Optimization of phase-field damage

Robert Haller-Dintelmann[1], Hannes Meinlschmidt[2], Masoumeh Mohammadi[1],
Ira Neitzel[3], Thomas Wick[4], Winnifried Wollner[1]

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[1] TU-Darmstadt, [2] RICAM, [3] U-Bonn, [4] U-Hannover

Outline of the Talk

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The Phase-Field Model
- The Crack-Propagation Model and its Regularizations
- Improved Differentiability

An Optimization Problem for Regularized Crack Propagation
- Limit in $\gamma \to \infty$

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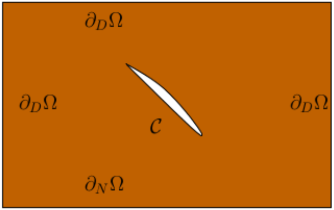
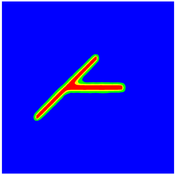
The Forward Griffith's Model





Minimize the total energy in each time-step

$$E(q;u,\mathcal{C}) = \frac{1}{2}(\mathbb{C}e(u),e(u))_{\Omega\setminus\mathcal{C}} - (q,u)_{\partial_N\Omega} + \mathcal{H}^{d-1}(\mathcal{C}),$$

$$E_\varepsilon(q;u,\varphi) = \frac{1}{2}\Big(g(\varphi)\mathbb{C}e(u),e(u)\Big) - (q,u)_{\partial_N\Omega} + \frac{1}{2\varepsilon}\|1-\varphi\|^2 + \frac{\varepsilon}{2}\|\nabla\varphi\|^2,$$

subject to $\quad 0 \le \varphi(t_i) \le \varphi(t_{i-1}) \le 1 \quad \forall i = 1,\dots,N$

Simulations from ongoing SPP1748 project

Basava, Mang, Walloth, Wick, W.

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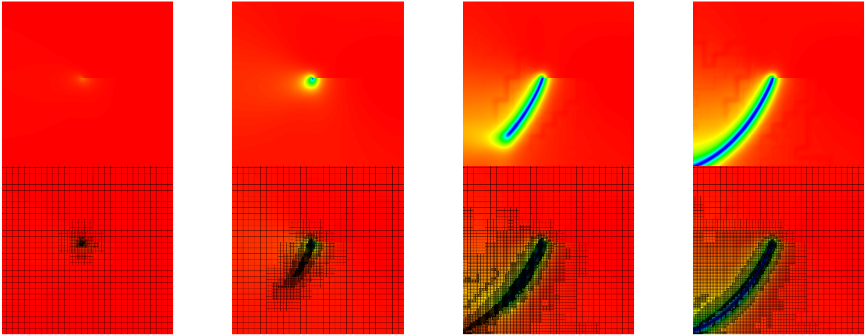

Questions (ongoing work):

- Incompressible materials
- Pressure robust discretization
- Convergence (rates?)
- Optimization

Troubleshooting

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- Minimizers of E_ε not unique.
- Necessary conditions for minimizing E_ε give a sequence of obstacle problems.
- Trouble in optimization, e.g., optimality conditions, (non-adapted) algorithms may converge to non-stationary limits...
- $\longrightarrow$ More regularization!

Given q^i and φ^{i-1} solve

$$\min_{\mathbf{u}} E_\varepsilon^\gamma(u^i, \varphi^i) := E_\varepsilon(q^i; u^i, \varphi^i) + \gamma R(\varphi^{i-1}; \varphi^i) + \eta \|\varphi^i - \varphi^{i-1}\|^2 \qquad (\mathrm{C}^{\gamma,\eta})$$

with $0 \le \gamma \to \infty$ and

$$R(\varphi^{i-1}; \varphi^i) = \frac{1}{4}\|(\varphi^i - \varphi^{i-1})^+\|_{L^4}^4.$$

The Problem $(\mathrm{C}^{\gamma,\eta})$

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Formally, any minimizer of $(\mathrm{C}^{\gamma,\eta})$ satisfies for any $(v,\psi) \in V = H^1_D(\Omega;\mathbb{R}^2) \times H^1(\Omega)$.

