Shape Optimization and a posteriori error estimates

Application to an Inverse Problem

O. Pantz, a join work with Matteo Giacomini and Karim Trabelsi

www.cmap.polytechnique.fr/~pantz

Shape Optimization

General Setting

The aim is to solve

$$\min_{\Omega \in \mathcal{U}} J(\Omega)$$

$\mathcal{U} =$ set of admissible shapes ; $J =$ cost function.

Basic Examples

Minimal Surface

$$J(S) = \mathcal{H}^{N-1}(S); \qquad \mathcal{U} = \{S \subset \mathbb{R}^N \ : \ K \subset \partial S\},$$

where $\mathcal{H}^{N-1}$ is the $N-1$ dimensional Hausdorff measure.

Willmore functional

$$J(S) = \int_S |H|^2 \, ds; \qquad \mathcal{U} = \{S \subset \mathbb{R}^N \ : \ \mathcal{H}^{N-1}(S) = A\},$$

where H is the mean curvature, $A \in \mathbb{R}^+$ given.

Gradient Method in Shape optimization

Shape Derivative

The cost function J is said to be X-differentiable at $\Omega \in \mathcal{U}$ if there exists a continuous linear form $dJ(\Omega)$ on X, such that $\forall \theta \in X$, we have

$$J((\mathrm{Id} + \theta)(\Omega)) = J(\Omega) + \langle dJ(\Omega), \theta \rangle + o(\theta),$$

Gradient Method

Given an initial guess $\Omega_0 \in \mathcal{U}$, set $n = 0$ and iterate :

1. Compute a descent direction $\theta_n \in X$, such that $\forall \delta\theta \in X$,

$$(\theta_n, \delta\theta)_X + \langle dJ(\Omega_n), \delta\theta \rangle = 0.$$

2. Update the shape $\Omega_{n+1} = (\mathrm{Id} + \mu_n \theta_n)(\Omega_n)$, where $\mu_n > 0$ is a *small* time step.
3. Repeat till $\|\theta_n\|_X < \varepsilon$.

Cost functions depending on a state equation

Let V be a Banach space and j be a map from $\mathcal{U} \times V$ into $\mathbb{R}$. We consider the case where J can be written as

$$J(\Omega) = j(\Omega, u(\Omega)),$$

where $u(\Omega) \in V$ is the solution of a variational formulation

$$a_\Omega(u(\Omega), v) = L_\Omega(v), \qquad \forall v \in V,$$

with a_Ω and L_Ω are respectively bilinear and linear forms on V depending on Ω.

Examples

Compliance of an elastic structure

$$J(\Omega) = \int_\Omega f \cdot u(\Omega)\, dx,$$

with $u(\Omega) \in V := \{v \in H^1(\Omega)^N \ : \ v = 0 \text{ on } \Gamma_D\}$

$$\int_\Omega \lambda e(u(\Omega)) : e(v) + \lambda \mathrm{div}(u(\Omega))\mathrm{div}(v) = \int_\Omega f \cdot v\, dx$$

Electrical Impedance Tomography (Kohn-Vogelius functional)

$$J(\Omega) = \frac{1}{2}\int_D k_\Omega |\nabla(u^N(\Omega) - u^D(\Omega))|^2 + |u^N(\Omega) - u^D(\Omega)|^2\, dx,$$

with $u^D(\Omega)$, $u^D = u_0$ on ∂D and $u^N(\Omega) \in H^1(D)$ such that $\forall v^N \in H^1(D)$ and $v^D \in H^1_0(D)$, we have for $i = N, D$,

$$\int_D k_\Omega \nabla u^i(\Omega) \cdot \nabla v^i + u^i(\Omega) v^i\, dx = \begin{cases} \int_{\partial D} g v^N\, dx & \text{if } i = N \\ 0 & \text{if } i = D, \end{cases}$$

where $k_\Omega = k_0 \chi_\Omega + k_1(1 - \chi_\Omega)$.

