Topology optimization based on a Numerical Topological-Shape Derivative

Michael Gfrerer

Joint work with Peter Gangl (RICAM Linz)

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Outline

1. Continuous stetting
   $\rightarrow$ Unification of shape and topological derivative

2. Numerical stetting
   $\rightarrow$ Explicit formulas for numerical topological-shape derivative

3. Numerical results
   $\rightarrow$ Verification
   $\rightarrow$ Optimization example

Continuous stetting

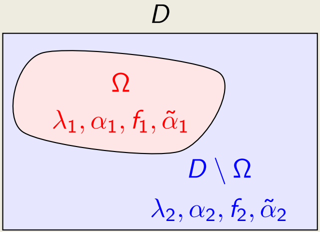
Topology optimization

Model problem

$$\min_{\Omega \in \mathcal{A}} \; g(\Omega, u)$$

subject to

$$\begin{aligned} -\lambda_\Omega \Delta u + \alpha_\Omega u &= f_\Omega && \text{in } D \\ u &= g_D && \text{on } \Gamma_D \\ \lambda_\Omega \partial_n u &= g_N && \text{on } \Gamma_N \end{aligned}$$



Area + Tracking type cost function

$$g(\Omega, u) = c_1 |\Omega| + c_2 \int_D \tilde{\alpha}_\Omega |u - \hat{u}|^2 \, \mathrm{d}x$$

$\hat{u} \ldots$ given desired state

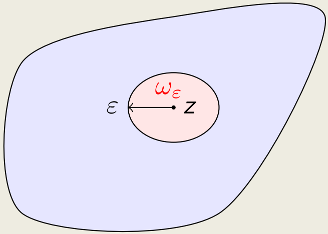
Reduced objective function: $\mathfrak{g}(\Omega) = g(\Omega, u(\Omega))$

Topological derivative

Definition

Let $\omega \subset \mathbb{R}^d$ with $0 \in \omega$.
For a point $z \in \Omega \cup (D \setminus \overline{\Omega})$, let $\omega_\varepsilon := z + \varepsilon\omega$ denote a perturbation of the domain around z of size ε and of shape ω.
The continuous topological derivative is defined by

$$d\mathfrak{g}(\Omega)(z) = \begin{cases} \lim_{\varepsilon \searrow 0} \frac{\mathfrak{g}(\Omega \cup \omega_\varepsilon) - \mathfrak{g}(\Omega)}{|\omega_\varepsilon|} & \text{for } z \in D \setminus \overline{\Omega} \\ \lim_{\varepsilon \searrow 0} \frac{\mathfrak{g}(\Omega \setminus \bar{\omega}_\varepsilon) - \mathfrak{g}(\Omega)}{|\omega_\varepsilon|} & \text{for } z \in \Omega \end{cases}$$



Shape derivative

Domain perturbation via a sufficiently smooth vector field V

$$\Omega_t = (\mathrm{id} + tV)(\Omega)$$

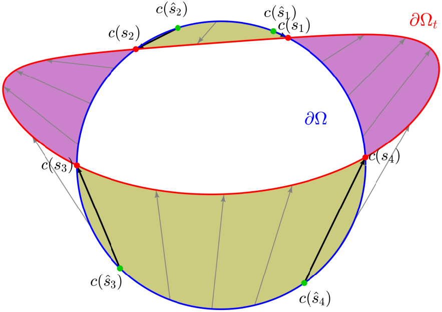
Definition (Classical Shape derivative)

$$d\mathfrak{g}(\Omega)(V) = \lim_{t \searrow 0} \frac{\mathfrak{g}(\Omega_t) - \mathfrak{g}(\Omega)}{t}$$

Definition (Modified shape derivative)

$$\hat{d}\mathfrak{g}(\Omega)(V) = \lim_{t \searrow 0} \frac{\mathfrak{g}(\Omega_t) - \mathfrak{g}(\Omega)}{|\Omega_t \triangle \Omega|} \quad \text{with} \quad \Omega_t \triangle \Omega := (\Omega_t \setminus \overline{\Omega}) \cup (\Omega \setminus \overline{\Omega}_t)$$

Shape derivative



Lemma

Let Ω and V smooth. It holds

$$\hat{d}\mathfrak{g}(\Omega)(V) = \frac{d\mathfrak{g}(\Omega)(V)}{\int_{\partial\Omega} |V \cdot n| \, dS_x}$$