$$\Big(g(\varphi^i)\mathbb{C}e(u^i), e(v)\Big) - (q^i, v)_{\partial_N\Omega} = 0$$

$$\varepsilon(\nabla\varphi^i, \nabla\psi) - \frac{1}{\varepsilon}(1-\varphi^i,\psi) + (1-\kappa)(\varphi^i\mathbb{C}e(u^i) : e(u^i),\psi) \qquad (\mathrm{EL}^{\gamma,\eta})$$

$$+\gamma([(\varphi^i - \varphi^{i-1})^+]^3,\psi) + \eta(\varphi^i - \varphi^{i-1},\psi) = 0.$$

for any $(v,\psi) \in V = H^1_D(\Omega;\mathbb{R}^2) \times H^1(\Omega)$.

But: Not immediately clear, if well-defined!

Theorem (Neitzel, Wick, W. 2017)

Given some assumptions on the data, there are minimizers, solving $(\mathrm{EL}^{\gamma,\eta})$*.*
Any solution (u,φ) *to* $(\mathrm{EL}^{\gamma,\eta})$ *satisfies (for some* $p > 2$*):*

$$\varphi \in H^1(\Omega) \qquad 0 \le \varphi \le 1$$

$$u \in W^{1,p}(\Omega) \cap H^1_D(\Omega) \qquad \|u\|_{1,p} \le c\|q\|$$

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The Problem

- Nice: $u \in W^{1,p}$ is sufficient to have well-defined products (in 2d).
- Not so nice: In optimization - q varies (converges weakly!) then u does so in $W^{1,p}$, but products of weak-convergent sequences are not nice $\mapsto$ trouble in the second equation! (Can be circumvented by compensated compactness)
- Not so nice: In numerics - approximation theory gives rates if a gap in differentiability is present (we only have integrability). $\mapsto$ only qualitative convergence $o(1)$ as $h \to 0$ can be expected (not uniform in the data q, φ^0).
- If $g(\varphi) \in L^\infty$ there is nothing we can do!

The Problem

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- Not so nice: In numerics - approximation theory gives rates if a gap in differentiability is present (we only have integrability). $\mapsto$ only qualitative convergence $o(1)$ as $h \to 0$ can be expected (not uniform in the data q, φ^0).
- If $g(\varphi) \in L^\infty$ there is nothing we can do!
- For the φ-equation with $\varphi \in L^\infty$ the right hand side

$$-G_c\varepsilon\Delta\varphi + \frac{G_c}{\varepsilon}\varphi = \frac{G_c}{\varepsilon}(1,\cdot) - (1-\kappa)(\varphi\mathbb{C}e(u), e(u)\cdot) - \gamma([(\varphi-\varphi^-)^+]^3,\cdot).$$

is in $L^{p/2}$, i.e., for a nice domain $\varphi \in W^{2,p/2}$. (better than L^∞ but not $W^{1,\infty}$!)

Improved Differentiability

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Theorem (Haller-Dintelmann, Meinlschmidt, W. 2019)

Given some assumptions on the domain, assuming a Gårding inequality, and each coefficient (matrix) $A^{i,j}$ being a multiplier on $H^\varepsilon(\Omega)^d$ for some $0 \leq \varepsilon < \frac{1}{2}$. Then there exist $\gamma \geq 0$ and $0 < \delta \leq \varepsilon$ such that for any $|\theta| < \delta$ the elliptic system

$$-\nabla \cdot A\nabla u + \gamma u = f \quad \text{in } H_D^{\theta-1}(\Omega)$$

has a unique solution $u \in H_D^{\theta+1}(\Omega)$ satisfying

$$\|u\|_{H_D^{\theta+1}(\Omega)} \leq C\|f\|_{H_D^{\theta-1}(\Omega)}$$

for some constant $C \geq 0$ independent of f
– C depends on multiplier norm of A but not A.
– If coercive then $\gamma = 0$ can be chosen.

