Topology Optimization with Isogeometric Analysis in a Phase Field Approach

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Design processes often involve or require some optimization of the geometry (CAD).

- **Shape Optimization:**
  find the optimal shape of a body;

- **Topology Optimization:**
  find the optimal distribution of the material in a domain or component.
Current **Engineering procedures** based on the **Finite Element Analysis** do **not** allow a straightforward use of optimization tools.

This is principally due to the **CAD geometry-mesh mapping**.
Design, Analysis, Optimization

**Example: Shape Optimization**

\[
\text{find } \partial \Omega \text{ s.t. } J(u; \partial \Omega) \text{ is minimum, with:} \\
L(u)u = f \text{ in } \Omega \text{ & BCs.}
\]

[Jamenson, Mohammadi, Pironneau, Sokolowski, Svanberg, Zolesio, …]

**Difficulties:**
- nonlinearities/differentiation/optimization tech.
- re-meshing
- geometrical information

![Shape Optimization Diagram]
Design, Analysis, Optimization

Difficulties in geometry optimization are inherited by drawbacks in Finite Element Analysis:

- Computational geometry and analysis are separate fields
  - Finite Element Method (FEM), started in 1950’s
  - Computer Aided Design (CAD) and Computational Geometry (CG), started in 1970’s
- Geometry is a foundation of CAD
- Geometry is a foundation of computational analysis
- CAD and FEM use different representations of geometry
- Mesh generation is a bottleneck in Design through Analysis.
Design, Analysis, Optimization

Encapsulate the exact CAD geometry in:
- Analysis
- Design
- Optimization:
  - Shape Optimization
  - Topology Optimization

Isogeometric Analysis

[Hughes, Cottrell, Bazilevs, 2005]
Isogeometric Analysis

- Analysis framework built on the primitives (basis functions) of CAD and Computational Geometry
  - Original instantiation based on Non-Uniform Rational B-Splines (NURBS)
  - Framework extended to more advanced discretizations (e.g., T-splines, Subdivision)

- Generalizes and improves on Finite Element Analysis
  - Encapsulates “exact geometry” and its parameterization at the coarsest level of discretization
  - Allows for smooth basis functions
  - Allows for $h$-, $p$- and $k$-refinement
  - Geometry and its parameterization unchanged during refinement
Objects of B-spline geometry

Linear combination of the spline basis in \( \hat{\Omega} = (0,1)^{\alpha} \) \( \alpha = 1, \ldots, d \)
and objects in \( \mathbb{R}^d \)

\[
\Omega = F(\xi) = \langle C, N \rangle(\xi) = \sum_{i=1}^{n} C_i N_i(\xi) \quad \forall \xi \in \hat{\Omega} = (0,1)^{\alpha}
\]

\( \alpha = 1 \) gives rise to a \textit{B-spline curve} in \( \mathbb{R}^d \)
\( \alpha = 2 \) gives rise to a \textit{B-spline surface} in \( \mathbb{R}^d \)
\( \alpha = 3 \) gives rise to a \textit{B-spline solid} in \( \mathbb{R}^d \)

\( \text{Control points.} \)
\( \text{Their multi-linear interpolation forms} \)
\( \text{Control mesh} \)

\textit{Cannot represent conic sections (i.e. circles, ellipses) exactly. Need NURBS.}
Univariate (1-D) splines

Knot vector on $\hat{\Omega}$ and $p$-order

$$\Xi = \{ \xi_1, \xi_2, \xi_3, \ldots, \xi_{n+p+1} \}$$

$n = \text{number of basis functions}$

Start with piece-wise constants

Knots $\xi_i$ with multiplicity $m_i$

B-spline basis on $\hat{\Omega}$ by recursion:

$$N_{i,0}(\xi) = \begin{cases} 
1 & \text{if } \xi_i \leq \xi < \xi_{i+1}, \\
0 & \text{otherwise}
\end{cases}$$

