Euler-Lagrange system

Formulation

Define $V := H_0^1(B), W_{in} := \{w \in H^1(B) | \, w \leq \varphi^{old} \leq 1 \text{ a.e. on } B\}$, *and* $W := H^1(B)$. *For the loading steps* $n = 1, 2, 3, \ldots$: *Find vector-valued displacements and a scalar-valued phase-field variable* $(u^n, \varphi^n) := (u, \varphi) \in \{u_D + V\} \times W$ *such that*

$$\Big(\big((1-\kappa)\varphi^2 + \kappa\big) \, \sigma(u), e(w) \Big) = 0 \quad \forall w \in V, \tag{1}$$

and

$$\begin{aligned} &(1-\kappa)(\varphi \, \sigma(u) : e(u), \psi - \varphi) \\ &+ G_c \Big(-\frac{1}{\varepsilon}(1-\varphi, \psi - \varphi) + \varepsilon(\nabla \varphi, \nabla(\psi - \varphi)) \Big) \geq 0 \quad \psi \in W_{in} \cap L^\infty(B) \end{aligned} \tag{2}$$

Therein, $\varepsilon, \kappa > 0$ *and* $\kappa = o(\varepsilon)$, *and* G_c *is the critical energy release rate. Moreover,*

$$\sigma := \sigma(u) = 2\mu e(u) + \lambda \, tr(e(u)) I.$$

Here, μ *and* λ *are material parameters,* $e(u) = \frac{1}{2}(\nabla u + \nabla u^T)$ *is the strain tensor, and* I *the identity matrix.*

Active set solution algorithm as a combined Newton solver [7]

At time t^n:

For $k = 0, 1, 2, \ldots$

repeat

Assemble residual $R(U_k)$

Compute active set $\mathcal{A}_k = \{i \mid (B^{-1})_{ii}(R_k)_i + c(\delta U_k)_i > 0\}$

Assemble matrix $G = \nabla^2 E_\varepsilon(U_k)\delta U_k$ and right-hand side $F = -\nabla E_\varepsilon(U_k)$

Eliminate rows and columns in $\mathcal{A}_k$ from G and F to obtain $\widetilde{G}$ and $\widetilde{F}$

Solve the linear system with GMRES and block-diagonal preconditioning

$$\widetilde{A}'(U_k)(\delta U_k, \Psi) = -\widetilde{A}(U_k)(\Psi) \quad \forall \Psi \in V \times W$$

Find a step size $0 < \omega \leq 1$ using line search to get

$$U_{k+1} = U_k + \omega \delta U_k,$$

with $\widetilde{R}(U_{k+1}) < \widetilde{R}(U_k)$.

until Stopping criterium:

$$\mathcal{A}_{k+1} = \mathcal{A}_k \qquad \text{and} \qquad \widetilde{R}(U_k) < \mathrm{TOL}\,.$$

- Primal-dual active set can be related to a semi-smooth Newton method (super-linear convergence)[6]

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[6] Hintermüller/Ito/Kunisch; SIAM Journal on Optimization, 2002

[7] Heister, Wheeler, Wick; CMAME (2015)

1 Motivation and problems

2 Attempts in verification
- Some positive attempts
- A still questionable test

3 Phase-field fracture model and numerical modeling
- A posteriori error estimation and mesh adaptivity

4 A phase-field fracture model for nearly incompressible solids
- Modeling
- Numerical tests

5 Further validation attempts
- Collaboration with DIK (German Kautschuk Institute)

6 Conclusions

Enhancing accuracy and efficiency

- Parallel computing
- Heuristic adaptivity (for instance the previously predictor-corrector): ONLY mesh refinement, NO error estimation!
- A posteriori error estimation
  - Residual-based estimators
  - Goal-oriented estimators: extremely interesting since specific target functionals (quantities of interest QoI) can be observed

$\rightarrow$ Extract local error indicators for mesh refinement and adaptive solver control

Predictor-corrector mesh adaptivity

- Only mesh adaptivity, but no error estimation
- Designed for problems with moving interfaces or moving discontinuities

Why?

- Problem 1: in fracture propagation the crack path is a priori unknown
- Problem 2: Relationship between h and ε (see also our simplified numerical analysis). For a given (small) ε, propagating fracture(s) might violate the condition $\varepsilon > h$. Do not change ε during a computation since this would change the entire model.

$\Rightarrow$ Predictor-corrector mesh adaptivity:

1. Predict the future crack path (solid discontinuity)
2. Redo the computation and correct the solution

Predictor-corrector mesh adaptivity

- $J(U) = \varphi < c$ with $c = 0.5$ for example.
- The key challenge is the relation of the model regularization parameter ε and the spatial mesh size h (high mesh resolution required!) since $h < \varepsilon$.
- Wish: Fix a (very) small ε during the entire computation.

