A guaranteed *a posteriori* error estimator for certified boundary variation algorithm

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Joint work with **Olivier Pantz** (CMAP École Polytechnique) and **Karim Trabelsi** (IPSA)

Outline

1. Shape optimization and shape identification problems
   - A scalar model problem
   - Differentiation with respect to the shape
   - The boundary variation algorithm
2. A posteriori estimators of the error in the shape derivative
   - Goal-oriented residual-type error estimator
   - Validation of the goal-oriented estimator
3. Adaptive shape optimization procedure
   - A first test case
   - Improved adaptive shape optimization procedure

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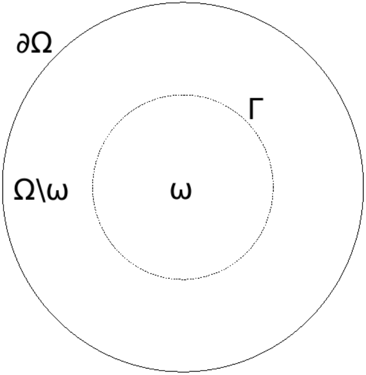
Electrical Impedance Tomography

Neumann problem (N):

$$\begin{cases} -k\Delta u_N + u_N = 0 & \text{in } \Omega \setminus \Gamma \\ [\![u_N]\!] = 0 & \text{on } \Gamma \\ [\![k\nabla u_N \cdot \mathbf{n}]\!] = 0 & \text{on } \Gamma \\ k_1 \nabla u_N \cdot \mathbf{n} = g & \text{on } \partial\Omega \end{cases}$$

Dirichlet problem (D):

$$\begin{cases} -k\Delta u_D + u_D = 0 & \text{in } \Omega \setminus \Gamma \\ [\![u_D]\!] = 0 & \text{on } \Gamma \\ [\![k\nabla u_D \cdot \mathbf{n}]\!] = 0 & \text{on } \Gamma \\ u_D = U_D & \text{on } \partial\Omega \end{cases}$$



$$k = k_0\chi_\omega + k_1(1-\chi_\omega)$$

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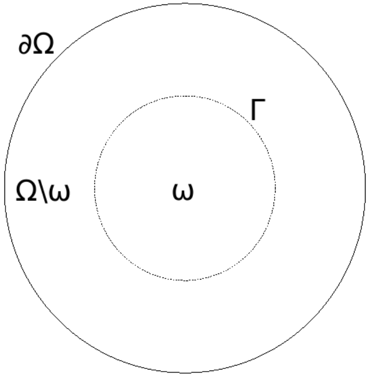


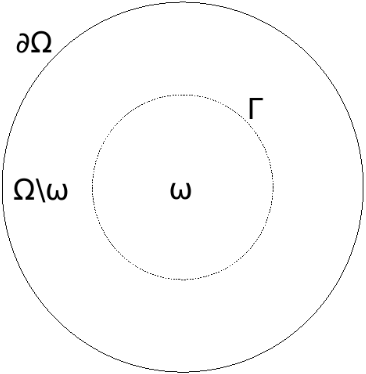
$$k = k_0\chi_\omega + k_1(1-\chi_\omega)$$

Objective functional:

$$J(\omega) = \frac{1}{2}\int_\Omega k\boldsymbol{\nabla}(u_N(\omega) - u_D(\omega)) \cdot \boldsymbol{\nabla}(u_N(\omega) - u_D(\omega))d\mathbf{x} + \frac{1}{2}\int_\Omega (u_N(\omega) - u_D(\omega))^2 d\mathbf{x}$$

Electrical Impedance Tomography

$$a(u, v) = \int_{\Omega} \Big(k \boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v + uv \Big) d\mathbf{x}$$



