PDE constrained optimization

Grégoire Allaire

Department of Applied Mathematics, Ecole Polytechnique

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Numerical algorithms
Parametric optimization

Model problem: thickness optimization

Consider a plate occupying a bounded domain Ω in $\mathbb{R}^N$, with forces $f \in L^2(\Omega)$ and displacement $u \in H^1_0(\Omega)$ solution of the membrane model

$$\left\{ \begin{array}{rcll} -\operatorname{div}(h\nabla u) & = & f & \text{in } \Omega, \\ u & = & 0 & \text{on } \partial\Omega. \end{array} \right.$$

The variable is the thickness h. It is called parametric optimization because the computational domain Ω is fixed. The thickness $h(x)$ is just a parameter.

The admissible set is defined by

$$\mathcal{U}_{ad} = \left\{ h \in L^2(\Omega), 0 < h_{min} \le h(x) \le h_{max} \text{ in } \Omega, \int_\Omega h(x)dx = \bar{h}|\Omega| \right\}.$$

Parametric optimization

Parametric optimization problem:

$$\inf_{h \in \mathcal{U}_{ad}} J(h) = \int_\Omega j(u)\, dx$$

where u depends on h through the state equation, and j is a C^1 function from $\mathbb{R}$ to $\mathbb{R}$ such that $|j(u)| \leq C(u^2+1)$ and $|j'(u)| \leq C(|u|+1)$.

Examples:

- Compliance or work done by the load (a measure of rigidity)

$$j(u) = fu$$

- Least square criterion to reach a target displacement $u_0 \in L^2(\Omega)$

$$j(u) = |u - u_0|^2$$

Derivative of the objective function

$$\inf_{h\in\mathcal{U}_{ad}} J(h) = \int_\Omega j(u)\, dx$$

$$\mathcal{U}_{ad} = \left\{ h \in L^2(\Omega), 0 < h_{min} \leq h(x) \leq h_{max} \text{ in } \Omega, \int_\Omega h(x)dx = \bar{h}|\Omega| \right\}.$$

with u solution of

$$\left\{ \begin{array}{rcll} -\operatorname{div}(h\nabla u) & = & f & \text{in } \Omega, \\ u & = & 0 & \text{on } \partial\Omega. \end{array} \right.$$

Theorem. The objective function is differentiable in $L^2(\Omega)$ and $J'(h) = \nabla u \cdot \nabla p$ with the adjoint p solution of

$$\left\{ \begin{array}{rcll} -\operatorname{div}(h\nabla p) & = & -j'(u) & \text{in } \Omega \\ p & = & 0 & \text{on } \partial\Omega. \end{array} \right.$$

1. For a general objective function we suggest a projected gradient algorithm.
2. For compliance minimization a more efficient optimality criteria algorithm is proposed.

The projected gradient algorithm is illustrated below on the counter-example of non-existence of optimal design.

Projected gradient algorithm

1. Initialization of the thickness $h_0 \in \mathcal{U}_{ad}$ (for example, a constant function which satisfies the constraints).
2. Iterations until convergence, for $n \geq 0$:

$$h_{n+1} = P_{\mathcal{U}_{ad}}\Big(h_n - \mu J'(h_n)\Big),$$

where $\mu > 0$ is a descent step, $P_{\mathcal{U}_{ad}}$ is the projection operator on the closed convex set $\mathcal{U}_{ad}$ and the derivative is given by

$$J'(h_n) = \nabla u_n \cdot \nabla p_n$$

with the state u_n and the adjoint p_n (associated with the thickness h_n).

To make the algorithm fully explicit, we have to specify what is the (orthogonal) projection operator $P_{\mathcal{U}_{ad}}$.

Projection operator

The projection operator $P_{\mathcal{U}_{ad}}$ is defined by

$$\Big(P_{\mathcal{U}_{ad}}(h)\Big)(x) = \max\left(h_{min}, \min\left(h_{max}, h(x) + \ell\right)\right)$$

where ℓ is the unique Lagrange multiplier such that

$$\int_\Omega P_{\mathcal{U}_{ad}}(h)\, dx = h_0|\Omega|.$$

The determination of the constant ℓ is not explicit: we must use an iterative algorithm based on the property of the function

$$\ell \to F(\ell) = \int_\Omega \max\left(h_{min}, \min\left(h_{max}, h(x) + \ell\right)\right)\, dx$$

which is strictly increasing and continuous on an interval $[\ell^-, \ell^+]$ such that $F([\ell^-, \ell^+]) = [h_{min}|\Omega|, h_{max}|\Omega|]$. Thus, a simple iterative algorithm is: first, bracket the root by an interval $[\ell^1, \ell^2]$ such that

$$F(\ell^1) \le h_0|\Omega| \le F(\ell^2),$$

second, proceed by dichotomy to find the root ℓ.