Bootstrap recursively to $p$

$$N_{i,p}(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi)$$

$n = \text{number of basis functions}$
Univariate (1-D) splines

*Knot vector* on $\hat{\Omega}$ and *order* 2

- control points
- knots
Objects of NURBS geometry

Linear combination of the spline basis in \( \hat{\Omega} = (0,1)^\alpha \) \( \alpha = 1,\ldots,d \) and objects in \( \mathbb{R}^{d+1} \) projected back into \( \mathbb{R}^d \) by a \textit{projective transformation}:

\[
\Omega = F(\xi) = \Pi \left( \sum_{i=1}^{n} \{ C_i, w_i \} N_i(\xi) \right) = C_{i,w_i}
\]

Part of geometrical map. NURBS basis is geometry-specific.

Conic sections represented exactly.
Objects of NURBS geometry
From NURBS to Isogeometric Analysis

\[ \Omega = \left\{ x \in \mathbb{R}^d, x = F(\xi) = \sum_{i=1}^{n} C_i R_i(\xi), \forall \xi \in \hat{\Omega} = (0,1)^a \right\} \]

Physical domain

Parametric domain

\[ u \in V \text{ solution of PDE} \]

Isogeometric Analysis

\[ u_h \in V_h = \text{span}\left\{ R_i \circ F^{-1} \right\}_{i=1, \ldots, n} \subset V \]

Basis (Isoparametric construction)

NURBS approximation space over physical domain

\[ u_h = \hat{u}_h \circ F^{-1} \quad \hat{u}_h(\xi) = \sum_{i=1}^{n} u_i R_i(\xi) \quad \text{in } \hat{\Omega} \]
Optimization with Isogeometric Analysis

- Initial CAD Geometry
- Topology Optimization
- Geometry generation
  - CAD (NURBS or T-splines)
    - [J.Zhang]
- Shape Optimization
- Optimal CAD Geometry
Topology Optimization

Applications:

• Beams/Trusses/Bridges [Bendsoe, Kikuchi, Sigmund, …]
• Aeronautical structures [Bendsoe]
• Crashworthiness design [Pedersen]
• MEMS devices / Piezoelectric micro-tools
  [Buhl, Carbonari, Sigmund, Silva, Paulino,…]
• Dynamical systems [Jensen]
• Acoustics / Photonic / Thermal / Fluid problems
  [Bendsoe, Gersborg-Hansen, Jensen, Sigmund, …]

- 2D/3D problems
- Single or multi-material
Topology Optimization

[ Bendsoe, Kikuchi, Sigmund, Stolpe, Svanberg, … ]

\[
\text{find } \rho = \{0,1\} \text{ in } \Omega \subset R^d \text{ s.t. } J_E(\rho,u) \text{ minimum, with:}
\]
\[
\begin{cases}
-\text{div } \sigma(u) = f \text{ in } \{\rho = 1\} \subseteq \Omega \\
u = 0 \text{ on } \Gamma_D, \\
\sigma(u) \cdot n = t \text{ on } \Gamma_N, \\
\sigma(u) \cdot n = 0 \text{ on } \partial \Omega \setminus (\Gamma_D \cup \Gamma_N)
\end{cases}
\]

& inequality constraints

\[
( u = u(\rho) \text{ and } \sigma(u) = \sigma(u(\rho)) )
\]

Structural Topology Optimization:
Linear Elasticity
Minimum Compliance

[Bendsoe, Kikuchi, Sigmund, Pedersen]

Find the optimal distribution of $\rho$ in the domain $\Omega$ in order to minimize the compliance $J_E(\rho)$ of the system under a volume constraint $V$ (equality or inequality)

$$J_E(\rho) = \int_{\Omega} f \cdot u(\rho) + \oint_{\Gamma_N} t \cdot u(\rho)$$

$$\int_{\Omega} \rho \leq V < |\Omega|$$

Alternative criterion: minimize weight of the structure under stress constraints
SIMP Approach

- \( \rho = \{0,1\} \rightarrow 0 \leq \rho \leq 1 \) (with inequality constraints)