A topological-shape derivative

Level-set representation: $\phi : D \to \mathbb{R}$

$$\phi(\mathbf{x}) < 0 \iff \mathbf{x} \in \Omega$$
$$\phi(\mathbf{x}) > 0 \iff \mathbf{x} \in D \setminus \overline{\Omega}$$
$$\phi(\mathbf{x}) = 0 \iff \mathbf{x} \in \Gamma$$

Indirect perturbation of Ω by perturbing ϕ

$$\phi_\varepsilon = O_\varepsilon \phi$$

with some operator $O_\varepsilon : C^0(D) \to C^0(D)$ dependent on $\varepsilon > 0$ with the property

$$\Omega(O_0\phi) = \Omega(\phi)$$

Definition (Continuous topological-shape derivative)

$$d\mathcal{J}(\phi)(O_\varepsilon) = \lim_{\varepsilon \searrow 0} \frac{\mathcal{J}(\phi_\varepsilon) - \mathcal{J}(\phi)}{|\Omega(\phi_\varepsilon) \triangle \Omega(\phi)|} \qquad \text{with} \qquad \mathcal{J}(\phi) := \mathfrak{g}(\Omega(\phi))$$

Numerical stetting

Discretization

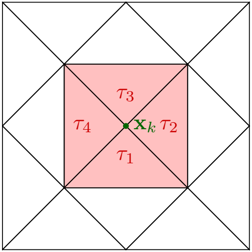
Assume fixed finite element mesh $\mathcal{T}$ covering D with

- M nodes $\{\mathbf{x}_k\}_{k=1}^{M}$
- and N triangular elements τ_l

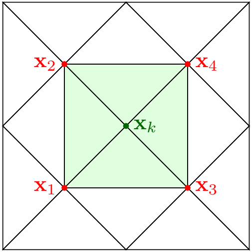
Index-sets:

$$I_{\mathbf{x}_k} := \{l \in \{1,\ldots,N\} : \mathbf{x}_k \in \bar{\tau}_l\} \quad \text{for } k = 1,\ldots,M.$$

$$R_{\mathbf{x}_k} := \{i \in \{1,\ldots,M\} | \exists l \in I_{\mathbf{x}_k} : \mathbf{x}_i \in \tau_l\} \quad \text{for } k = 1,\ldots,M.$$



$I_{\mathbf{x}_k} = \{1,\ 2,\ 3,\ 4\}$



$R_{\mathbf{x}_k} = \{k,\ 1,\ 2,\ 3,\ 4\}$

Discretization

Linear finite elements

$$S_h^1(D) = \{v \in H^1(D) : v|_T \in P_1 \text{ for all } T \in \mathcal{T}\} = \text{span}\{\varphi_1, \dots, \varphi_M\}$$

Discretize the state and the level-set function: $u \in S_h^1(D)$, $\phi \in S_h^1(D)$
System of linear equations

$$(\mathbf{M} + \mathbf{K})\mathbf{u} = \mathbf{f}$$

with

$$\mathbf{M}[i,j] = \int_D \alpha_\Omega \varphi_j \varphi_i \, \mathrm{d}x,$$

$$\mathbf{K}[i,j] = \int_D \lambda_\Omega \nabla \varphi_j \cdot \nabla \varphi_i \, \mathrm{d}x,$$

$$\mathbf{f}[i] = \int_D f_\Omega \varphi_i \, \mathrm{d}x.$$

Numerical topological-shape derivative

Definition

$$d\mathcal{J}(\phi)(\mathbf{x}_k) = \begin{cases} \lim_{\varepsilon \searrow 0} \frac{\mathcal{J}(T^{-\to+}_{k,\varepsilon}\phi) - \mathcal{J}(\phi)}{|\Omega(T^{-\to+}_{k,\varepsilon}\phi)\Delta\Omega(\phi)|} & \text{for } \mathbf{x}_k \in \mathfrak{T}^- = \{\mathbf{x}_k \in \mathcal{T} | \forall i \in R_{\mathbf{x}_k} : \phi_i \leq 0\} \\ \lim_{\varepsilon \searrow 0} \frac{\mathcal{J}(T^{+\to-}_{k,\varepsilon}\phi) - \mathcal{J}(\phi)}{|\Omega(T^{+\to-}_{k,\varepsilon}\phi)\Delta\Omega(\phi)|} & \text{for } \mathbf{x}_k \in \mathfrak{T}^+ = \{\mathbf{x}_k \in \mathcal{T} | \forall i \in R_{\mathbf{x}_k} : \phi_i \geq 0\} \\ \lim_{\varepsilon \searrow 0} \frac{\mathcal{J}(S_{k,\varepsilon}\phi) - \mathcal{J}(\Omega(\phi))}{|\Omega(S_{k,\varepsilon}\phi)\Delta\Omega(\phi)|} & \text{for } \mathbf{x}_k \in \mathfrak{S} = \mathcal{T} \setminus (\mathfrak{T}^- \cup \mathfrak{T}^+) \end{cases}$$

