of wing crack formation with a combined phase-field and experimental approach, Geophys. Res. Lett. 43 (15) (2016) 7946–7952, http://dx.doi.org/10.1002/2016GL069979.

[28] S. Lee, M.F. Wheeler, T. Wick, S. Srinivasan, Initialization of phase-field fracture propagation in porous media using probability maps of fracture networks, Mech. Res. Commun. 80 (2017) 16–23, http://dx.doi.org/10.1016/j.mechrescom.2016.04.002, Multi-Physics of Solids at Fracture, URL http://www.sciencedirect.com/science/article/pii/S0093641316300106.

[29] S. Lee, A. Mikelić, M. Wheeler, T. Wick, Phase-field modeling of two phase fluid filled fractures in a poroelastic medium, Multiscale Model. Simul. 16 (4) (2018) 1542–1580.

[30] N. Noii, T. Wick, A phase-field description for pressurized and non-isothermal propagating fractures, Comput. Methods Appl. Mech. Engrg. 351 (2019) 860–890, http://dx.doi.org/10.1016/j.cma.2019.03.058, URL http://www.sciencedirect.com/science/article/pii/S0045782519301975.

[31] K. Mang, T. Wick, W. Wollner, A phase-field model for fractures in nearly incompressible solids, Comput. Mech. 65 (2020) 61–78.

[32] A. Mesgarnejad, B. Bourdin, M. Khonsari, Validation simulations for the variational approach to fracture, Comput. Methods Appl. Mech. Engrg. 290 (2015) 420–437.

[33] N. Noii, F. Aldakheel, T. Wick, P. Wriggers, An adaptive global-local approach for phase-field modeling of anisotropic brittle fracture, Comput. Methods Appl. Mech. Engrg. 361 (2020) 112744, http://dx.doi.org/10.1016/j.cma.2019.112744, URL http://www.sciencedirect.com/science/article/pii/S0045782519306346.

[34] F. Aldakheel, N. Noii, T. Wick, P. Wriggers, A global-local approach for hydraulic phase-field fracture in poroelastic media, 2020, arXiv:2001.06055.

[35] K. Mang, T. Wick, Numerical Methods for Variational Phase-Field Fracture Problems, Institutionelles Repositorium der Leibniz Universität Hannover, Hannover, 2019, http://dx.doi.org/10.15488/5129.