- Solid Isotropic Material with Penalization (SIMP)
  \[ E(\rho) = \rho^P E_0, \quad P \geq 3 \]
  (Young modulus depends on density)

- Finite Element approximation; Low Order \( \rho \) piecewise constant over mesh elements

- Constrained Optimization procedure; e.g.: MMA (Method of Moving Asymptotes), [Svanberg]
**SIMP Approach**

**Advantages:**
- simplicity & flexibility
- low number of DOFs

**Drawbacks:**
- instabilities & check-board phenomenon
  - Required: regularization techniques, filters, sensitivity filters, perimeter limitation
- high number of inequality constraints
- non-convex optimization
- ability to provide geometric information
- manufacturability - integration with CAD
Multiphase Approach

[Bourdin, Burger, Chambolle, Stainko, Wang, Zhou]

\[ \rho = \{0, 1\} \in L^\infty(\Omega) \rightarrow \rho \in H^1(\Omega) \cap L^\infty(\Omega) \]

Sharp interfaces approximated by thin layers

Add to cost functional a total free energy term (Cahn-Hilliard type):

\[
J(\rho) = J_E(\rho) + \frac{1}{\varepsilon} J_{BLK}(\rho) + \varepsilon J_{INT}(\rho)
\]

\[
J_{BLK}(\rho) = \int_{\Omega} \rho(1 - \rho) \, d\Omega
\]

\[
J_{INT}(\rho) = \frac{1}{2} \int_{\Omega} |\nabla \rho|^2 \, d\Omega
\]

\(\varepsilon > 0\)

“Filtering” & perimeter limitation

Finite Element approximation: order \(\geq 1\)
Multiphase Approach

Advantages:
- sharp & smooth interfaces
- geometrical information
- filtering and perimeter limitation embedded in $J_{\text{INT}}(\rho)$
- possibility to remove inequality constraints $0 \leq \rho \leq 1$ by choosing $J_{\text{BLK}}(\rho)$

Drawbacks:
- non-convex optimization
  $\rightarrow$ strong dependence on the optimization solver used
- dependence on parameters
Multiphase Approach

Continuation method

• Quasi-Newton optimization method

• Continuation method (progressive reduction of $\varepsilon = \chi^L \varepsilon_0$); the final solution is obtained as a sequence of optimal states for increasing values of $L$

$$J(\rho) = J_E(\rho) + \frac{1}{\varepsilon} J_{BLK}(\rho) + \varepsilon J_{INT}(\rho)$$

• Isogeometric Analysis, order 3

Linear Elasticity, Plane Stress

$E_0 = 1, \ v = 0.3, \ f = 0, \ t = -0.5\hat{y}$

$\Omega = (0,2) \times (0,1), \ \int_{\Omega} \rho \leq 0.35$

$E(\rho) = \rho^P E_0, \ P = 5$

$\varepsilon_0 = 1.5, \ \chi = 0.25$

# d.o.f. = 3960 (IsoG.)
Multiphase Approach

\[ t = -0.5 \]

\[ \Gamma_N \]

\[ \Omega \]

\[ \Gamma_D \]

\[ \Gamma_D \]

\[ L=0 \]

\[ L=1 \]

\[ L=2 \]

\[ L=3 \]

\[ L=4 \]
The Multiphase approach in Topology Optimization shows analogies with Multiphase problems, in particular with the:

**Cahn-Hilliard equation** (1957)

which describe the transition of two phases from a mixed status to a fully separated configuration.