Neumann problem (N): $u_N \in H^1(\Omega)$

$$a(u_N, v) = F_N(v) \quad \forall v \in W_N = H^1(\Omega)$$

$$F_N(v) = \int_{\partial\Omega} gv \; d\sigma$$

Dirichlet problem (D): $u_D \in H^1_{U_D}(\Omega)$

$$a(u_D, v) = F_D(v) \quad \forall v \in W_D = H^1_0(\Omega)$$

$$F_D(v) = 0$$

$$k = k_0 \chi_\omega + k_1 (1 - \chi_\omega)$$

Objective functional:

$$\boxed{J(\omega) = \frac{1}{2} a \left(u_N(\omega) - u_D(\omega), u_N(\omega) - u_D(\omega) \right)}$$

Shape optimization approach

PDE-constrained optimization problem: $\omega^* = \text{argmin}_\omega J(\omega)$

$\Longrightarrow$ **Optimization variable:** Shape and location of the inclusion ω

Shape optimization startegy:

```
Given the domain Ω^(0), set ℓ = 0 and iterate:
1. Compute the solutions u_N^(ℓ) and u_D^(ℓ);
2. Compute a descent direction θ^(ℓ) and an admissible step μ^(ℓ);
3. Move the interface Γ^(ℓ+1) = (I + μ^(ℓ) θ^(ℓ)) Γ^(ℓ);
4. While stopping criterion not fulfilled, ℓ = ℓ + 1 and repeat.
```

Shape optimization approach

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Given the domain $\Omega^{(0)}$, set $\ell = 0$ and iterate:

1. Compute the solutions $u_N^{(\ell)}$ and $u_D^{(\ell)}$;
2. Compute a descent direction $\boldsymbol{\theta}^{(\ell)}$ and an admissible step $\mu^{(\ell)}$;
3. Move the interface $\Gamma^{(\ell+1)} = (\mathbf{I} + \mu^{(\ell)}\boldsymbol{\theta}^{(\ell)})\Gamma^{(\ell)}$;
4. While stopping criterion not fulfilled, $\ell = \ell + 1$ and repeat.

Classical optimization

$$\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x}) \quad , \quad f : \mathbb{R}^n \to \mathbb{R}$$

Steepest descent direction at point $\mathbf{x}$: $\boxed{\mathbf{v}(\mathbf{x}) = -\nabla f(\mathbf{x})}$

$$\mathbf{x}^{(\ell+1)} = \mathbf{x}^{(\ell)} + \mu^{(\ell)}\, \mathbf{v}(\mathbf{x}^{(\ell)})$$

Shape optimization

$$\min_{\omega\in\mathcal{U}_{ad}} J(\omega) \quad , \quad J : \mathcal{U}_{ad} \to \mathbb{R}$$

$$\mathcal{U}_{ad} = \{\text{Open sets in } \Omega \subset \mathbb{R}^d\}$$

Gradient-based descent direction at ω: $\boxed{\boldsymbol{\theta} \text{ s.t. } \langle dJ(\omega), \boldsymbol{\theta}\rangle < 0}$

$$\omega^{(\ell+1)} = (\mathbf{I} + \mu^{(\ell)}\boldsymbol{\theta}^{(\ell)})\omega^{(\ell)}$$

Shape derivative

Let $\boldsymbol{\theta} \in W^{1,\infty}(\Omega, \mathbb{R}^2)$ be an admissible smooth deformation of Ω s.t. the external boundary is fixed: $\boldsymbol{\theta} = \mathbf{0}$ on $\partial\Omega$

$\Longrightarrow$ **Small perturbation of the domain:** $\Omega(\boldsymbol{\theta}) = (\mathbf{I} + t\boldsymbol{\theta})\Omega$

If the map $\mathcal{J}_\Omega : \boldsymbol{\theta} \mapsto J(\Omega(\boldsymbol{\theta}))$ is differentiable at $\boldsymbol{\theta} = \mathbf{0}$, we define the shape derivative:

$$\langle dJ(\omega), \boldsymbol{\theta} \rangle = \langle \mathcal{J}'_\Omega(0), \boldsymbol{\theta} \rangle = \lim_{t \searrow 0} \frac{J((\mathbf{I} + t\boldsymbol{\theta})\Omega) - J(\Omega)}{t}$$