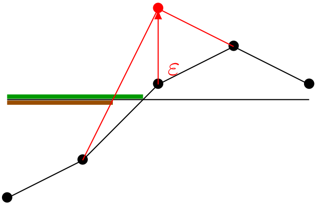
with

$$T^{-\to+}_{k,\varepsilon}\phi(\mathbf{x}) = \phi(\mathbf{x}) - (\phi(\mathbf{x}_k) - \varepsilon)\varphi_k$$

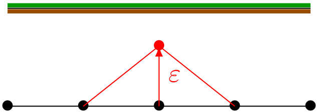
$$T^{+\to-}_{k,\varepsilon}\phi(\mathbf{x}) = \phi(\mathbf{x}) - (\phi(\mathbf{x}_k) + \varepsilon)\varphi_k.$$

$$S_{k,\varepsilon}\phi(\mathbf{x}) := \phi(\mathbf{x}) + \varepsilon\varphi_k(\mathbf{x}).$$

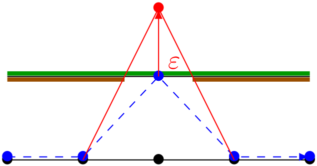
Discrete perturbations



(a) Shape derivative



(b) No effect



(c) Topological derivative

$$T_{k,\varepsilon}^{-\to+}\phi(\mathbf{x}) = \phi(\mathbf{x}) - (\phi(\mathbf{x}_k) - \varepsilon)\varphi_k$$

Numerical topological-shape derivative

Lemma

Let $\mathbf{u}_l = [u_{l_1}, u_{l_2}, u_{l_3}]\top$ and $\mathbf{p}_l = [p_{l_1}, p_{l_2}, p_{l_3}]\top$ be the nodal values for τ_l and $\mathbf{k}_{0,l}[i,j] = \left(J_l^{-1}\nabla_\xi \psi_j\right)^\top \left(J_l^{-1}\nabla_\xi \psi_i\right)$.
For $\mathbf{x}_k \in \mathfrak{T}^-$ the numerical topological derivative reads

$$d\mathcal{J}(\phi)(\mathbf{x}_k) = -c_1 - \Delta\lambda \frac{\sum_{l\in I_{\mathbf{x}_k}} \frac{\mathbf{p}_l^\top \mathbf{k}_{0,l}\mathbf{u}_l |\det J_l|}{\phi_{l_2}\phi_{l_3}}}{\sum_{l\in I_{\mathbf{x}_k}} \frac{|\det J_l|}{\phi_{l_2}\phi_{l_3}}} - \Delta\alpha p_k u_k + \Delta f p_k - c_2\Delta\tilde{\alpha}(u_k - \hat{u}_k)^2$$

whereas for $\mathbf{x}_k \in \mathfrak{T}^+$ we have

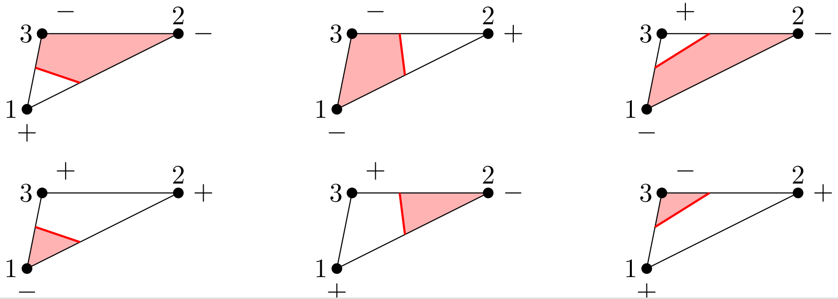
$$d\mathcal{J}(\phi)(\mathbf{x}_k) = c_1 + \Delta\lambda \frac{\sum_{l\in I_{\mathbf{x}_k}} \frac{\mathbf{p}_l^\top \mathbf{k}_{0,l}\mathbf{u}_l |\det J_l|}{\phi_{l_2}\phi_{l_3}}}{\sum_{l\in I_{\mathbf{x}_k}} \frac{|\det J_l|}{\phi_{l_2}\phi_{l_3}}} + \Delta\alpha p_k u_k - \Delta f p_k + c_2\Delta\tilde{\alpha}(u_k - \hat{u}_k)^2$$

Numerical topological-shape derivative

Lemma cont.