→ The CH eq. is a 4\textsuperscript{th} order nonlinear parabolic PDE
Cahn - Hilliard Equation

\[
\begin{aligned}
\frac{\partial \rho}{\partial t} &= \nabla \cdot (M(\rho) \nabla \mu_{\text{CH}}(\rho)) \quad \text{in } \Omega \times (0,T) \\
\nabla \rho \cdot n &= 0 \quad \text{on } \partial \Omega \times (0,T) \\
M(\rho) \nabla \mu_{\text{CH}}(\rho) \cdot n &= 0 \quad \text{on } \partial \Omega \times (0,T) \\
\rho &= \rho_0 \quad \text{in } \Omega \times \{t=0\}
\end{aligned}
\]

\[
J_{\text{CH}}(\rho) = \int_{\Omega} F(\rho) d\Omega + \frac{1}{2} \lambda \int_{\Omega} \nabla \rho \cdot \nabla \rho d\Omega \quad \lambda > 0
\]

\[
\mu_{\text{CH}}(\rho) : = \langle \mu_{\text{CH}}(\rho), \varphi \rangle = \frac{dJ_{\text{CH}}}{d\rho}(\rho)[\varphi] \quad \forall \varphi \text{ test function}
\]

\[
\mu_{\text{CH}}(\rho) = \frac{dF}{d\rho}(\rho) - \lambda \Delta \rho
\]

\[
V = \int_{\Omega} \rho_0 d\Omega \equiv \int_{\Omega} \rho(t) d\Omega \quad \forall t \in (0,T)
\]

\[
M(\rho) = D \rho (1 - \rho) \quad \text{mobility}
\]
Cahn - Hilliard Equation

Time approximation:
• generalized α-method (fully implicit, second order accurate)
• adaptive time-scheme (based on comparison of Backward Euler and α-method)

Spatial approximation:
• IsoGeometric Analysis, order ≥ 2

\[ \lambda = \tau h^2 \]

Interface thickness
Depending on resolution

\[ F(\rho) \text{ logarithmic, } \theta = 1.5, \ M = D\rho(1-\rho), \ D = 1, \]
Initial random distribution: \textit{Volume} ± 0.50 %
\textit{IGA}: order \( p,q = 2 \), Gauss pt.s = 3, \( h = L_0 / 45 \)

[Gomez, Calo, Bazilevs, Hughes, 2007]
Cahn - Hilliard Equation

Volume = 0.50, Periodic BCs

$t = 4e-4$

Steady state

$J_{CH}$
Cahn - Hilliard Equation

Volume = 0.37, Periodic BCs

\( t = 9 \times 10^{-5} \)

Steady state

\( J_{CH} \)
Cahn - Hilliard Equation

Volume = 0.50

Volume = 0.37
Topology Opt. with Phase Field

**Generalized Cahn-Hilliard equations**

\[ J(\rho) = J_{CH}(\rho) + \gamma J_E(u(\rho)) \]

\[ J_{CH}(\rho) = \int_{\Omega} F(\rho) d\Omega + \frac{1}{2} \lambda \int_{\Omega} \nabla \rho \cdot \nabla \rho d\Omega \quad \lambda > 0 \]

\[ J_E(u(\rho)) = \int_{\Gamma_N} t \cdot u(\rho) d\Gamma_N \]

\[ \mu(\rho, u(\rho)) = \mu(\rho) : < \mu(\rho), \varphi > = \frac{dJ}{d\rho}(\rho)[\varphi] \quad \forall \varphi \text{ test function} \]

\[ \mu(\rho) = \mu_{CH}(\rho) + \mu_E(\rho, u(\rho)) = \frac{dF}{d\rho}(\rho) - \lambda \Delta \rho - \gamma P \rho^{p-1} \tilde{\sigma}(u(\rho)) : \varepsilon(u(\rho)) \]

\[ \sigma(\rho, u) = \rho^p \tilde{\sigma}(u) \]

\[ V = \int_{\Omega} \rho_0 d\Omega \equiv \int_{\Omega} \rho(t) d\Omega \quad \forall t \in (0, T) \]

\[ M(\rho) = D \rho (1 - \rho) \quad \text{mobility} \]
Topology Opt. with Phase Field