Shape derivative of the objective functional $J(\omega)$[1]:

$$\begin{aligned} \langle dJ(\omega), \boldsymbol{\theta} \rangle =& \frac{1}{2} \int_\Omega k\mathbf{M}(\boldsymbol{\theta}) \boldsymbol{\nabla}(u_N(\omega) + u_D(\omega)) \cdot \boldsymbol{\nabla}(u_N(\omega) - u_D(\omega)) d\mathbf{x} \\ &- \frac{1}{2} \int_\Omega \boldsymbol{\nabla} \cdot \boldsymbol{\theta} \ (u_N(\omega) + u_D(\omega))(u_N(\omega) - u_D(\omega)) d\mathbf{x} \end{aligned}$$

$$\mathbf{M}(\boldsymbol{\theta}) = \boldsymbol{\nabla}\boldsymbol{\theta} + \boldsymbol{\nabla}\boldsymbol{\theta}^T - (\boldsymbol{\nabla} \cdot \boldsymbol{\theta})\mathbf{I}$$

[1] O. Pantz. *Sensibilité de l'équation de la chaleur aux sauts de conductivité*. C. R. Acad. Sci. Paris, Ser. I(341):333-337 (2005)

The boundary variation algorithm

Gradient-based strategy:

$$\langle \boldsymbol{\theta}, \boldsymbol{\delta\theta} \rangle_{[H^1(\Omega)]^d} + \langle dJ(\omega), \boldsymbol{\delta\theta} \rangle = 0 \quad \forall \boldsymbol{\delta\theta} \in [H^1(\Omega)]^d$$

$\Longrightarrow$ **Descent direction:** $\boldsymbol{\theta}$ such that $\langle dJ(\omega), \boldsymbol{\theta} \rangle < 0$

There are two possible approaches to numerical shape optimization:

- Discretize-then-Optimize
- Optimize-then-Discretize

The boundary variation algorithm

Gradient-based strategy:

$$\langle \boldsymbol{\theta}, \boldsymbol{\delta\theta} \rangle_{[H^1(\Omega)]^d} + \langle dJ(\omega), \boldsymbol{\delta\theta} \rangle = 0 \quad \forall \boldsymbol{\delta\theta} \in [H^1(\Omega)]^d$$

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There are two possible approaches to numerical shape optimization:

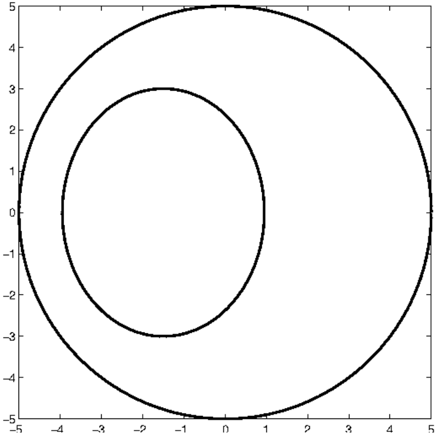
- Discretize-then-Optimize
- Optimize-then-Discretize $\Longrightarrow$ Discretized gradient-based strategy:

$$\langle \boldsymbol{\theta}^h, \boldsymbol{\delta\theta}^h \rangle_{[X_h^p]^d} + \langle d_h J, \boldsymbol{\delta\theta}^h \rangle \simeq 0 \quad \forall \boldsymbol{\delta\theta}^h \in [X_h^p]^d$$

$\Longrightarrow$ **Certified descent direction:** $\boldsymbol{\theta}^h$ such that $\langle d_h J, \boldsymbol{\theta}^h \rangle + |E^h| < 0$