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Corollary

Let $q \in H^{\theta_0 - 1}$. Then there exists $0 < \bar{\theta} \leq \theta_0$ such that the solution $(u, \varphi) \in \left(W^{1,p}(\Omega) \cap H^1_D(\Omega)\right) \times \left(H^1(\Omega) \cap L^\infty(\Omega)\right)$ of $(\mathrm{EL}^{\gamma,\eta})$ admits the additional regularity $u \in H^{\theta+1}(\Omega)$ and $\varphi \in H^{\theta+1}(\Omega)$ for any θ satisfying $0 < \theta < \bar{\theta}$. Moreover, we obtain the estimate

$$\|u\|_{H_D^{1+\theta}(\Omega)} \leq C\|q\|_{H_D^{\theta_0 - 1}(\Omega)}$$

with a constant $C = C(\|q\|^2_{H^{-1,p}}, \gamma, \eta, \varepsilon)$.

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Model Problem

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Given $(u^0, \varphi^0) \in V$ with $0 \leq \varphi^0 \leq 1$.
Find $(q, \mathbf{u}) = (q, (u, \varphi)) \in (Q \times V)^M$ solving

$$\min_{q,\mathbf{u}} J(q, \mathbf{u}) := \frac{1}{2} \sum_{i=1}^{M} \|u^i - u_d^i\|^2 + \frac{\alpha}{2} \sum_{i=1}^{M} \|q^i\|^2_{\partial_N \Omega} \qquad (\mathrm{NLP}^\gamma)$$

$$\text{s.t. } (q, \mathbf{u}) \text{ satisfy } (\mathrm{EL}^{\gamma,\eta}).$$

where $u_d \in (L^2(\Omega))^M$ is a given desired displacement, $\alpha > 0$.

Theorem (Neitzel, Wick, W. (2017))

There exists at least one global minimizer $(q, \mathbf{u}) \in (Q \times V)^M$ *to* (NLP^γ).

Under the assumptions of the previous slides, any such minimizer satisfies the additional regularity $u \in H^{1+s}$, $\varphi \in W^{2,p/2}$.

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Lemma (Neitzel, Wick, W. (2017))

For any given $(u_k, \varphi_k) \in (V \cap (W^{1,p}(\Omega;\mathbb{R}^2) \times L^\infty(\Omega))^M$ *the linear operators* $A_i\colon V \to V^*$ *corresponding to the the linearized fracture equation, i.e.,*

$$\begin{aligned}\langle A_i(u,\varphi),(v,\psi)\rangle_{V^*,V} &= a_i(u,\varphi;v,\psi)\\ &= \Big(g(\varphi_k^i)\mathbb{C}e(u), e(v)\Big) + 2(1-\kappa)(\varphi_k^i\mathbb{C}e(u_k^i)\varphi, e(v))\\ &\quad + \varepsilon(\nabla\varphi,\nabla\psi) + (\frac{1}{\varepsilon}+\eta)(\varphi,\psi) + (1-\kappa)(\varphi\mathbb{C}e(u_k^i) : e(u_k^i),\psi)\\ &\quad + 3\gamma([(\varphi_k^i - \varphi_k^{i-1})^+]^2\varphi,\psi) + 2(1-\kappa)(\varphi_k^i\mathbb{C}e(u_k^i) : e(u),\psi)\end{aligned}$$

are Fredholm of index zero.
The same is true for the $\mathcal{A}\colon V^M \to (V^*)^M$ *assembling all time-steps, thus injectivity is a constraint qualification.*

A QP-Approximation

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Let $(q_k, \mathbf{u}_k) = (q_k, u_k, \varphi_k) \in Q^M \times (V \cap W^{1,p}(\Omega;\mathbb{R}^2) \times L^\infty(\Omega))^M$.

Find $(q, \mathbf{u}) \in Q^M \times V^M$ solving

$$\min_{(q,\mathbf{u})} J_{\text{lin}}(q, \mathbf{u}) := \frac{1}{2} \sum_{i=1}^{M} \|u - (u_d - u_k)\|^2 + \frac{\alpha}{2} \sum_{i=1}^{M} \|q + q_k\|^2_{\partial_N \Omega} (+ \dots) \qquad (\text{QP}^\gamma)$$

$$\text{s.t. } \mathcal{A}\mathbf{u} = \mathcal{B}q.$$

Where $\mathcal{B} \colon Q^M \to (V^*)^M$ is

$$\langle \mathcal{B}q, v \rangle_{(V^*)^M, V^M} := \sum_{i=1}^{M} (q^i, v^i)_{\partial_N \Omega}$$

For suitably chosen $p > 2$ any solution $\mathbf{u}$ of the linear equation satisfies the desired regularity, e.g., the regularity does not degenerate.