Computation of the shape gradient I

Fast derivation method of Céa

We introduce the Lagrangian

$$\mathcal{L}(\Omega, u, p) = j(\Omega, u) + a_\Omega(u, p) - L_\Omega(p),$$

and let $p(\Omega) \in V$ such that for all $q \in V$,

$$a_\Omega(q, p(\Omega)) + \left\langle \frac{\partial j}{\partial u}(\Omega, u(\Omega)), q \right\rangle = 0,$$

we have

$$\langle dJ(\Omega), \theta \rangle = \left\langle \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega, u(\Omega), p(\Omega)), \theta \right\rangle.$$

Computation of the shape gradient II

Material Derivative

Let φ be a differomorphism of $\mathbb{R}^N$ and u and $p \in V$. We set

$$\Omega_\varphi = \varphi(\Omega), \quad u_\varphi = u \circ \varphi^{-1} \text{ and } p_\varphi = p \circ \varphi^{-1}.$$

We say that $\mathcal{L}$ admits a material derivative at (Ω, u, p) if there exists a linear form $\partial \mathcal{L} / \partial \varphi$ such that

$$\mathcal{L}(\Omega_\varphi, u_\varphi, p_\varphi) = \mathcal{L}(\Omega, u, p) + \left\langle \frac{\partial \mathcal{L}}{\partial \varphi}(\Omega, u, p), \theta \right\rangle + o(\theta),$$

where $\varphi = \mathrm{Id} + \theta$. In this case, we have also

$$\langle dJ(\Omega), \theta \rangle = \left\langle \frac{\partial \mathcal{L}}{\partial \varphi}(\Omega, u(\Omega), p(\Omega)), \theta \right\rangle.$$

Kohn-Vogelius functional

Surface expression

The K-V functional is self-adjoint. We get $p^D = 0$ and $p^N = u^N - u^D$.

$$\langle dJ(\Omega), \theta \rangle = \frac{1}{2} \int_{\partial\Omega} \left([k] \left(\left| \frac{\partial u^N}{\partial \tau} \right|^2 - \left| \frac{\partial u^D}{\partial \tau} \right|^2 \right) \right.$$
$$\left. - [k^{-1}] \left(\left| k \frac{\partial u^N}{\partial n} \right|^2 - \left| k \frac{\partial u^D}{\partial n} \right|^2 \right) \right) (\theta \cdot n) \, ds$$

where n is the outward normal to Ω, $[k] = k_1 - k_0$, $[k^{-1}] = k_1^{-1} - k_0^{-1}$.

Kohn-Vogelius functional

Volume expression

$$\langle dJ(\Omega), \theta \rangle = \langle G(\Omega, u^N) - G(\Omega, u^D), \theta \rangle,$$

$$\langle G(\Omega, u), \theta \rangle = \frac{1}{2} \int_D kM(\theta) |\nabla u|^2 - (\nabla \cdot \theta) u^2 \, dx,$$

and

$$M(\theta) = \nabla\theta + \nabla\theta^T - (\nabla \cdot \theta)\mathrm{Id}.$$

No regularity on the solutions u^N and u^D needed.

Discretization

Two possible Strategies

Discretize-then-Optimize Apply the gradient method to an approximation J_h of the cost function

Pro Stopping criterion reached.

Cons Can't be applied to Level-Set formulation ; Interaction between optimization and discretization.

Optimize-then-Discretize Apply the gradient method using an approximation $d_h J$ of the shape gradient

Pro Can be applied to Level-Set formulation.

Cons Stopping criterion difficult to define.

? Choice of the discretization of $dJ(\Omega)$.

Discretized Gradient Method

Given an initial guess $\Omega_0 \in \mathcal{U}$, set $n = 0$ and iterate

1. Compute u_n^h and $p_n^h \in V_h$
2. Compute a guessed descent direction $\theta_n^h \in X$ solution of

$$(\theta_n^h, \delta\theta)_X + \langle d_h J(\Omega_n), \delta\theta \rangle = 0, \qquad \forall \delta\theta \in X,$$

   where

$$\langle d_h J(\Omega_n), \delta\theta \rangle = \left\langle \frac{\partial \mathcal{L}}{\partial \varphi}(\Omega_n, u_n^h, p_n^h), \delta\theta \right\rangle.$$

3. Update the shape

$$\Omega_{n+1} = (\mathrm{Id} + \mu_n \theta_n^h)(\Omega_n),$$

   where $\mu_n > 0$ is a *small* time step.