For $\mathbf{x}_k \in \mathfrak{S}$ the numerical shape derivative reads

$$d\mathcal{J}(\phi)(\mathbf{x}_k) = -c_1 + \Delta\lambda \frac{\sum_{l\in C_k} \mathbf{p}_l^\top \mathbf{k}_{0,l}\mathbf{u}_l \, d_k a_l}{d_k \tilde{a}} + \Delta\alpha \frac{\sum_{l\in C_k} \mathbf{p}_l^\top d_k \mathbf{m}_l^l \mathbf{u}_l}{d_k \tilde{a}} - \Delta f \frac{\sum_{l\in C_k} \mathbf{p}_l^\top d_k \mathbf{f}_l^l}{d_k \tilde{a}} + c_2 \Delta\tilde{\alpha} \frac{\sum_{l\in C_k} (\mathbf{u}_l - \hat{\mathbf{u}}_l)^\top d_k \mathbf{m}_l^l (\mathbf{u}_l - \hat{\mathbf{u}}_l)}{d_k \tilde{a}}$$



Comparison

Continuous topological derivative at $z \in D \setminus \Omega$:

$$d\mathfrak{g}(\Omega)(z) = c_1 + 2\lambda_2 \frac{\Delta\lambda}{\lambda_1 + \lambda_2} \nabla u(z) \cdot \nabla p(z) + \Delta\alpha u(z) p(z) - \Delta f p(z) + c_2 \Delta\tilde{\alpha}(u(z) - \hat{u}(z))^2$$

Numerical topological derivative for node $x_k \in \mathfrak{T}^+$:

$$d\mathcal{J}(\phi)(\mathbf{x}_k) = c_1 + \Delta\lambda \frac{\sum_{l \in \boldsymbol{I}_{\mathbf{x}_k}} \frac{\mathbf{p}_l^\top \mathbf{k}_{0,l} \mathbf{u}_l |\det J_l|}{\phi_{l_2}\phi_{l_3}}}{\sum_{l \in \boldsymbol{I}_{\mathbf{x}_k}} \frac{|\det J_l|}{\phi_{l_2}\phi_{l_3}}} + \Delta\alpha p_k u_k - \Delta f p_k + c_2 \Delta\tilde{\alpha}(u_k - \hat{u}_k)^2$$

$\rightarrow$ Mesh and basis functions are assumed to be fixed and independent of ε!

Numerical results

Problem setting

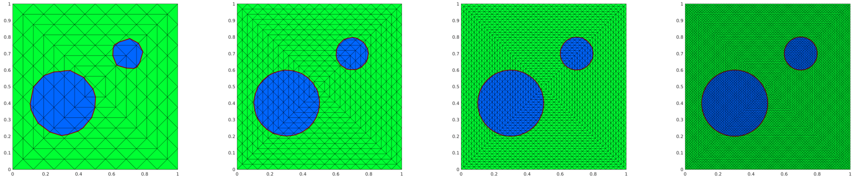
Unit square $D = \{(x, y) \in \mathbb{R}^2 | 0 \leq x \leq 1, 0 \leq y \leq 1\}$
Mixed Dirichlet-Neumann problem

$$\Gamma_D = \{(x, y) \in \partial D | y = 0 \text{ or } y = 1\} \qquad \Gamma_N = \partial D \cap \Gamma_D$$

$$g_D = y \qquad g_N = 0$$

Desired shape

$$\bar{\phi}_d(x, y) = \left((x - 0.3)^2 + (y - 0.4)^2 + 0.2^2\right)\left((x - 0.7)^2 + (y - 0.7)^2 + 0.1^2\right)$$



$\tilde{\alpha}_1$	$\tilde{\alpha}_2$	α_1	α_2	λ_1	λ_2	f_1	f_2
1	0.9	1	0.2	1	0.6	1	0.5