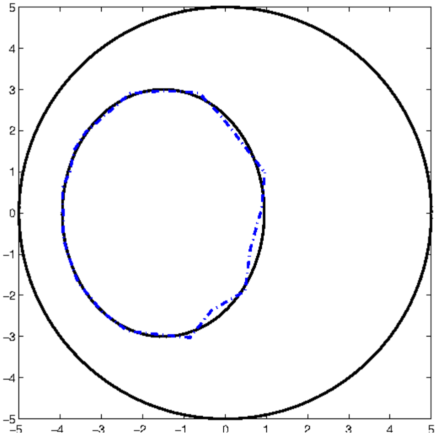
Numerical error in the shape derivative: $\boxed{E^h = \langle dJ(\omega^h), \boldsymbol{\theta}^h \rangle - \langle d_h J, \boldsymbol{\theta}^h \rangle}$

Why coupling error estimates with shape optmization?

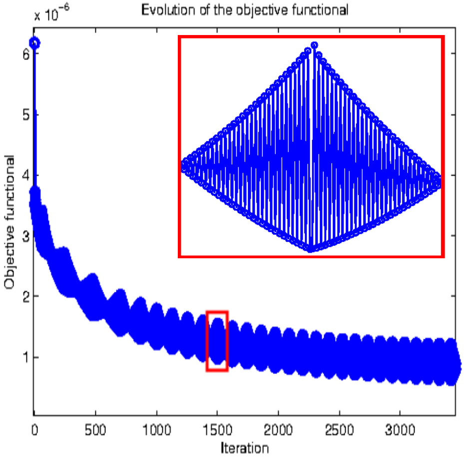


Initial interface

Why coupling error estimates with shape optmization?



Reconstructed interface



Objective functional

The adaptive boundary variation algorithm

Given the domain $\Omega^{(0)}$ and tol $= 10^{-8}$, set the $\ell = 0$ and iterate:

1. Construct a coarse mesh $\mathcal{T}_h^{(\ell)} \subset \Omega^{(\ell)}$;
2. Compute the primal solutions $u_N^{h^{(\ell)}}$ and $u_D^{h^{(\ell)}}$;
3. Compute a descent direction $\boldsymbol{\theta}^{h^{(\ell)}}$;
4. Compute the upper bound $\overline{E}$ of the numerical error $|E^h|$;
5. While $\langle d_h J, \boldsymbol{\theta}^{h^{(\ell)}} \rangle + \overline{E} > 0$, repeat:
    (a) Adapt the computational mesh $\mathcal{T}_h^{(\ell)}$;
    (b) Re-compute the primal solutions $u_N^{h^{(\ell)}}$ and $u_D^{h^{(\ell)}}$;
    (c) Re-compute a descent direction $\boldsymbol{\theta}^{h^{(\ell)}}$;
    (d) Re-compute the upper bound $\overline{E}$ of $|E^h|$ and $\langle d_h J, \boldsymbol{\theta}^{h^{(\ell)}} \rangle + \overline{E}$;
6. Compute an admissible step size $\mu^{h^{(\ell)}}$;
7. Move the mesh $\mathcal{T}_h^{(\ell+1)} = (\mathbf{I} + \mu^{h^{(\ell)}} \boldsymbol{\theta}^{h^{(\ell)}}) \mathcal{T}_h^{(\ell)}$;
8. While $|\langle d_h J, \boldsymbol{\theta}^{h^{(\ell)}} \rangle| + \overline{E} >$ tol, $\ell = \ell + 1$ and repeat.

The adaptive boundary variation algorithm

Given the domain $\Omega^{(0)}$ and $\texttt{tol} = 10^{-8}$, set the $\ell = 0$ and iterate:

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Error in the Quantity of Interest

Error operator:

$$\mathcal{G}_{\boldsymbol{\theta}^h}(u,v) = \frac{1}{2}\int_{\Omega}\Big(k\mathbf{M}(\boldsymbol{\theta}^h)\boldsymbol{\nabla}(u+v)\cdot\boldsymbol{\nabla}(u-v) - \boldsymbol{\nabla}\cdot\boldsymbol{\theta}^h(u+v)(u-v)\Big)d\mathbf{x}$$