4. Repeat till $\|\theta_n\|_X < \varepsilon$. NOT REACHED!!!

Improve Discretized Gradient Method

Main Idea

- Use a posteriori error estimates on the computations of the state u and the adjoint state p to evaluate the error made on the computation of the gradient.
- Refine the discretization if no gradient descent could be found.

Advantages

- Stopping criterion is reached.
- Save time ? Only coarse discretizations are needed at the beginning of the optimization. Finer ones are only required when the gradient of the cost function is small.

Drawback

Constant-free a posteriori errors should be computed. [it takes time.]

Improved Discretized Gradient Method

Given an initial guess $\Omega_0 \in \mathcal{U}$, set $n = 0$ and iterate

1. Compute u_n^h and $p_n^h \in V_h$
2. Compute a guessed descent direction $\theta_n^h \in X$ solution of

$$(\theta_n^h, \delta\theta)_X + \langle d_h J(\Omega_n), \delta\theta \rangle = 0 \forall \delta\theta \in X,$$

3. Compute an upper bound E_n^h of the error on the gradient

$$|\langle (dJ - d_h J(\Omega_n), \theta_n^h \rangle| \leq E_n^h$$

4. If $E_n^h + \langle d_h J(\Omega_n), \theta_n^h \rangle > 0$, refine the discretization size h and go back to step 1.

3. Update the shape $\Omega_{n+1} = (\mathrm{Id} + \mu_n \theta_n^h)(\Omega_n)$.

4. Repeat till $\|\theta_n^h\| + E_n^h < \varepsilon$.

Error Estimation of the shape Gradient

$$
\begin{aligned}
\langle (dJ - d_hJ)(\Omega), \theta \rangle &= \left\langle \frac{\partial \mathcal{L}}{\partial \varphi}(\Omega, u(\Omega), p(\Omega) - \frac{\partial \mathcal{L}}{\partial \varphi}(\Omega, u_h(\Omega), p_h(\Omega), \theta \right\rangle \\
&\approx \frac{\partial^2 \mathcal{L}}{\partial \varphi \partial u}(\Omega, u_h(\Omega), p_h(\Omega))(\theta, (u - u_h)(\Omega)) \\
&\quad + \frac{\partial^2 \mathcal{L}}{\partial \varphi \partial p}(\Omega, u_h(\Omega), p_h(\Omega))(\theta, (p - p_h)(\Omega))
\end{aligned}
$$

Let r and $s \in V$ be the adjoint states such that $\forall \delta s$ and $\delta r \in V$,

$$
a_\Omega(r(\Omega), \delta r) = \frac{\partial^2 \mathcal{L}}{\partial \varphi \partial u}(\Omega, u_h(\Omega), p_h(\Omega))(\theta, \delta r)
$$

and

$$
a_\Omega(s(\Omega), \delta s) = \frac{\partial^2 \mathcal{L}}{\partial \varphi \partial p}(\Omega, u_h(\Omega), p_h(\Omega))(\theta, \delta s)
$$

We denote r_h and s_h Finite Elements approximations of r and s in V_h.

We get

$$
\begin{aligned}
|\langle (dJ - d_h J)(\Omega), \theta \rangle| &\approx |a_\Omega(r, u - u_h) + a_\Omega(s, p - p_h)| \\
&= |a_\Omega(r - r_h, u - u_h) + a_\Omega(s - s_h, p - p_h)| \\
&\leq \|r - r_h\|_\Omega \|u - u_h\|_\Omega + \|s - s_h\|_\Omega \|p - p_h\|_\Omega,
\end{aligned}
$$

where $\| \cdot \|_\Omega^2 = a_\Omega(\cdot, \cdot)$.