$\rightarrow$ Predictor-corrector mesh adaptivity with hanging nodes (the mesh grows with the fracture).

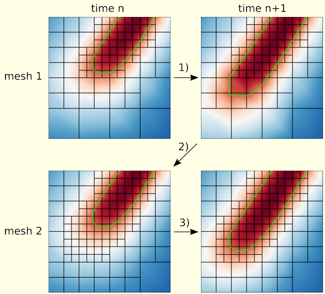
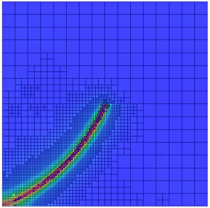


Figure: Predictor-corrector scheme: 1. advance in time, crack leaves fine mesh. 2. refine and go back in time (interpolate old solution). 3. advance in time on new mesh. Repeat until mesh doesn't change anymore. Refinement is triggered for $\varphi < C = 0.2$ (green contour line) here.

Adaptive refinement via residual-based estimator

- Improve the quality of the solution for given computational resources
- Resolve the transition zone (between $\varphi = 0$ and $\varphi = 1$)
- Resolve the fracture tip
- No overrefinement in full-contact zone ($\varphi^n = \varphi^{n-1}$)



$\Rightarrow$ Residual-based a posteriori error estimator of the variational inequality[8, 9]

- Containing interior, jump and complementarity residuals
- Providing a robust upper bound of the error measure and local lower bounds
- Used for an optimized refinement strategy

[8] M. Walloth, *Residual-type A Posteriori Estimators for a Singularly Perturbed Reaction-Diffusion Variational Inequality – Reliability, Efficiency and Robustness.*, Preprint 2018, arXiv No. 1812.01957.

[9] K. Mang, M. Walloth, T. Wick, W. Wollner; GAMM-Mitteilungen 2019

Residual-based a posteriori error estimator

Error estimator

$$\eta := \sum_{k=1}^{4} \eta_k$$

with (p denotes the node) $\alpha_p := \min_{x\in\omega_p} \left\{ \frac{G_c}{\epsilon} + (1-\kappa)(\boldsymbol{\sigma}^+(\boldsymbol{u}_h^n) : \boldsymbol{E}_{\mathrm{lin}}(\boldsymbol{u}_h^n)) \right\}$, and $h_p := \mathrm{diam}(\omega_p)$ and

$$\eta_1 := \left(\sum_{p\in\mathfrak{N}\setminus\mathfrak{N}^{fC}} \eta_{1,p}^2 \right)^{\frac{1}{2}}, \qquad \eta_{1,p} := \min\left\{ \frac{h_p}{\sqrt{G_c\epsilon}}, \alpha_p^{-\frac{1}{2}} \right\} \|r(\varphi_h)\|_{\omega_p},$$

$$\eta_2 := \left(\sum_{p\in\mathfrak{N}^I\setminus\mathfrak{N}^{fC}} \eta_{2,p}^2 \right)^{\frac{1}{2}}, \qquad \eta_{2,p} := \min\left\{ \frac{h_p}{\sqrt{G_c\epsilon}}, \alpha_p^{-\frac{1}{2}} \right\}^{\frac{1}{2}} (G_c\epsilon)^{-\frac{1}{4}} \|G_c\epsilon[\nabla\varphi_h]\|_{\gamma_p^I},$$

$$\eta_3 := \left(\sum_{p\in\mathfrak{N}^\Gamma\setminus\mathfrak{N}^{fC}} \eta_{3,p}^2 \right)^{\frac{1}{2}}, \qquad \eta_{3,p} := \min\left\{ \frac{h_p}{\sqrt{G_c\epsilon}}, \alpha_p^{-\frac{1}{2}} \right\}^{\frac{1}{2}} (G_c\epsilon)^{-\frac{1}{4}} \|G_c\epsilon\nabla\varphi_h\|_{\gamma_p^\Gamma},$$

$$\eta_4 := \left(\sum_{p\in\mathfrak{N}^{sC}} \eta_{4,p}^2 \right)^{\frac{1}{2}}, \qquad \eta_{4,p} := \left(s_p \int_{\tilde{\omega}_p} (I_h^n \varphi_h^{n-1} - \varphi_h)\varphi_p \, \mathrm{d}x \right)^{\frac{1}{2}}.$$

Residual-based A Posteriori Error Estimator [10]

Proposition

For linear (bilinear) finite elements, the above error estimator η for the phase-field variable φ is ***robust*** *and* ***efficient****. (Some technical issues are included!)*
It detail:

1. *Robustness/reliability:* $\|\varphi - \varphi_h\| \leq c_2\, \eta$, *where* $c_2 > 0$
2. *Efficiency:* $c_1\, \eta \leq \|\varphi - \varphi_h\|$, *where* $c_1 > 0$

In words: if both estimates are fulfilled that we can guarantee that the estimator approximates the true error.