Existence of Solutions to (QP^γ) and optimality conditions

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Theorem (Neitzel, Wick, W. (2017))

Given $(u_k, \varphi_k) \in (V \cap W^{1,p}(\Omega;\mathbb{R}^2) \times L^\infty(\Omega))^M$ and $q_k \in Q^M$, the problem (QP^γ) has a unique solution $(\overline{q}, \overline{\mathbf{u}}) \in Q^M \times V^M$.
Further, regardless of the invertibility of $\mathcal{A}$, there exists a Lagrange multiplier, $\overline{z} \in V^M$ satisfying

$$\begin{aligned} \mathcal{A}\overline{u} &= \mathcal{B}\overline{q} && \text{in } (V^*)^M, \\ \mathcal{A}^*\overline{z} &= \overline{u} - (u_d - u_k) && \text{in } (V^*)^M, \\ \alpha(\overline{q} + q_k) + \overline{z} &= 0 && \text{on } \partial_N\Omega. \end{aligned} \tag{KKT$^\gamma$}$$

Due to convexity, any such triplet gives rise to a solution of (QP^γ).

Error estimates for the SQP-Step

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Theorem (Mohammadi, W. (2018))

Under the previous assumptions, assuming in addition that $\mathcal{A}$ is an isomorphism, there exists $h_0 > 0$ such that for any $h \leq h_0$ then for any $q \in Q$ the solution $\mathbf{u} \in V$ to $\mathcal{A}\mathbf{u} = \mathcal{B}q$ and its Galerkin-approximation $\mathbf{u}_h \in V_h$ exist and satisfy the following quasi best-approximation property

$$\|\mathbf{u} - \mathbf{u}_h\|_V \lesssim \inf_{\mathbf{v}_h \in V_h} \|\mathbf{u} - \mathbf{v}_h\|_V.$$

Theorem (Mohammadi, W. (2018))

Under the previous assumptions, there exists $\theta > 0$ such that the solution $(\bar{q}, \bar{\mathbf{u}})$ to (QP^γ), and its variational discretization $(\bar{q}_h, \bar{\mathbf{u}}_h)$ satisfy

$$\alpha\|\bar{q} - \bar{q}_h\|^2_{\partial_N\Omega} + \|\bar{u} - \bar{u}_h\|^2 \leq c(1 + \frac{1}{\alpha})h^{2\theta}$$

Content

The Phase-Field Model

The Crack-Propagation Model and its Regularizations

Improved Differentiability

An Optimization Problem for Regularized Crack Propagation

Limit in $\gamma \to \infty$

Formal Limit Problem

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We expect, that solutions of (EL$^{\gamma,\eta}$)

$$\Big(g(\varphi^i)\mathbb{C}e(u^i), e(v)\Big) - (q^i, v)_{\Gamma_N} = 0,$$

$$\varepsilon(\nabla\varphi^i, \nabla\psi) - \frac{1}{\varepsilon}(1-\varphi^i, \psi) + \eta(\varphi^i - \varphi^{i-1}, \psi)$$
$$+(1-\kappa)(\varphi^i\mathbb{C}e(u^i) : e(u^i), \psi) + \gamma([(\varphi^i - \varphi^{i-1})^+]^3, \psi) = 0$$

converge to solutions of the VI

$$\Big(g(\varphi^i)\mathbb{C}e(u^i), e(v)\Big) - (q^i, v)_{\Gamma_N} = 0,$$

$$\varepsilon(\nabla\varphi^i, \nabla\psi) - \frac{1}{\varepsilon}(1-\varphi^i, \psi) + \eta(\varphi^i - \varphi^{i-1}, \psi) \qquad (\mathrm{EL}^{\eta})$$
$$+(1-\kappa)(\varphi^i\mathbb{C}e(u^i) : e(u^i), \psi) + (\lambda^i, \psi) = 0,$$
$$\varphi^i \le \varphi^{i-1}, \quad \lambda^i \ge 0, \quad (\lambda^i, \varphi^i - \varphi^{i-1}) = 0.$$