Details

- In practice, we rather use a projected gradient algorithm with a variable step (not optimal) which guarantees the decrease of the functional: $J(h_{n+1}) < J(h_n)$.
- The overhead generated by the adjoint computation is very modest : one has to build a new right-hand-side (using the state) and solve the corresponding linear system (with the same stiffness matrix).
- Convergence is detected when the optimality condition is satisfied with a threshold $\epsilon > 0$

$$\left| h_n - \max\left(h_{min}, \min\left(h_{max}, h_n - \mu_n J'(h_n) + \ell_n\right)\right)\right| \leq \epsilon \mu_n h_{max}.$$

The self-adjoint case: the compliance

When $j(u) = fu$, we find $p = -u$ since $j'(u) = f$. This particular case is said to be **self-adjoint**. It is a rare case where there exists an optimal solution !

For this, we use the dual or complementary energy

$$\int_\Omega fu\,dx = \min_{\substack{\tau\in L^2(\Omega)^N \\ -\mathrm{div}\tau=f \text{ in } \Omega}} \int_\Omega h^{-1}|\tau|^2 dx \; .$$

We can rewrite the optimization problem as a double minimization

$$\inf_{h\in\mathcal{U}_{ad}} \min_{\substack{\tau\in L^2(\Omega)^N \\ -\mathrm{div}\tau=f \text{ in } \Omega}} \int_\Omega h^{-1}|\tau|^2 dx \; ,$$

and the order of minimization can be changed.

Optimality conditions

Lemma. Take $\tau \in L^2(\Omega)^N$. The problem

$$\min_{h\in\mathcal{U}_{ad}} \int_\Omega h^{-1}|\tau|^2 dx$$

admits a unique minimizer $h(\tau)$ in $\mathcal{U}_{ad}$ given by

$$h(\tau)(x) = \begin{cases} h^*(x) & \text{if } h_{min} < h^*(x) < h_{max} \\ h_{min} & \text{if } h^*(x) \leq h_{min} \\ h_{max} & \text{if } h^*(x) \geq h_{max} \end{cases} \qquad \text{with } h^*(x) = \frac{|\tau(x)|}{\sqrt{\ell}},$$

where $\ell \in \mathbb{R}_+$ is the Lagrange multiplier such that
$\displaystyle\int_\Omega h(x)\, dx = h_0|\Omega|$.

Proof. The function $h \to \int_\Omega h^{-1}|\tau|^2 dx$ is strictly convex from $\mathcal{U}_{ad}$ into $\mathbb{R}$ and we easily find the stationary point of the Lagrangian

$$\int_\Omega h^{-1}|\tau|^2 dx + \ell \left(\int_\Omega h(x)\, dx - h_0|\Omega| \right).$$

New numerical algorithm for the compliance

Instead of using a projected gradient algorithm (as before), we rely on the optimality condition.

We perform an alternate minimization in h and τ.

This is called an optimality criteria method.

Optimality criteria method

1. Initialization of the thickness $h_0 \in \mathcal{U}_{ad}$.
2. Iterations until convergence, for $n \geq 0$:
   1. Computation of the state τ_n, unique solution of

      $$\min_{\substack{\tau \in L^2(\Omega)^N \\ -\operatorname{div}\tau = f \text{in } \Omega}} \int_\Omega h_n^{-1} |\tau|^2 dx \,,$$

      with the previous thickness h_n.
   2. Update of the thickness :

      $$h_{n+1} = h(\tau_n),$$

      where $h(\tau)$ is the minimizer defined by the optimality condition. The Lagrange multiplier is computed by dichotomy.

Details

Remark that minimizing in τ is equivalent to solving the equation

$$\begin{cases} -\operatorname{div}(h_n \nabla u_n) = f & \text{in } \Omega \\ u_n = 0 & \text{on } \partial\Omega, \end{cases}$$

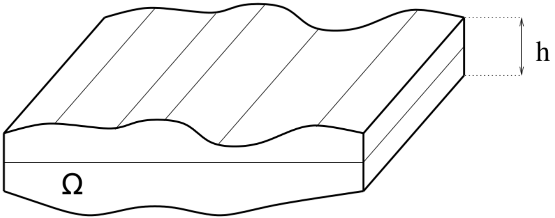
and we recover τ_n by the formula$\tau_n = h_n \nabla u_n$.

This algorithm is an alternate minimization in τ and h of the objective function. In particular, we deduce that the objective function **always decreases** through the iterations

$$J(h_{n+1}) = \int_\Omega h_{n+1}^{-1} |\tau_{n+1}|^2 dx \leq \int_\Omega h_n^{-1} |\tau_{n+1}|^2 dx \leq \int_\Omega h_n^{-1} |\tau_n|^2 dx = J(h_n).$$

This algorithm can also be interpreted as an optimality criteria method (a fixed point algorithm on the optimality conditions).

