Relating phase field and sharp interface approaches to structural topology optimization

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1 Introduction into structural topology optimization

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3 Sharp interface limit of the phase field approximation

4 Numerics
Problem setting in structural topology optimization

- Domain $\Omega$ to be designed:
  1. solid domain $\Omega^M$ with fixed given volume $|\Omega^M| = m$
  2. void $\Omega \setminus \Omega^M$

- Volume forces $f$ given

- Surface loads $g$, Traction forces given
Problem setting in structural topology optimization

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Aim of the structural topology optimization:

Distribute a limited amount of material $\Omega^M$ in a design domain $\Omega$ such that an objective functional $J$ is minimized.
### Mathematical formulation:

Given a design domain $\Omega \subset \mathbb{R}^d$ and $m$

$$\min_{\Omega^M \in U_{ad}} J(\Omega^M)$$

Admissible set: $U_{ad} = \{ \Omega^M \subset \Omega \text{ such that } |\Omega^M| = m \}$
Mathematical formulation:

Given a design domain $\Omega \subset \mathbb{R}^d$ and $m$

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Solve simultaneously the elasticity equation (solid domain modeled as linear elastic material)

$$-\text{div}(C^M \mathcal{E}(u)) = f \text{ in } \Omega^M \text{ and boundary conditions}$$

- elasticity tensor $C^M$
- linearized strain tensor $\mathcal{E}(u) = \frac{1}{2}(\nabla u + \nabla u^T)$
- Displacement field $u$
Possible objective functionals

First choice

Maximize stiffness or equivalently Minimize compliance (work done by the load)

\[ J_1(\Omega^M) = \int_{\Omega^M} f \cdot u + \int_{\Gamma_g} g \cdot u. \]
Possible objective functionals

First choice

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Concrete examples for mean compliance

Michell type structure

Cantilever beam configuration
Possible objective functionals (tracking-type)

Second choice

Error compared to target displacement

\[ J_2(\Omega^M) = \left( \int_{\Omega^M} c(x)|u - u_\Omega|^2 \right)^\kappa, \quad \kappa \in (0, 1] \]

- \( c(x) \): given weighting factor,
- \( u_\Omega \): target displacement
- \( \kappa = \frac{1}{2} \) in applications, \( \kappa = 1 \) least square minimization
Second choice

Error compared to target displacement

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- \(c(x)\): given weighting factor,
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- \(\kappa = \frac{1}{2}\) in applications, \(\kappa = 1\) least square minimization

Concrete example for compliant mechanism

Minimize error to given target displacement

Push configuration
Structural optimization problem

Minimize \( J(\Omega^M) = \alpha J_1(\Omega^M) + \beta J_2(\Omega^M) \) subject to

\[
-\text{div}(\mathbb{C}^M \mathcal{E}(u)) = f \quad \text{in} \quad \Omega^M \\
(\mathbb{C}^M \mathcal{E}(u)) n = 0 \quad \text{on} \quad \Gamma_0 \\
(\mathbb{C}^M \mathcal{E}(u)) n = g \quad \text{on} \quad \Gamma_g \\
u = 0 \quad \text{on} \quad \Gamma_D
\]
Possible objective functionals

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\]
\[
u = 0 \quad \text{on} \quad \Gamma_D
\]

Problem is not well-posed!

A possible path to well-posedness

Add the perimeter: \( P(\Omega^M) = \int_{(\partial \Omega^M) \cap \Omega} ds \):

\[
J(\Omega^M) = \alpha J_1(\Omega^M) + \beta J_2(\Omega^M) + \gamma P(\Omega^M)
\]
Approaches used to tackle structural optimization problems

- Classical method of shape calculus: Boundary variations based on a parametric approach
  - drawbacks: topology changes difficult / serious remeshing necessary
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- Homogenization methods and variants of it (Allaire, Bendsoe, Sigmund and many others)
  (power law materials, Solid Isotropic Material with Penalization (SIMP) method)
  - Applicability restricted to particular objective functionals
Approaches used to tackle structural optimization problems