Known stability properties for (NLP$^\gamma$)

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For $q = p/2$ and some $p > 2$ we know, that solutions to (EL$^{\gamma,\eta}$) satisfy

$$\|u_\gamma^i\|_{1,p} \le c\|q^i\|,$$
$$\|\varphi_\gamma^i\|_{2,q} \le c\Big(1 + \|q^i\|^2 + \gamma\|((\varphi_\gamma^i - \varphi_\gamma^{i-1})^+)^3\|_q + \eta\|\varphi_\gamma^i - \varphi_\gamma^{i-1}\|_q\Big),$$
$$\|u_\gamma^i\|_{1+s} \le c_\varphi^i\|q^i\|.$$

Trouble for the limit:

- c_φ^i depends on $\|\varphi_\gamma^i\|_{2,q}$.
- $\|\varphi_\gamma^i\|_{2,q}$ depends on $\lambda_\gamma^i = \gamma((\varphi_\gamma^i - \varphi_\gamma^{i-1})^+)^3$ in L^q (approximate multiplier for obstacle-constraint).
- Elementary estimates only for $\lambda_\gamma^i \in (H^1)^* \cap L^1$.

Convergence and improved stability estimates

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Theorem (Neitzel, Wick, W. (2019))

Under suitable conditions on the initial data φ^0 and control q it is true that for $\gamma \to \infty$ (up to a subsequence)

- $u_\gamma \to u_\infty$ *in* H^1_D,
- $\varphi_\gamma \to \varphi_\infty$ *in* H^1.

If $\varphi^0 \in W^{2,q}$ *than*

- $\|\lambda_\gamma\|_q \leq C$, *(depending on number of time-steps)*
- $\varphi_\gamma \to \varphi_\infty$ *in* $C^{0,\alpha}$,
- $u_\gamma \to u_\infty$ *in* H^{1+s}_D.

Moreover any such limit-point satisfies the corresponding VI (EL^η)

This remains true, mutatis mutandis, if $q_n \rightharpoonup q$ is considered.

Approximability of local minimizers

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Theorem (Neitzel, Wick, W. (2019))

Let $\bar{q} \in Q^M$ be an isolated local minimizer of (NLP^γ) *subject to* (EL^η) *and assume that the corresponding state* $\bar{\mathbf{u}} = (u, \varphi)$, $\bar{\lambda}$ *is the unique solution of* (EL^η). *Then, for* γ *sufficiently large, there exists a sequence* $q_\gamma, \mathbf{u}_\gamma$ *of local minimizers of* (NLP^γ) *such that*

$$
\begin{aligned}
q_\gamma &\to \bar{q} && \text{in } Q^M,\\
\mathbf{u}_\gamma &\to \bar{\mathbf{u}} && \text{in } V^M \cap (H^{1+s}(\Omega) \times C^{0,\alpha}(\Omega))^M,\\
\lambda_\gamma &\rightharpoonup \bar{\lambda} && \text{in } L^{p/2}(\Omega)^M
\end{aligned}
$$

γ	$J[\times 10^{-5}]$	Iter.	Residual	$\|\lambda_\gamma\|_1$	$\|\lambda_\gamma\|_2^2$	$\|\max(\varphi^i_\gamma, \varphi^{i-1}) - \varphi^i_\gamma\|^2_{H^1(\Omega)}$
10^8	1.0533	4	$8.7 \cdot 10^{-13}$	1.1	244	$6 \cdot 10^{-3}$
10^9	1.0531	1	$9.4 \cdot 10^{-13}$	1.1	254	$2 \cdot 10^{-3}$
10^{10}	1.0531	1	$4.6 \cdot 10^{-13}$	1.1	258	$7 \cdot 10^{-4}$
10^{11}	1.0532	1	$3.4 \cdot 10^{-13}$	1.1	260	$3 \cdot 10^{-4}$
10^{12}	1.0532	0	$4.0 \cdot 10^{-13}$	1.1	262	$6 \cdot 10^{-5}$
10^{13}	1.0532	0	$9.6 \cdot 10^{-13}$	1.1	262	$2 \cdot 10^{-5}$

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Thank you for the attention!