$\Longrightarrow$ **Numerical error:** $\left|E^h\right| = \left|\mathcal{G}_{\boldsymbol{\theta}^h}(u_N, u_N^h) - \mathcal{G}_{\boldsymbol{\theta}^h}(u_D, u_D^h)\right|$

Error in the Quantity of Interest

Error operator:

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$$\widetilde{\mathcal{G}}_{\boldsymbol{\theta}^h}(u) = \frac{1}{2}\int_\Omega \Big(k\mathbf{M}(\boldsymbol{\theta}^h)\boldsymbol{\nabla}u\cdot\boldsymbol{\nabla}u - \boldsymbol{\nabla}\cdot\boldsymbol{\theta}^h u^2\Big) d\mathbf{x}$$

$\Longrightarrow$ **Numerical error:**
$$\begin{aligned} \left|E^h\right| &= \left|\mathcal{G}_{\boldsymbol{\theta}^h}(u_N,u_N^h) - \mathcal{G}_{\boldsymbol{\theta}^h}(u_D,u_D^h)\right| \\ &\le \left|\widetilde{\mathcal{G}}_{\boldsymbol{\theta}^h}(u_N) - \widetilde{\mathcal{G}}_{\boldsymbol{\theta}^h}(u_N^h)\right| + \left|\widetilde{\mathcal{G}}_{\boldsymbol{\theta}^h}(u_D) - \widetilde{\mathcal{G}}_{\boldsymbol{\theta}^h}(u_D^h)\right| \end{aligned}$$

Error in the Quantity of Interest

Error operator:

$$\mathcal{G}_{\boldsymbol{\theta}^h}(u,v) = \frac{1}{2}\int_\Omega \Big(k\mathbf{M}(\boldsymbol{\theta}^h)\nabla(u+v)\cdot\nabla(u-v) - \nabla\cdot\boldsymbol{\theta}^h(u+v)(u-v)\Big)d\mathbf{x}$$

$$\widetilde{\mathcal{G}}_{\boldsymbol{\theta}^h}(u) = \frac{1}{2}\int_\Omega \Big(k\mathbf{M}(\boldsymbol{\theta}^h)\nabla u\cdot\nabla u - \nabla\cdot\boldsymbol{\theta}^h u^2\Big)d\mathbf{x}$$

$\Longrightarrow$ **Numerical error:**

$$\begin{aligned} \left|E^h\right| &= \left|\mathcal{G}_{\boldsymbol{\theta}^h}(u_N,u_N^h) - \mathcal{G}_{\boldsymbol{\theta}^h}(u_D,u_D^h)\right| \\ &\leq \Big|\underbrace{\widetilde{\mathcal{G}}_{\boldsymbol{\theta}^h}(u_N) - \widetilde{\mathcal{G}}_{\boldsymbol{\theta}^h}(u_N^h)}_{E_N^h}\Big| + \Big|\underbrace{\widetilde{\mathcal{G}}_{\boldsymbol{\theta}^h}(u_D) - \widetilde{\mathcal{G}}_{\boldsymbol{\theta}^h}(u_D^h)}_{E_D^h}\Big| \end{aligned}$$

Adjoint problems: $a^*(p_i,\varphi) = \mathcal{F}_i(\varphi) \quad \forall\varphi\in W_i \ , \ i=N,D$

$$\mathcal{F}_i(\varphi) = \int_\Omega \Big(k\mathbf{M}(\boldsymbol{\theta}^h)\nabla u_i^h\cdot\nabla\varphi - \nabla\cdot\boldsymbol{\theta}^h u_i^h\varphi\Big)d\mathbf{x}$$

Goal-oriented residual-type error estimator

Variational formulation of the error via the adjoint problems ($i = N, D$):

$$E_i^h = \widetilde{\mathcal{G}}_{\boldsymbol{\theta}^h}(u_i) - \widetilde{\mathcal{G}}_{\boldsymbol{\theta}^h}(u_i^h) \simeq \mathcal{F}_i(e_i) = a^*(p_i, e_i) = a^*(p_i - p_i^h, e_i) = a(e_i, \epsilon_i)$$