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  (power law materials, Solid Isotropic Material with Penalization (SIMP) method)
  - Applicability restricted to particular objective functionals

- Level set methods (Sethian, Osher, Allaire, Burger and many others)
  (Applicable to a wide range of problems)
  - drawbacks: difficult to create holes / (topological derivatives would help)
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Multi-material phase field approach

- another strategy: Phase field method
- approximate $P(\Omega^M)$ by Ginzburg-Landau functional
- allows for *topology changes* (nucleation or elimination of holes),
- easy to construct a *multi-phase model* (more than one material and void possible)
- In the following
another strategy: Phase field method

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allows for topology changes (nucleation or elimination of holes),

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In the following

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Multi-material phase field approach

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- asymptotic analysis: formal
- rigorous justification by \( \Gamma \)-convergence machinery, still ongoing research
## Phase field approach, earlier work

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Phase field approach, earlier work


Common: focus on numerical aspects and formal analysis,
Phase field approach: Introduction

- phase field $\varphi := (\varphi^i)_{i=1}^N$; phase-fraction $\varphi^i$; void $\varphi^N$; $\varepsilon > 0$ interface width
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- \( \mathcal{G} := \{ v \in H^1(\Omega, \mathbb{R}^N) \mid v(x) \in G \; \text{a.e. in} \; \Omega \} \)
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- \( G^m := \{ v \in G | \int_{\Omega} v = m \} \)
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- $\mathcal{G} := \{ v \in H^1(\Omega, \mathbb{R}^N) | v(x) \in G \text{ a.e. in } \Omega \}$
- $\mathcal{G}^m := \{ v \in \mathcal{G} | \int_{\Omega} v = m \}$

Example: 3 materials

![Diagram showing phases and material properties]
Phase field approach: Introduction

**mechanical properties of the system**

- linear elasticity
- elasticity tensors in material for each phase $C^i, i \in \{1, \ldots, N - 1\}$

- void is modeled as a very soft "ersatz material" with a very small elasticity tensor $C^N = C_N(\varepsilon) = \varepsilon^2 \tilde{C}_N$ (quadratic rate in $\varepsilon$ accelerates the convergence in the void as $\varepsilon \to 0$ and is hence chosen in the numerical computations)

- elasticity tensor in the interfacial region: $C(\phi) = C(\phi) + C_N(\varepsilon)\phi_N, \forall \phi \in G$

  $C(\phi) := \sum_{i=1}^{N-1} C_i \phi_i$
Phase field approach: Introduction

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- elasticity tensor in the interfacial region: $\overline{C}(\varphi) = \overline{C}(\varphi) + C^N(\varepsilon)\varphi^N, \forall \varphi \in G,$
  $\overline{C}(\varphi) := \sum_{i=1}^{N-1} C^i \varphi^i$
Phase field approach

- Ginzburg-Landau functional

\[ E^\varepsilon(\varphi) := \int_{\Omega} \left( \frac{\varepsilon}{2} |\nabla \varphi|^2 + \frac{1}{\varepsilon} \Psi(\varphi) \right) dx, \quad \varepsilon > 0, \]

- Prototype examples for \( \Psi \) are given by

\[ \Psi(\varphi) := \frac{1}{2} (1 - \varphi \cdot \varphi) \quad \text{and} \quad \Psi(\varphi) := \frac{1}{2} \varphi \cdot \nabla \varphi \]
Phase field approach

- Ginzburg-Landau functional

\[ E^\varepsilon(\varphi) := \int_\Omega \left( \frac{\varepsilon}{2} |\nabla \varphi|^2 + \frac{1}{\varepsilon} \Psi(\varphi) \right) \, dx, \quad \varepsilon > 0, \]

- Prototype examples for \( \Psi \) are given by

\[ \Psi(\varphi) := \frac{1}{2} (1 - \varphi \cdot \varphi) \quad \text{and} \quad \Psi(\varphi) := \frac{1}{2} \varphi \cdot \mathcal{W} \varphi \]