Thickness optimization of an elastic plate in planar deformation



$$\begin{cases} -\mathrm{div}\sigma = f & \text{in } \Omega \\ \sigma = hAe(u) = h\left(2\mu\, e(u) + \lambda\, \mathrm{tr}(e(u))\, \mathrm{Id}\right) & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \sigma n = g & \text{on } \Gamma_N \end{cases}$$

with the strain tensor $e(u) = \frac{1}{2}\left(\nabla u + (\nabla u)^t\right)$.

Compliance minimization

Set of admissible thickness:

$$\mathcal{U}_{ad} = \left\{ h \in L^2(\Omega),\ h_{max} \geq h(x) \geq h_{min} > 0 \text{ in } \Omega, \int_\Omega h(x)dx = h_0|\Omega| \right\}.$$

The compliance optimization can be written

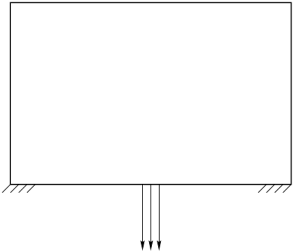
$$\min_{h \in \mathcal{U}_{ad}} J(h) = \int_\Omega f \cdot u \, dx + \int_{\Gamma_N} g \cdot u \, ds.$$

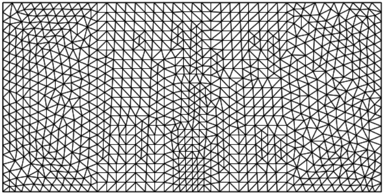
The theoretical results are the same and the problem rewrites

$$\inf_{h \in \mathcal{U}_{ad}} \min_{\substack{\sigma \in L^2(\Omega)^{N \times N} \\ -\mathrm{div}\sigma = f \text{ in } \Omega,\ \sigma n = g \text{ on } \Gamma_N}} \int_\Omega h^{-1} A^{-1} \sigma : \sigma \, dx \, .$$

We apply the optimality criteria method.

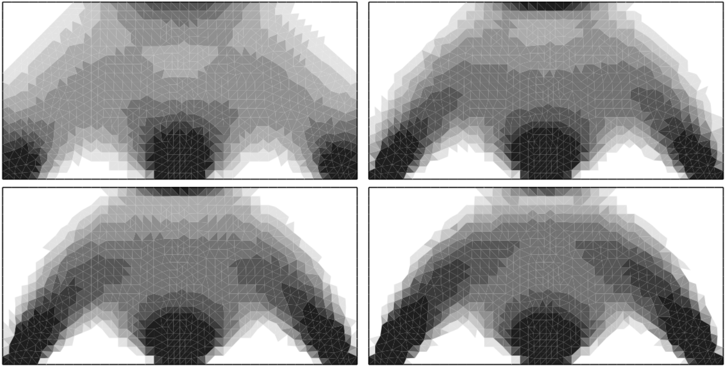
Boundary conditions and mesh for an elastic plate





FreeFem++ computations ; scripts available on the web page
http://www.cmap.polytechnique.fr/~allaire/cours_X_annee3.html

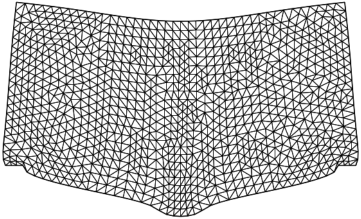
Thickness at iterations 1, 5, 10, 30 (uniform initialization).

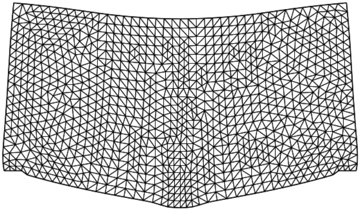


$h_{min} = 0.1$, $h_{max} = 1.0$, $h_0 = 0.5$ (increasing thickness from white to black)

Numerical results

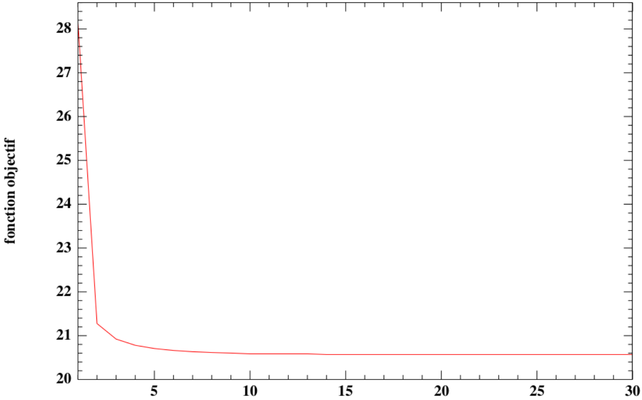
Comparing the initial and final deformed shapes