Generalized Cahn-Hilliard equations

\[ \begin{aligned}
\frac{\partial \rho}{\partial t} &= \nabla \cdot (M(\rho) \nabla \mu(\rho,u)) \quad \text{in } \Omega \times (0,T) \\
\nabla \rho \cdot n &= 0 \quad \text{on } \partial \Omega \times (0,T) \\
M(\rho) \nabla \mu(\rho,u) \cdot n &= 0 \quad \text{on } \partial \Omega \times (0,T) \\
\rho &= \rho_0 \quad \text{in } \Omega \times \{t = 0\}
\end{aligned} \]

\[ \begin{aligned}
-\text{div} \, \sigma(\rho,u) &= f \quad \text{in } \Omega \times (0,T) \\
u &= 0 \quad \text{on } \Gamma_D \times (0,T) \\
\sigma(\rho,u) \cdot n &= t \quad \text{on } \Gamma_N \times (0,T) \\
\sigma(\rho,u) \cdot n &= 0 \quad \text{on } \partial \Omega \setminus (\Gamma_D \cup \Gamma_N) \times (0,T)
\end{aligned} \]
Topology Opt. with Phase Field

**Generalized Cahn-Hilliard equations**

- Mass/volume conservative $\Rightarrow$ topology optimization is volume constrained

$$
\int_\Omega \rho = \int_\Omega \rho_0 = V \quad \forall t \geq 0
$$

- The cost functional $J(\rho)$ corresponds to the energy of the generalized CH eqs. and it is a Liapunov functional

$$
\frac{dJ}{dt}(\rho) = - \int_\Omega M(\rho) |\nabla \mu(\rho)|^2 \leq 0 \quad \forall t \geq 0
$$

- The steady state of the generalized CH eqs. corresponds to the minimum of the energy and hence to the minimum of the cost functional
Topology Opt. with Phase Field

Generalized Cahn-Hilliard equations

Advantages:
• optimal topology is obtained as steady state of CH eqs.
• no optimization procedure
• provide geometrical information
• no use of “filtering” techniques

Drawbacks:
• set of 4\textsuperscript{th} order nonlinear parabolic PDEs
• ability to capture sharp interfaces → resolution
• computational expensive
Isogeometric Analysis

- $C^q(\Omega), q \geq 1$, continuous basis
- adaptive time stepping method + implicit solver, $\alpha$-method
- accurate and stable results capturing thin layers
- NO geometrical approximation of CAD geometries
- perform topology opt. in regions and components of existing structures
The choice of the parameters $\lambda$ and $\gamma$

$$J(\rho) = J_{CH}(\rho) + \gamma J_E(u(\rho))$$

$$J_{CH}(\rho) = \int_{\Omega} F(\rho) d\Omega + \frac{1}{2} \lambda \int_{\Omega} \nabla \rho \cdot \nabla \rho d\Omega \quad \lambda > 0$$

$$J_E(u(\rho)) = \int_{\Gamma_N} t \cdot u(\rho) d\Gamma_N$$

$$\lambda = \tilde{\lambda} h^2, \quad \gamma = \tilde{\gamma} \gamma_E$$

• To balance the compliance and the CH parts of the energy, we choose:

$$\gamma_E = \frac{J_{CH}(\rho_0)}{J_E(\rho_0)}$$

$$\tilde{\lambda}, \tilde{\gamma} = \text{dimensionless, chosen by user (depend on each other, load case, volume fraction, penalization P, ...)}$$
Topology Opt. with Phase Field

\[ \Omega = (0, 2.0 m) \times (0, 1.0 m), \quad V = 0.50 |\Omega|, \quad \rho_0 = 0.5 \]
plane stress, \( E_0 = 200 \text{GPa}, \quad \nu = 0.3, \quad |t| = 200 \text{MPa} \]
\[ P = 5, \quad \text{Gauss points: } 5 \times 5 \]

Order \( p=q=2, \# \text{DOF} = 840 \)

\[ \tilde{\lambda} = 2.5 \quad \tilde{\gamma} = 5.0 \]

Steady state

dt vs. time
Topology Opt. with Phase Field

Steady state
Topology Opt. with Phase Field

Energy vs. time (dimensionless)