- mean compliance \( J_1 \) and compliant mechanism \( J_2 \)

\[ J_1(u, \varphi) = \int_\Omega (1 - \varphi^N) f \cdot u + \int_{\Gamma_g} g \cdot u, \]

\[ J_2(u, \varphi) := \left( \int_\Omega c (1 - \varphi^N) |u - u_\Omega|^2 \right)^\varsigma, \quad \varsigma \in (0, 1] \]
Similarities to optimal control problem, control: $\varphi$, state: $u$

$$\begin{aligned}
\min \ J^\varepsilon(u, \varphi) := \alpha J_1(u, \varphi) + \beta J_2(u, \varphi) + \gamma E^\varepsilon(\varphi),
\text{over} \quad (u, \varphi) \in H^1_D(\Omega, \mathbb{R}^d) \times H^1(\Omega, \mathbb{R}^N),
\text{s.t.} \quad SE \quad \begin{cases}
- \nabla \cdot [C(\varphi)E(u)] = (1 - \varphi^N) f & \text{in } \Omega, \\
u = 0 & \text{on } \Gamma_D, \\
[C(\varphi)E(u)] n = g & \text{on } \Gamma_g, \\
[C(\varphi)E(u)] n = 0 & \text{on } \Gamma_0,
\end{cases}
\varphi \in G^m \cap U_c,
\end{aligned}$$

$$U_c := \{ \varphi \in H^1(\Omega, \mathbb{R}^N) \mid \varphi^N = 0 \text{ a.e. on } S_0 \text{ and } \varphi^N = 1 \text{ a.e. on } S_1 \}.$$
**“Control-to-state” operator**

**Lemma:**

\[ S : L^\infty(\Omega, \mathbb{R}^N) \to H^1_D(\Omega, \mathbb{R}^d), \quad S(\varphi) := u \]

The control-to-state operator \( S : L^\infty(\Omega, \mathbb{R}^N) \to H^1_D(\Omega, \mathbb{R}^d) \) is Fréchet-differentiable.
“Control-to-state” operator

Lemma:

\[ S : L^\infty(\Omega, \mathbb{R}^N) \rightarrow H^1_D(\Omega, \mathbb{R}^d), \quad S(\varphi) := u \]

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Reduced cost-functional

Lemma:

\[ j(\varphi) := J^\varepsilon(S(\varphi), \varphi) = \alpha J_1(S(\varphi), \varphi) + \beta J_2(S(\varphi), \varphi) + \gamma E^\varepsilon(\varphi) \]

The reduced cost-functional \( j : H^1(\Omega, \mathbb{R}^N) \cap L^\infty(\Omega, \mathbb{R}^N) \rightarrow \mathbb{R} \) is Fréchet-differentiable.
the optimal control problem \((\mathcal{P}^\varepsilon)\) can be reformulated to

\[
\min_{\varphi \in \mathcal{G}^m \cap \mathcal{U}_c} j(\varphi).
\]

Then the following variational inequality is fulfilled:

\[
\frac{d}{d\varphi}(\tilde{\varphi} - \varphi) \geq 0 \quad \forall \tilde{\varphi} \in \mathcal{G}^m \cap \mathcal{U}_c.
\]

\[
j'(\varphi)(\tilde{\varphi} - \varphi) = J_{u\varphi}(u, \varphi) u^* + J_{\varphi}(u, \varphi)(\tilde{\varphi} - \varphi)
\]

\[
J_{u\varphi}(u, \varphi) u^* = -\langle E(p), E(u) \rangle_{\mathcal{C}'(\varphi) \bar{\varphi} - \varphi^N} - \int_\Omega (\tilde{\varphi}^N - \varphi^N) f \cdot p
\]
Theorem (optimality system)