Residual equations ($i = N, D$):

$$a(e_i, v) = \mathcal{R}_i(v) \quad \forall v \in W_i \quad , \quad \mathcal{R}_i(v) = F_i(v) - a(u_i^h, v)$$

$$a^*(\epsilon_i, \varphi) = \mathcal{R}_i^*(\varphi) \quad \forall \varphi \in W_i \quad , \quad \mathcal{R}_i^*(\varphi) = \mathcal{F}_i(\varphi) - a^*(p_i^h, \varphi)$$

$\Longrightarrow$ **Residual error estimator in the QoI [2]:**

$$\left| E_i^h \right| \leq \sum_{T \in \mathcal{T}_h} \eta_i \Big|_T \xi_i \Big|_T$$

η_i primal residue

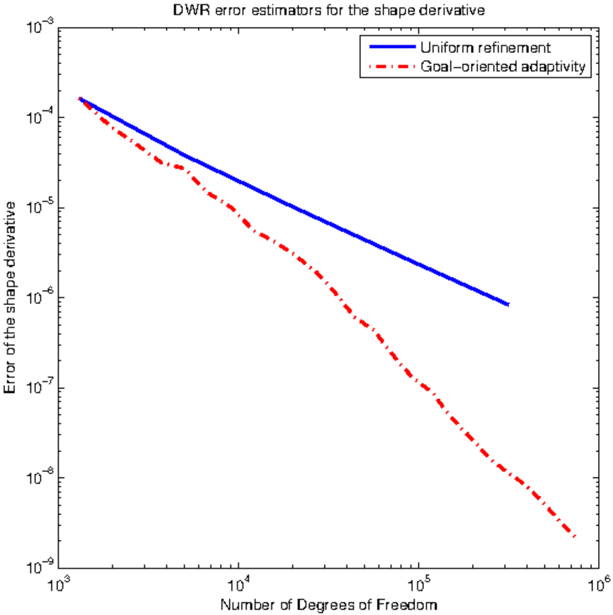
ξ_i adjoint residue

Global residual-type error estimator for the shape derivative:

$$\boxed{\zeta := \sum_{T \in \mathcal{T}_h} \left(\eta_N \Big|_T \xi_N \Big|_T + \eta_D \Big|_T \xi_D \Big|_T \right)}$$

[2] R. Becker, R. Rannacher. *An optimal control approach to a posteriori error estimation in Finite Element Methods*. Acta Numerica, 10:1-102 (2001)

Validation of the goal-oriented mesh adaptivity strategy



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Adaptive shape optimization procedure [3]

Given the domain $\Omega^{(0)}$ and $\mathrm{tol} = 10^{-8}$, set the $\ell = 0$ and iterate:

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2. Compute the primal solutions $u_N^{h^{(\ell)}}$ and $u_D^{h^{(\ell)}}$;
3. Compute a descent direction $\boldsymbol{\theta}^{h^{(\ell)}}$;
4. Compute the adjoint solutions $p_N^{h^{(\ell)}}$ and $p_D^{h^{(\ell)}}$;
5. Compute the error estimator $\zeta^{(\ell)}$;
6. While $\langle d_h J, \boldsymbol{\theta}^{h^{(\ell)}} \rangle + \zeta^{(\ell)} > 0$, repeat:
   (a) Adapt the computational mesh $\mathcal{T}_h^{(\ell)}$ w.r.t. $\zeta^{(\ell)}$;
   (b) Re-compute the primal solutions $u_N^{h^{(\ell)}}$ and $u_D^{h^{(\ell)}}$;
   (c) Re-compute a descent direction $\boldsymbol{\theta}^{h^{(\ell)}}$;
   (d) Re-compute the adjoint solutions $p_N^{h^{(\ell)}}$ and $p_D^{h^{(\ell)}}$;
   (e) Re-compute the error estimator $\zeta^{(\ell)}$ and $\langle d_h J, \boldsymbol{\theta}^{h^{(\ell)}} \rangle + \zeta^{(\ell)}$;
7. Compute an admissible step size $\mu^{h^{(\ell)}}$;
8. Move the mesh $\mathcal{T}_h^{(\ell+1)} = (\mathbf{I} + \mu^{h^{(\ell)}} \boldsymbol{\theta}^{h^{(\ell)}}) \mathcal{T}_h^{(\ell)}$;
9. While $|\langle d_h J, \boldsymbol{\theta}^{h^{(\ell)}} \rangle| + \zeta^{(\ell)} > \mathrm{tol}$, $\ell = \ell + 1$ and repeat.