It remains to evaluate the error made in energy norm on u, p, r and s.

We need EXPLICIT bounds.

For instance, the Complementary Energy Principle can be used.

Adjoint states

For the Kohn-Vogelius Functional

The adjoint states $r^D(\Omega) \in H_0^1(D)$ and $r^N(\Omega) \in H^1(D)$ are defined by

$$a_\Omega(r^D(\Omega), s) = \left\langle \left\langle \frac{\partial G}{\partial u}(\Omega, u_h^D), s \right\rangle, \theta \right\rangle \qquad \forall s \in H_0^1(D)$$

and

$$a_\Omega(r^N(\Omega), s) = \left\langle \left\langle \frac{\partial G}{\partial u}(\Omega, u_h^N), s \right\rangle, \theta \right\rangle \qquad \forall s \in H^1(D),$$

with

$$\left\langle \left\langle \frac{\partial G}{\partial u}(\Omega, u), s \right\rangle, \theta \right\rangle = \int_D k_\Omega M(\theta)\nabla u \cdot \nabla s - (\nabla \cdot \theta) u s \, dx.$$

A posteriori Error Estimates

Using Complementary Energy Principle

Let $e_h^D = u_h^D - u^D$ be the error on the computation of the Dirichlet Problem.

$$\|e_h^D\|_\Omega^2 \leq \int_D k_\Omega^{-1}|\sigma - k\nabla u_h^D|^2 + |\nabla\cdot\sigma - u_h^D|^2\,dx \qquad \forall\sigma\in H(\mathrm{div};D).$$

Let $\sigma_h \in W_h \subset H(\mathrm{div};\Omega)$ the flux approximation defined by

$$\int_D k^{-1}\sigma_h^D\cdot\delta\sigma + (\nabla\cdot\sigma_h^D)(\nabla\cdot\delta\sigma)\,dx = \int_{\partial D} u_0(\delta\sigma\cdot n)\,ds, \qquad \forall\delta\sigma\in W_h.$$

We have

$$\|e_h^D\|_\Omega^2 \leq \int_D k_\Omega^{-1}|\sigma_h^D - k\nabla u_h^D|^2 + |\nabla\cdot\sigma_h^D - u_h^D|^2\,dx.$$

[Note : Similar result for e_h^N.]

A posteriori Error Estimates

For the adjoint states

Let $\epsilon_h^D = r_h^D - r^D$ be the error on the computation of the Dirichlet Adjoint Problem. $\forall \tau \in H(\text{div}; D)$,

$$\|\epsilon_h^D\|_\Omega^2 \leq \int_D k_\Omega^{-1} |\tau - k\nabla r_h^D + kM(\theta)\nabla u_h^D|^2 + |\nabla \cdot \tau - r_h^D - (\nabla \cdot \theta) u_h^D|^2 \, dx$$

Let $\tau_h^D \in W_h$ defined by $\forall \delta\tau \in W_h$,

$$\int_D k^{-1} \tau_h^D \cdot \delta\tau + (\nabla \cdot \tau_h^D)(\nabla \cdot \delta\tau) \, dx = \int_D (\nabla \cdot \theta) u_h^D \nabla \cdot \delta\tau - M(\theta)\nabla u_h^D \cdot \delta\tau \, dx.$$

We have

$$\|\epsilon_h^D\|_\Omega^2 \leq \int_D k_\Omega^{-1} |\tau_h^D - k\nabla r_h^D + kM(\theta)\nabla u_h^D|^2 + |\nabla \cdot \tau_h^D - r_h^D - (\nabla \cdot \theta) u_h^D|^2 \, dx$$

[Note : Similar result for ϵ_h^N.]