[10] K. Mang, M. Walloth, T. Wick, W. Wollner; GAMM-Mitteilungen 2019

Goal-oriented error estimation using duality arguments [11]

- So far only mesh refinement around the crack or global norms based on residual-based estimation ...
- ... but often our goal measurements are somewhere else located
- Such quantities can be of technical nature such as stresses, displacements, point values.
- These can be formulated in terms of a goal functional $J(\cdot)$.
- We restrict our attention to:

$$|J(U) - J(U_{\varepsilon,h})| \leq |J(U) - J(U_\varepsilon)| + |J(U_\varepsilon) - J(U_{\varepsilon,h})|$$

[11] Becker/Rannacher; Acta Numerica, 2001

Ingredients

- Define a goal functional $J(u)$:

$$J(u) = u(x_0, y_0), \quad J(u) = \int_\Gamma \sigma(u) \cdot n \, dx, \quad \text{or} \quad J(\varphi) = \int_\Gamma \varphi \, ds,$$

  or a global norm.

- Key idea: Formulate a minimization problem (recall $U_\varepsilon = \{u_\varepsilon, \varphi_\varepsilon\}$)

$$\min(J(U_\varepsilon) - J(U_{\varepsilon,h})) \quad \text{s.t. } A(U_\varepsilon)(\Psi) = 0 \quad \text{(PDE)}$$

- Define the Lagrangian (as in optimization):

$$L(U_\varepsilon, \lambda) = (J(U_\varepsilon) - J(U_{\varepsilon,h})) - A(U_\varepsilon)(\lambda)$$

- Differentiating the Lagrangian yields the optimality system for U (adjoint problem) and λ (primal problem)
- The adjoint problem will yield sensitivity measures that are then used for error estimation (dual-weighted residuals - DWR)
- To localize the error estimator to obtain indicators for refinement, keep the weak form (in contrast to the classical method) and add a partition-of-unity (PU)
  (There is another weak form localization using special interpolation and patched meshes by Braack/Ern; 2003)

PU-DWR[12] for goal functional evaluations

Proposition (DWR phase-field fracture (Wick, 2016))

For the finite element approximation of the phase-field fracture problem, we have the a posteriori error estimate

$$|J(U) - J(U_h)| \le \eta(u_h) := \sum_{i=1}^{N} |\eta_i|$$

with

$$\begin{aligned}
\eta_i &= (f, (z - i_h z)\psi_i) - a(U, (Z - i_h Z)\psi_i) \\
&= (f, (z_u - i_h z_u)\psi_i) - \Big([(1-\kappa)\varphi^2 + \kappa]\mu \nabla u, \nabla((z_u - i_h z_u)\psi_i)\Big) \\
&\quad - \Big((1-\kappa)\varphi\mu|\nabla u|^2, ((z_\varphi - i_h z_\varphi)\psi_i)\Big) + (\frac{G_C}{\epsilon}(1-\varphi), ((z_\varphi - i_h z_\varphi)\psi_i)) \\
&\quad - (G_C \epsilon \nabla \varphi, \nabla((z_\varphi - i_h z_\varphi)\psi_i)) \\
&\quad + \gamma([\varphi - \varphi^0]^+, ((z_\varphi - i_h z_\varphi)\psi_i))
\end{aligned}$$

Here $U = (u, \varphi)$ *and* $Z = (z_u, z_\varphi)$.

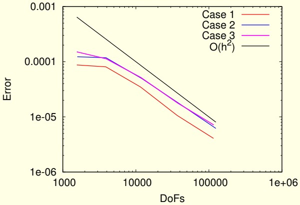
[12] Richter/Wick, JCAM, 2015

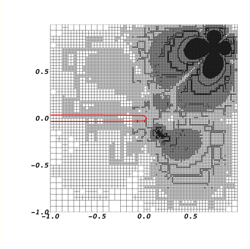
Numerical results[13]

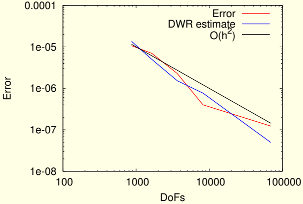
Top: point functional evaluation in the slit domain (but the slit is not given in the geometry but through phase-field).