[3] M. Giacomini, O. Pantz, K. Trabelsi. *An adaptive shape optimization strategy driven by fully-computable goal-oriented error estimators.* (In preparation)

A first test case

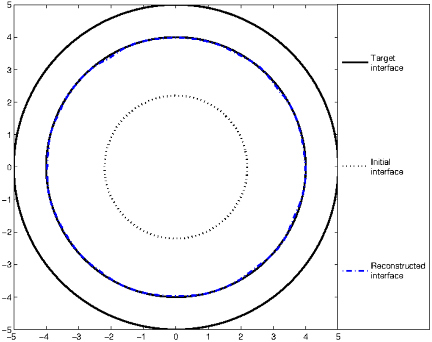
Evolution of the interface

Objective functional

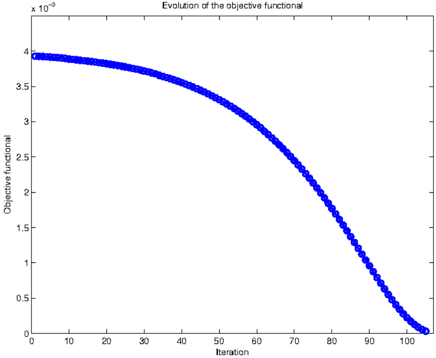
All the simulations were performed using `FreeFem++`.

F. Hecht. *New development in FreeFem++*. J. Numer. Math., 20(3-4):251-265 (2012)

A first test case



Reconstructed interface



Objective functional

Improved adaptive shape optimization procedure [4]

Given the domain $\Omega^{(0)}$ and tol $= 10^{-8}$, set the $\ell = 0$ and iterate:

1. Construct a coarse mesh $\mathcal{T}_h^{(\ell)} \subset \Omega^{(\ell)}$ and a fine mesh $\mathcal{S}_h^{(\ell)} \subset \Omega^{(\ell)}$;
2. Compute the primal solutions $u_N^{h^{(\ell)}}$ and $u_D^{h^{(\ell)}}$ on $\mathcal{S}_h^{(\ell)}$;
3. Compute a descent direction $\boldsymbol{\theta}^{h^{(\ell)}}$ on $\mathcal{S}_h^{(\ell)}$;
4. Compute the adjoint solutions $p_N^{h^{(\ell)}}$ and $p_D^{h^{(\ell)}}$ on $\mathcal{S}_h^{(\ell)}$;
5. Compute the error estimator $\zeta^{(\ell)}$;
6. While $\langle d_h J, \boldsymbol{\theta}^{h^{(\ell)}} \rangle + \zeta^{(\ell)} > 0$, repeat:
   (a) Adapt the computational mesh $\mathcal{S}_h^{(\ell)}$ w.r.t. $\zeta^{(\ell)}$;
   (b) Re-compute the primal solutions $u_N^{h^{(\ell)}}$ and $u_D^{h^{(\ell)}}$ on $\mathcal{S}_h^{(\ell)}$;
   (c) Re-compute a descent direction $\boldsymbol{\theta}^{h^{(\ell)}}$ on $\mathcal{S}_h^{(\ell)}$;
   (d) Re-compute the adjoint solutions $p_N^{h^{(\ell)}}$ and $p_D^{h^{(\ell)}}$ on $\mathcal{S}_h^{(\ell)}$;
   (e) Re-compute the error estimator $\zeta^{(\ell)}$ and $\langle d_h J, \boldsymbol{\theta}^{h^{(\ell)}} \rangle + \zeta^{(\ell)}$;
7. Compute an admissible step size $\mu^{h^{(\ell)}}$;
8. Move the coarse mesh $\mathcal{T}_h^{(\ell+1)} = (\mathbf{I} + \mu^{h^{(\ell)}} \boldsymbol{\theta}^{(\ell)}) \mathcal{T}_h^{(\ell)}$;
9. While $|\langle d_h J, \boldsymbol{\theta}^{h^{(\ell)}} \rangle| + \zeta^{(\ell)} >$ tol, $\ell = \ell + 1$ and repeat.