The functions \((u, \varphi, p) \in H^1_D(\Omega, \mathbb{R}^d) \times (g^m \cap U_c) \times H^1_D(\Omega, \mathbb{R}^d)\) fulfill

\[
\begin{align*}
\begin{cases}
-\nabla \cdot [C(\varphi)E(u)] &= \left(1 - \varphi^N\right)f & \text{in } \Omega, \\
u &= 0 & \text{on } \Gamma_D, \\
[C(\varphi)E(u)] n &= g & \text{on } \Gamma_g, \\
[C(\varphi)E(u)] n &= 0 & \text{on } \Gamma_0,
\end{cases}
\end{align*}
\]

the adjoint equations (AE)

\[
\begin{align*}
\begin{cases}
-\nabla \cdot [C(\varphi)E(p)] &= \alpha \left(1 - \varphi^N\right)f + \\
&+ 2\beta \kappa J_0(u, \varphi) \frac{\kappa - 1}{\kappa} c(1 - \varphi^N)(u - u_\Omega) & \text{in } \Omega, \\
p &= 0 & \text{on } \Gamma_D, \\
[C(\varphi)E(p)] n &= \alpha g & \text{on } \Gamma_g, \\
[C(\varphi)E(p)] n &= 0 & \text{on } \Gamma_0,
\end{cases}
\end{align*}
\]

and the gradient inequality (GI)

\[
\begin{align*}
\begin{cases}
\gamma \varepsilon \int_\Omega \nabla \varphi : \nabla (\tilde{\varphi} - \varphi) + \frac{\gamma}{\varepsilon} \int_\Omega \Psi'_0(\varphi) \cdot ( \tilde{\varphi} - \varphi) \\
- \beta \kappa J_0(u, \varphi) \frac{\kappa - 1}{\kappa} \int_\Omega c(\tilde{\varphi}^N - \varphi^N)|u - u_\Omega|^2 \\
- \int_\Omega (\tilde{\varphi}^N - \varphi^N)f \cdot (\alpha u + p) - \langle E(p), E(u) \rangle_{C'(\varphi)}(\tilde{\varphi} - \varphi) & \geq 0, \\
\forall \tilde{\varphi} \in g^m \cap U_c.
\end{cases}
\end{align*}
\]
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3. Sharp interface limit of the phase field approximation

4. Numerics
Asymptotic expansion

Interfacial regions have thickness $\varepsilon$

Structure of phase field across interface

Use rescaled variable $z = \frac{\text{dist}(x, \{\varphi_\varepsilon = \frac{1}{2}\})}{\varepsilon}$

Matched asymptotic expansions
Sharp interface limit as $\varepsilon \to 0$

- Domain $\Omega$ is partitioned into $N$ regions
- $\Omega^i$ separated by interfaces $\Gamma_{ij}$,
- $[w]^j_i$ jump across interface.
- We obtain for $i, j \in \{1, \ldots, N - 1\}$: (material-material)

\[
\begin{align*}
(\text{SE})^i & \quad \begin{cases}
- \nabla \cdot [C^i E(u)] = f & \text{in } \Omega^i, \\
[w]^j_i = 0 & \text{on } \Gamma_{ij}, \\
[C E(u) \nu]^j_i = 0 & \text{on } \Gamma_{ij},
\end{cases} \\
(\text{AE})^i & \quad \begin{cases}
- \nabla \cdot [C^i E(p)] = \alpha f + 2\beta \chi J_0(u, \varphi) \frac{\chi - 1}{\chi} c(u - u_\Omega) & \text{in } \Omega^i, \\
[p]^j_i = 0 & \text{on } \Gamma_{ij}, \\
[C E(p) \nu]^j_i = 0 & \text{on } \Gamma_{ij},
\end{cases}
\end{align*}
\]

and we have $(C^i E_i(u))\nu = (C^i E_i(p))\nu = 0$ on $\Gamma_{iN}$ (material-void).
Sharp interface limit as $\varepsilon \to 0$