$J(\rho)$

$J_E(\rho)$

$J_{CH}(\rho)$

$J_{BLK}(\rho)$

$J_{INT}(\rho)$
Topology Opt. with Phase Field

\[ \Omega = (0, 2.0m) \times (0, 1.0 m), \quad V = 0.50 \parallel \Omega, \quad \rho_0 = 0.5 \]
plane stress, \( E_0 = 200 GPa, \quad \nu = 0.3, \quad |t| = 200 MPa \]
\( P = 5, \quad \) Gauss points: \( 5 \times 5 \)

Order \( p=q=2, \# \text{DOF} = 680 \)

\[ \tilde{\lambda} = 2.5 \quad \tilde{\gamma} = 5.0 \]

Steady state

\[ t = 1404.3155 \]
Topology Opt. with Phase Field

Steady state
Topology Opt. with Phase Field

\[ \Omega = (0, 2.0m) \times (0, 1.0m), \quad V = 0.50 |\Omega|, \quad \rho_0 = 0.5 \]

plane stress, \( E_0 = 200 \text{GPa}, \quad \nu = 0.3, \quad |t| = 200 \text{MPa} \]

\( P = 5, \quad \text{Gauss points: } 5 \times 5 \)

Order \( p=q=2, \# \text{DOF} = 840 \)

\[ \tilde{\lambda} = 2.5 \quad \tilde{\gamma} = 5.0 \]
Topology Opt. with Phase Field

\[ \tilde{\lambda} = 2.5 \]

\[ \tilde{\lambda} = 1.375 \]

(limit value)

dt vs. time
Topology Opt. with Phase Field

\[ \Omega = (0, 2.0m) \times (0, 1.0 m), \quad V = 0.50 |\Omega|, \quad \rho_0 = 0.5 \]
plane stress, \( E_0 = 200 GPa, \quad \nu = 0.3, \quad |t| = 200 MPa \)
\( P = 5, \quad \text{Gauss points: } 5 \times 5 \)

Order \( p=q=2, \# \text{ DOF} = 840 \)

\[ \tilde{\lambda} = 1.5 \quad \tilde{\gamma} = 1.0 \]

**Diagram:**
- \( \Omega \)
- \( \Gamma_D \)
- \( \Gamma_N \)
- only \( u_1 = 0 \)
- \( t \)
- \( \omega \)

**Graphs:**
- \( dt \) vs. time
- \( J(\rho) \)
- \( J_{CH}(\rho) \)
- \( J_E(\rho) \)
Topology Opt. with Phase Field

- Exact geometry
- Steady state
Shape Optimization

- The NURBS map turns the infinite dimensional problem:

  \[
  \min_{\partial \Omega} J(\partial \Omega)
  \]

  s.t. \( g_i(\partial \Omega) \geq 0 \quad i = 1, 2, ..., n_{ineq} \)
  
  \( h_j(\partial \Omega) = 0 \quad j = 1, 2, ..., n_{eq} \)

  state eq. with b.c.'s

into a finite dimensional one:

  \[
  \min_{P_{i,j}} J(\partial \Omega(P_{i,j}))
  \]

  s.t. \( g_i(\partial \Omega(P_{i,j})) \geq 0 \quad i = 1, 2, ..., n_{ineq} \)
  
  \( h_j(\partial \Omega(P_{i,j})) = 0 \quad j = 1, 2, ..., n_{eq} \)

  state eq. with b.c.'s

Isogeometric Analysis \(\leftrightarrows\) Exact CAD geometries
Shape Optimization

Topology optimization

NURBS geometry
(sweeping technique, J. Zhang)

Shape Optimization

\[ J = 2.6148 \cdot 10^{-4} \]

\[ J = 2.1473 \cdot 10^{-4} \]
Conclusions & Future Developments

- We developed a pipeline for geometry optimization with Isogeometric Analysis encapsulating exact CAD geometries.

- We solved topology optimization problems in a phase field approach based on the generalized Cahn-Hilliard equations.

- Improve resolution for 2D problems (sharp interfaces)

- 3D problems