Final Algorithm

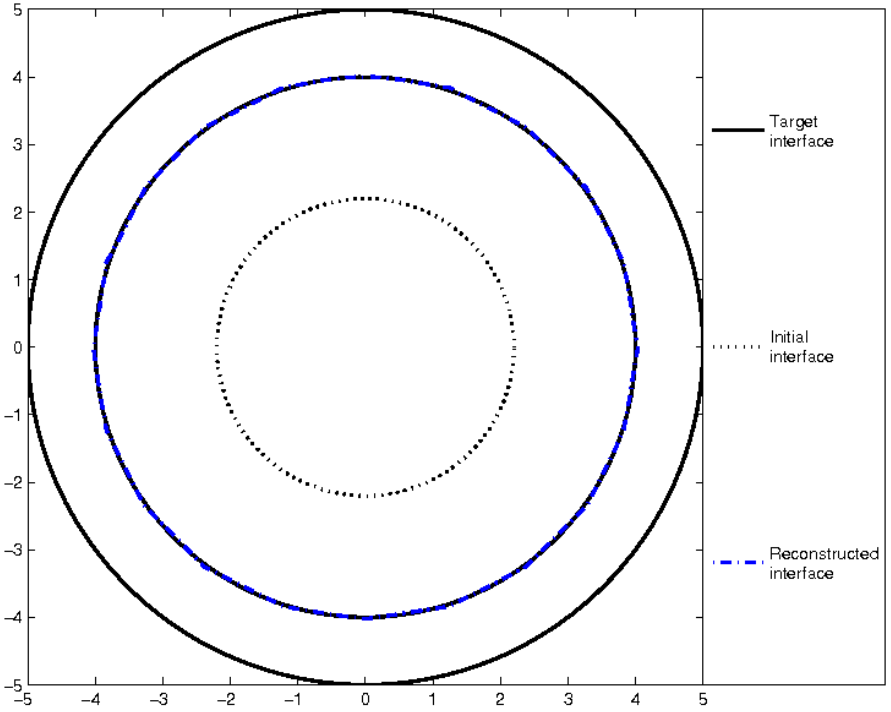
Given an initial guess $\Omega_0 \in \mathcal{U}$, set $n = 0$ and iterate

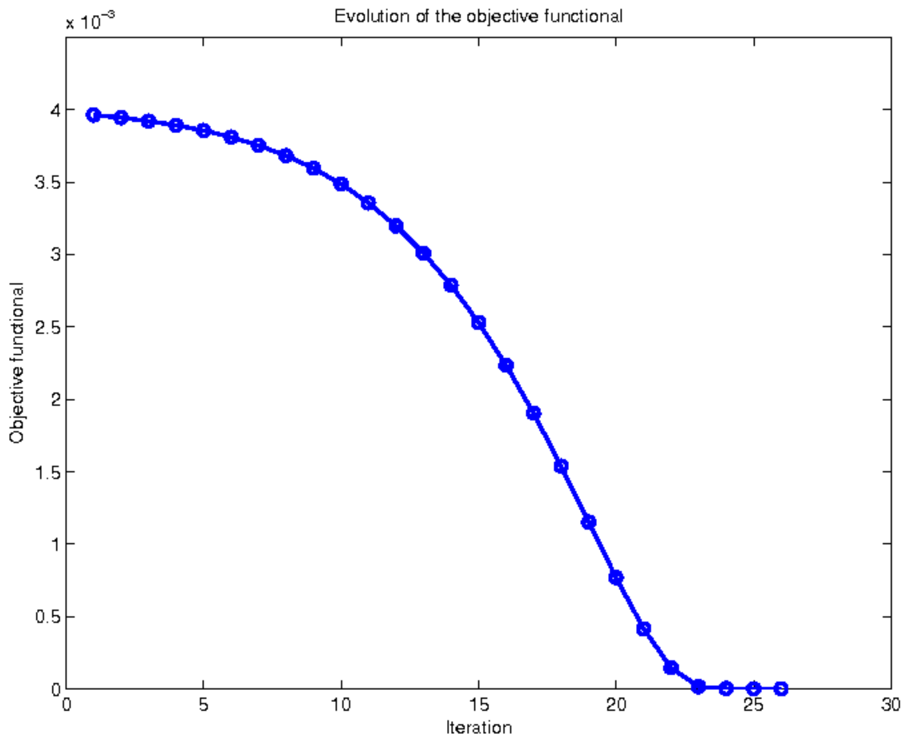
1. Compute u_n^h and $p_n^h \in V_h$
2. Compute a guessed descent direction $\theta_n^h \in X$ solution of
$$(\theta_n^h, \delta\theta)_X + \langle d_h J(\Omega_n), \delta\theta\rangle = 0 \qquad \forall \delta\theta \in X,$$
3. Compute an upper bound E_n^h of the error on the gradient
   (a) Compute the adjoint states r_n^h and s_n^h.
   (b) Compute the approximation of the flux of u_n^h, p_n^h, r_n^h and s_n^h.
4. If $E_n^h + \langle d_h J(\Omega_n), \theta_n^h\rangle > 0$, refine the discretization size h and go back to step 1.