For all $i, j \neq N$ (material-material) interface

$$0 = \gamma \sigma_{ij} \kappa - [\mathcal{C} \mathcal{E}(u) : \mathcal{E}(p)]_i^j + [\mathcal{C} \mathcal{E}(u) \nu \cdot (\nabla p) \nu]_i^j + [\mathcal{C} \mathcal{E}(p) \nu \cdot (\nabla u) \nu]_i^j - [\lambda_1]_i^j$$

Term $- [\mathcal{C} \mathcal{E}(u) : \mathcal{E}(p)]_i^j + [\mathcal{C} \mathcal{E}(u) \nu \cdot (\nabla p) \nu]_i^j + [\mathcal{C} \mathcal{E}(p) \nu \cdot (\nabla u) \nu]_i^j$ generalizes the Eshelby traction (compare materials science)

$$0 = \gamma \sigma_{iN} \kappa + \mathcal{C}^i \mathcal{E}_i(u) : \mathcal{E}_i(p)$$

$$- \beta \kappa J_0(u, \varphi) \frac{\kappa - 1}{\kappa} c |u - u_\Omega|^2 - f \cdot (\alpha u + p) + (\lambda_1)_i - (\lambda_1)_N.$$

(void-material) interface
Choose angle at triple junction

Example computation

- Typically angles at void should be $180^\circ$ or close to it (otherwise cracks are possible)
- Angles in phase field model are determined by energy $\Psi$ (Bronsard, Reitich; Bronsard, Garcke, Stoth)
- Important: Asymptotic analysis shows elasticity does not influence equilibrium angles
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Solving the gradient inequality

In order to solve the gradient inequality (GI), we use a $L^2$-gradient flow dynamic.

Allen-Cahn (2.order)

$$\varepsilon (\partial_t \varphi, \tilde{\varphi} - \varphi)_{L^2} + j'(\varphi)(\tilde{\varphi} - \varphi) \geq 0 \quad \forall \tilde{\varphi} \in G^m \cap U_c. \quad (4.1)$$

Setting $\frac{\partial \varphi}{\partial t} = 0$ in (4.1) we obtain a solution of (GI).

Cahn-Hilliard dynamics possible

- $H^{-1}$-gradient flow dynamics
- Leads to different evolution, fourth-order PDE (compare Voigt et al.)
- Computationally more "expensive"
**Numerical solution techniques**

- finite element approximation of $\varphi, u, p$
- semi-implicit in time: pseudo-time stepping approach to gradient inequality
- solve variational inequality with primal dual active set method (PDAS) (Hintermüller, Ito, Kunisch)
- Analyzed for Cahn-Hilliard variational inequality by Blank, Butz, Garcke
- Analyzed for Allen–Cahn systems by Blank, Garcke, Sarbu, Styles
- More efficient methods for the overall optimization problem Blank, Rupprecht
  $H^1$-gradient projection and SQP method
Michell construction $d = 2, N = 2, \beta = 0$ (red: material, blue: void)

Typical computation starting with checker-board

- Topology changes
Cantilever beam construction \( d = 2, N = 3, \beta = 0 \)

Here: two materials and void

Deformed state

\( t = 0.000 \)
\( t = 0.0015 \)
\( t = 0.01 \)
\( t = 0.02 \)
\( t = 0.04 \)
\( t = 0.3 \)

(red: hard material, green: soft material, blue: void)
Cantilever beam construction $d = 3, N = 2, \beta = 0$

(red: hard material, blue: void )

final state

boundary of material region
Push construction (red: material, blue: void)

Computation of adjoint state necessary
Summary / Conclusions

- Introduced a phase field method for multi-material structural topology optimization (based on earlier work by Bourdin/Chambolle, Wang/Zhou, Burger/Stainko)
- First order optimality conditions were rigorously derived
- Sharp interface limit was analyzed with the help of formally matched asymptotic expansions
  In the limit we obtained classical shape derivatives and some new shape derivatives for the multi-material situation
- With the help of asymptotics at the triple junction
- Numerical computations demonstrated the applicability of the approach

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Thank you for your Attention!