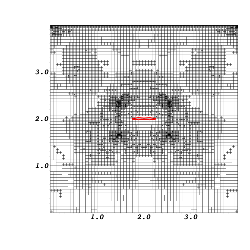
Bottom: Sneddon's test (elasticity with a given pressure p) and computation of the normal stress on the top boundary $\int_\Gamma \sigma(u) \cdot n \, ds$.

In both computations the crack tip is also refined - as expected.









[13] T. Wick; Comp. Mech, 2016

Software

- Open-source `C++` programming codes
- deal.II: differential equations analysis library, `www.dealii.org`
- DOpElib: Differential and optimization environment library, `www.dopelib.net`

- T. Heister, T. Wick: Variational phase-field fracture template: **primal-dual active set solver for crack irreversibility** and **adaptive mesh refinement** and **high-performance parallel computing** (Heister/Wick, 2018, PAMM):

`https://github.com/tjhei/cracks`

Difficulties for (nearly) incompressible solids

- Nearly incompressible means $\nu_s \to 0.5$ yielding $\lambda \to \infty$
- Standard Galerkin approaches yield large approximations errors (locking!)
- Solutions:
  1. DG
  2. Higher-order methods
  3. Mixed methods
- We adopt a mixed approach in the following

$\Rightarrow$ Novel for phase-field fracture type approaches

Modeling choices and assumptions

- We take the Euler-Lagrange PDE system and formulate a mixed system to deal with (nearly) incompressible solids
- **No attempt or claim** that this system Γ converges to some limit for $\varepsilon \to 0$
- **No attempt or claim** that an energy variational principle is fulfilled!

$\rightarrow$ ε fixed!

- **Questions** in which we were rather interested at this stage:
  - Can we proof that the inf-sup condition does hold for this system?
  - Based on this system, can be develop a robust numerical discretization?
  - Do we obtain anything useful out of this model?

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  - Do we obtain anything useful out of this model?
- **We are happy to get your input and discussions!**

Fracture Model in Mixed Form

One approach to avoid locking is a mixed problem formulation with penalty term:

$$p =: \lambda \nabla \cdot u \quad \text{with } p \in \mathcal{U} := L_2(\Omega).$$

Phase-field fracture problem in mixed form [14]:

Find $u \in \mathcal{V}$, $p \in \mathcal{U}$ and $\varphi \in \mathcal{K} \subset \mathcal{W}$ such that

$$(g(\varphi) 2\mu (E_{\text{lin}}(u) + p\,\mathbf{I}), E_{\text{lin}}(w)) = 0 \quad \forall w \in \mathcal{V},$$

$$(\nabla \cdot u, q) - \frac{1}{\lambda}(p, q) = 0 \quad \forall q \in \mathcal{U},$$

$$(1-\kappa)(\varphi 2\mu E_{\text{lin}}(u) + p\,\mathbf{I} : E_{\text{lin}}(u), \psi - \varphi) + G_c(-\frac{1}{\epsilon}(1-\varphi), \psi - \varphi)$$
$$+ G_c \epsilon (\nabla \varphi, \nabla(\psi - \varphi)) \geq 0 \quad \forall \psi \in \mathcal{K}.$$

[14] K. Mang, T. Wick, W. Wollner, Comp. Mech., 2019.

inf-sup condition for the solid [15]

We introduce the following bilinear forms:

$$\begin{aligned} a_\varphi(u,w) &:= (g(\varphi)E_{\text{lin}}(u), E_{\text{lin}}(w)), \\ b_\varphi(w,p) &:= (g(\varphi)\nabla\cdot w, p), \\ c_\varphi(p,q) &:= (g(\varphi)p, q). \end{aligned}$$

A compact bilinear form is summing up the single terms from before:

$$A_\varphi(u,p;w,q) := 2\mu a_\varphi(u,w) + b_\varphi(w,p) + b_\varphi(u,q) - \frac{1}{\lambda} c_\varphi(p,q).$$

Assume $g(0) = \kappa > 0$ and let the bilinear form be $\mathcal{V}$-elliptic. Then it holds the inf-sup condition

$$\inf_{(u,p)\in(\mathcal{V}\times\mathcal{U})} \sup_{(w,q)\in(\mathcal{V}\times\mathcal{U})} \frac{A_\varphi(u,p;w,q)}{(u,p)\cdot(w,q)} \geq \beta > 0,$$

with β independent of λ and $g(\varphi)$, assuming that $0 \leq \frac{1}{\lambda} \leq 1$ and $g(\varphi) \geq \kappa$.

[15] V. Girault, P.A. Raviart, *Finite element methods for Navier-Stokes equations: theory and algorithms*, Springer Science (2012).