Verification

Numerical experiments to show that the topological-shape derivative is correct

1. Finite difference like test

2. Test related to the complex step derivative

3. Test based on hyper-dual numbers

Verification: Finite difference

$$\delta \mathcal{J}_\varepsilon(\phi)(\mathbf{x}_k) = \frac{\mathcal{J}(O_{k,\varepsilon}\phi) - \mathcal{J}(\phi)}{|\Omega(O_{k,\varepsilon}\phi)\Delta\Omega(\phi)|}$$

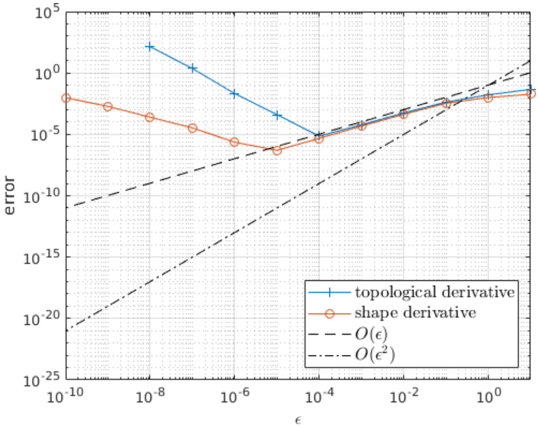
Compute the errors

$$e_S^{FD}(\varepsilon) = \sqrt{\sum_{\mathbf{x}_k \in \mathfrak{S}} (\delta \mathcal{J}_\varepsilon(\phi)(\mathbf{x}_k) - d\mathcal{J}(\phi)(\mathbf{x}_k))^2},$$

$$e_T^{FD}(\varepsilon) = \sqrt{\sum_{\mathbf{x}_k \in \mathfrak{T}^- \cup \mathfrak{T}^+} (\delta \mathcal{J}_\varepsilon(\phi)(\mathbf{x}_k) - d\mathcal{J}(\phi)(\mathbf{x}_k))^2}$$

for a decreasing sequence of values for ε.

Verification: Finite difference



Verification: Complex step derivative

Assume higher order expansion

$$\mathcal{J}(O_{k,\varepsilon}\phi) = \mathcal{J}(\phi) + \varepsilon^{o}\, d_k \tilde{a}\, d\mathcal{J}(\phi)(\mathbf{x}_k) + \varepsilon^{o+1}\, d_k \tilde{a}\, d^2\mathcal{J}(\phi)(\mathbf{x}_k) + \varepsilon^{o+2}\, d_k \tilde{a}\, d^3\mathcal{J}(\phi)(\mathbf{x}_k) + o(\varepsilon^{o+2})\dots$$

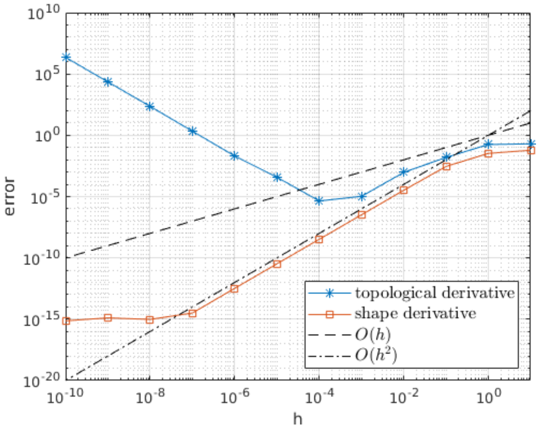
$o = 2$ for $\mathbf{x}_k \in \mathfrak{T}^- \cup \mathfrak{T}^+$
$o = 1$ for $\mathbf{x}_k \in \mathfrak{S}$

Set $\varepsilon = ih$ and compute

$$\delta\mathcal{J}_h^{CS}(\phi)(\mathbf{x}_k) := \begin{cases} \frac{\mathrm{Re}(\mathcal{J}(T_{k,ih}^{-\to+}\phi) - \mathcal{J}(\phi))}{-h^2\, d_k \tilde{a}}, & \mathbf{x}_k \in \mathfrak{T}^- \\ \frac{\mathrm{Re}(\mathcal{J}(T_{k,ih}^{+\to-}\phi) - \mathcal{J}(\phi))}{-h^2\, d_k \tilde{a}}, & \mathbf{x}_k \in \mathfrak{T}^+ \\ \frac{\mathrm{Im}(\mathcal{J}(S_{k,ih}\phi))}{h\, d_k \tilde{a}}, & \mathbf{x}_k \in \mathfrak{S} \end{cases}$$

$$d\mathcal{J}(\phi)(\mathbf{x}_k) = \delta\mathcal{J}_h^{CS}(\phi)(\mathbf{x}_k) + \mathcal{O}(h^2)$$