3. Update the shape $\Omega_{n+1} = (\mathrm{Id} + \mu_n \theta_n^h)(\Omega_n)$.
4. Repeat till $\|\theta_n^h\| + E_n^h < \varepsilon$.

Circular inclusion

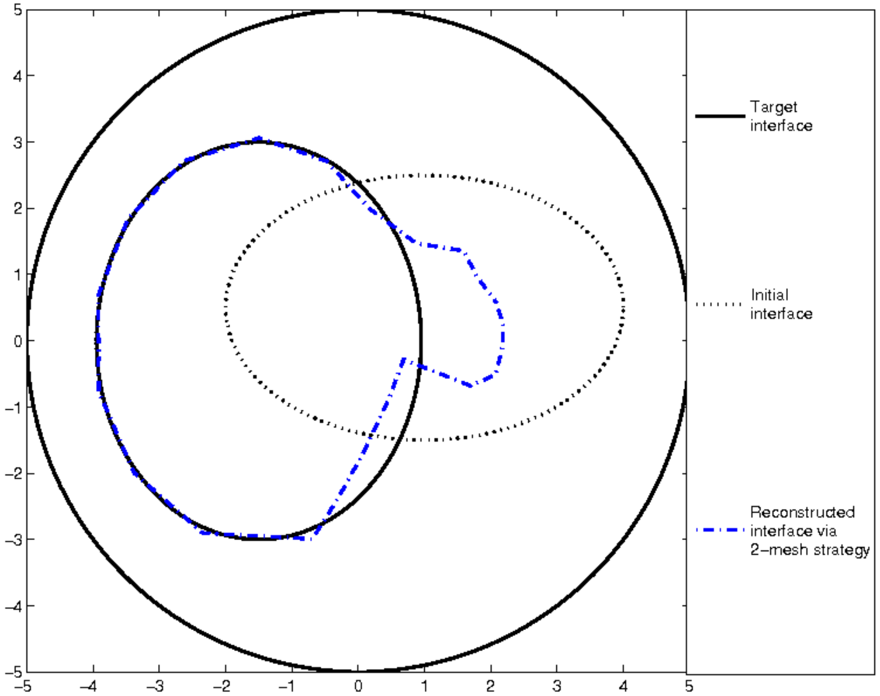
One measure on the boundary

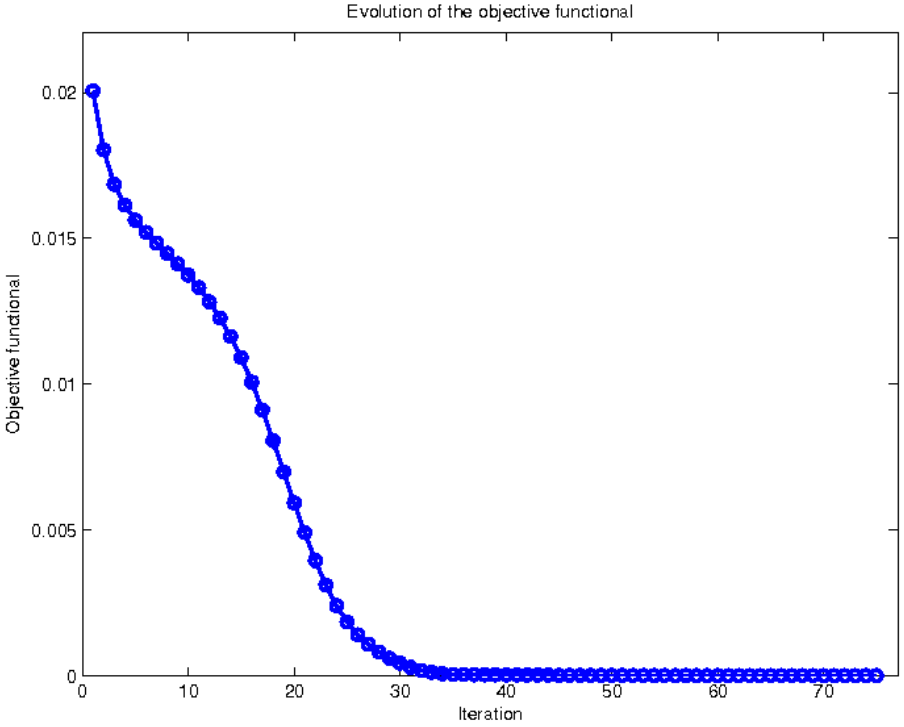




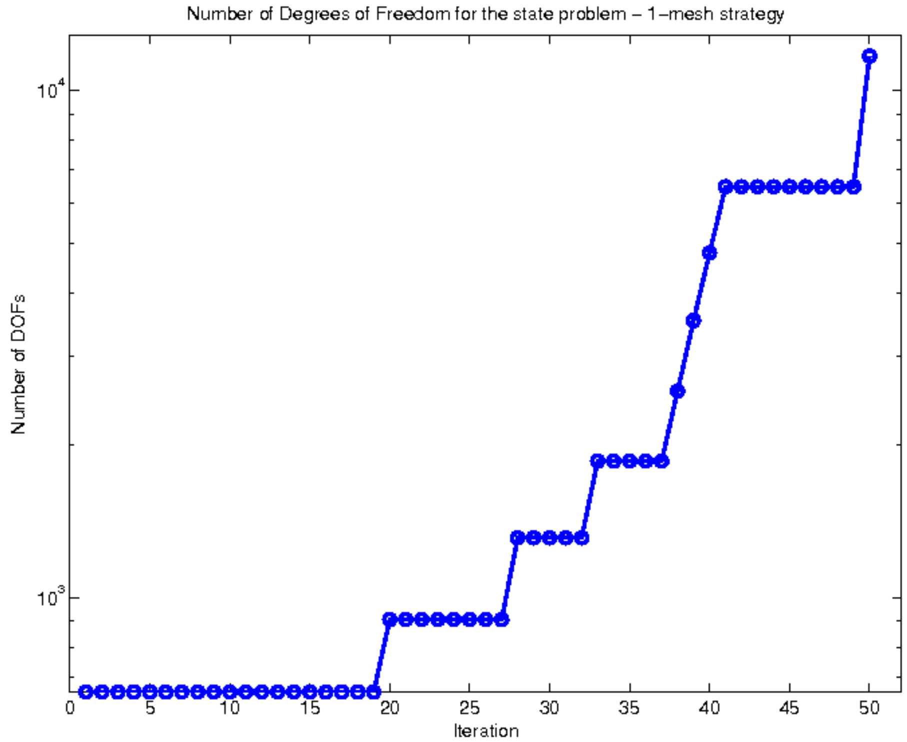
Elliptical inclusion

Ten measures on the boundary





Evolution of the degree of freedom



Conclusion

- Guaranteed shape optimization strategy using certified goal-oriented estimates for the error in the shape derivative.
- Increase the precision of computation of the states only when needed.
- Stopping criterion reached.

Perspectives

- Use less time consuming a posteriori estimators.
- Apply to structural optimization.
- Apply to Level-Set Methods.
- Select the direction of descent, considering the a posteriori error estimates.