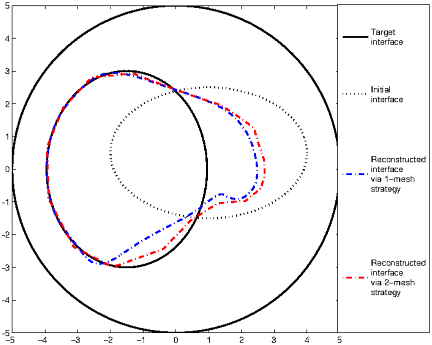
[4] G. Allaire, O. Pantz. *Structural optimization with FreeFem++*. Struct. Multidiscip. Optim. 32:3 (2006)

1-mesh VS 2-mesh optimization strategy

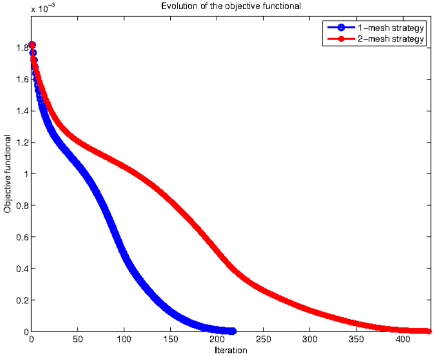
1-mesh strategy

2-mesh strategy

1-mesh VS 2-mesh optimization strategy



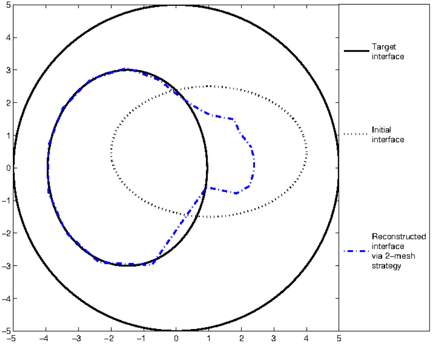
Reconstructed interfaces



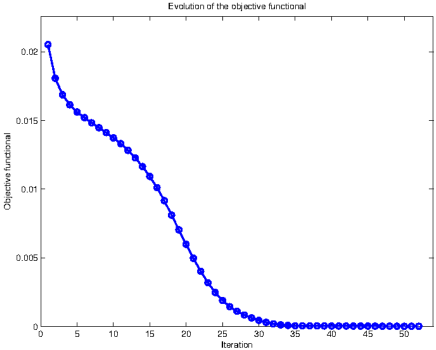
Objective functionals

The case of multiple measures

10 measures using 2-mesh strategy:



Reconstructed interface



Objective functional

Conclusions

- Guaranteed shape optimization strategy using certified goal-oriented estimates for the error in the shape derivative.
- Sharp bounds are obtained using DWR estimator.
- A reliable stopping criterion is derived.
- A 2-mesh strategy improves the convergence of the algorithm.

Special thanks to `FreeFem++` for:

- Powerful management of geometries and meshes.
- Adaptivity strategies using user-defined metrics.

Ongoing and future investigations:

- Application to compliance minimization in structural optimization.
- Goal-oriented anisotropic error estimators.