Verification: Complex step derivative



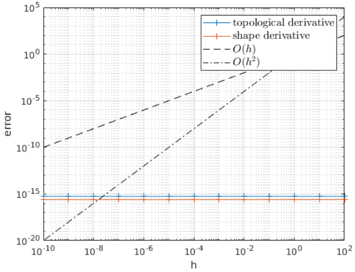
Verification: Hyper-dual numbers

- Three non-real components E_1, E_2 and E_1E_2
- $E_1^2 = E_2^2 = (E_1E_2)^2 = 0$

Set $\varepsilon = hE_1 + hE_2 + 0E_1E_2$ and compute

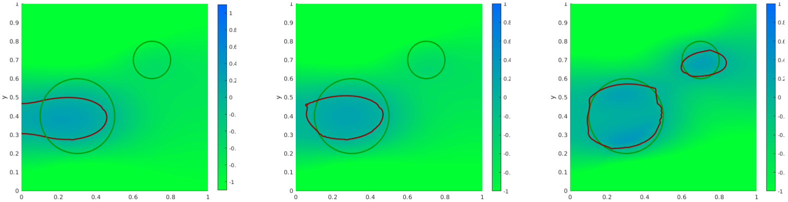
$$\delta\mathcal{J}_h^{HD}(\phi)(\mathbf{x}_k) := \begin{cases} \dfrac{E_1E_2\text{part}(\mathcal{J}(T^{-\to+}_{k,h_1E_1+h_2E_2+0E_1E_2}\phi))}{2h^2\, d_k\tilde{a}}, & \mathbf{x}_k \in \mathfrak{T}^- \\ \dfrac{E_1E_2\text{part}(\mathcal{J}(T^{+\to-}_{k,h_1E_1+h_2E_2+0E_1E_2}\phi))}{2h^2\, d_k\tilde{a}}, & \mathbf{x}_k \in \mathfrak{T}^+ \\ \dfrac{E_1\text{part}(\mathcal{J}(S_{k,h_1E_1+h_2E_2+0E_1E_2}\phi))}{h\, d_k\tilde{a}}, & \mathbf{x}_k \in \mathfrak{S} \end{cases}$$

$$d\mathcal{J}(\phi)(\mathbf{x}_k) = \delta\mathcal{J}_h^{HD}(\phi)(\mathbf{x}_k)$$

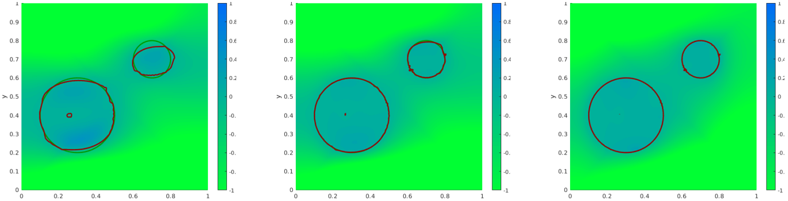


Optimization

Update the level-set function by spherical interpolation[1]



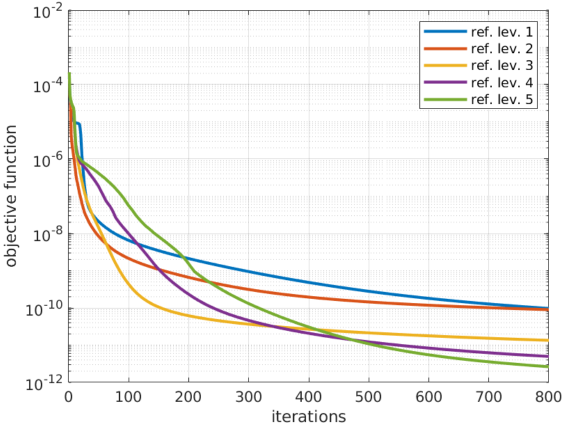
(a) 1 iteration (b) 2 iteration (c) 10 iteration



(d) 20 iteration (e) 100 iteration (f) 800 iteration

[1] Amstutz and Andrä 2006

Optimization



Summary

1. Unification of shape and topological derivative

2. Explicit formulas for the numerical topological-shape derivative

3. Verification
   1. Finite difference like test
   2. Complex numbers
   3. Hyper-dual numbers

4. Optimization based on the numerical topological-shape derivative

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