Numerical results

Convergence history

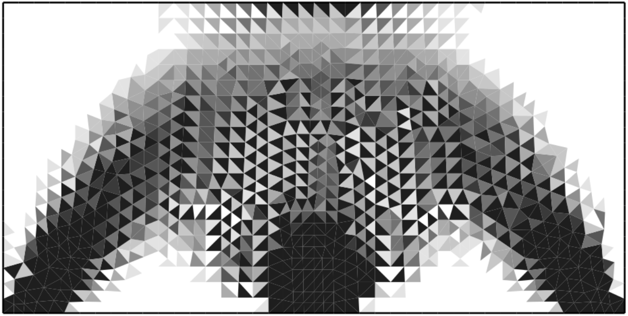


Numerical instabilities

Numerical instabilities (checkerboards)

- Finite elements $P2$ for u and $P0$ for $h \Rightarrow$ OK
- Finite elements $P1$ for u and $P0$ for $h \Rightarrow$ unstable !

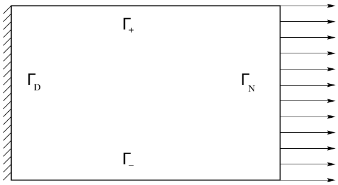
Hint (not a proof!): artificial rigidity of checkerboards.



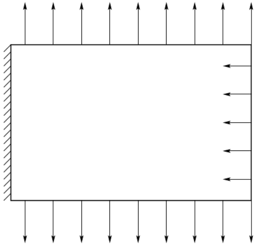
Result with $P1$ / $P0$ finite elements.

Numerical counter-example of non-existence of an optimal design (in elasticity)

We look for the design which horizontally is less deformed and vertically more deformed.



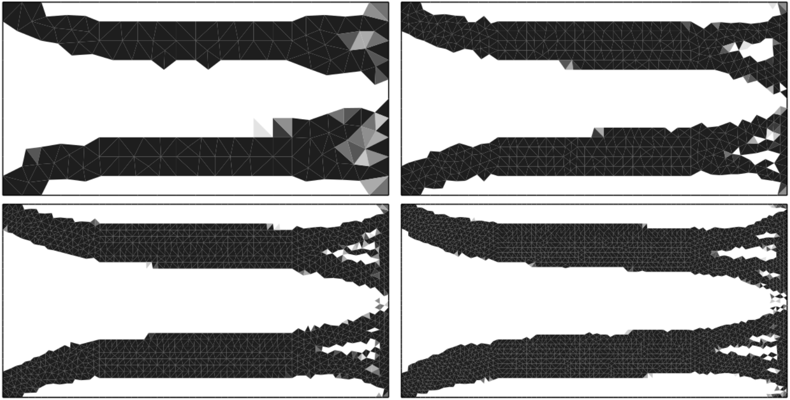
boundary conditions



target displacement u_0

$$\inf_{h \in \mathcal{U}_{ad}} J(h) = \int_\Omega |u - u_0|^2 \, dx$$

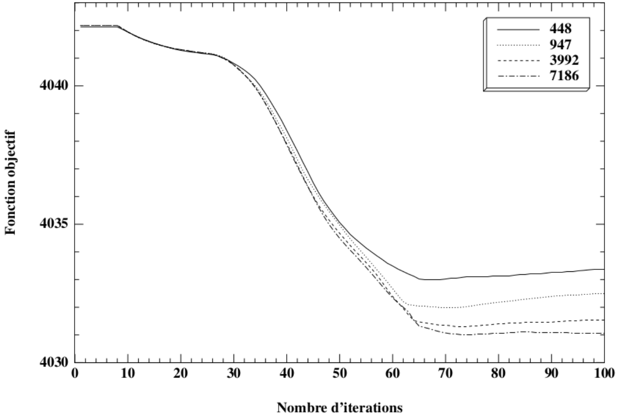
Optimal designs for meshes with 448, 947, 3992, 7186 triangles



No convergence under mesh refinement

Non existence of solutions can be seen numerically as no convergence under mesh refinement !

More and more details appear when the mesh size is decreased.
The value of the objective function decreases with the mesh size.



Regularization

Triple motivation:

1. To avoid instabilities when using $P1$ finite elements for u and $P0$ for h (less expensive than $P2$-$P0$).
2. To obtain an algorithm which converges by mesh refinement.
3. To adhere to the “regularized” framework of section 5.2.3 (with existence of optimal solutions).

$H^1(\Omega)$ scalar product

Recall that

$$\langle J'(h), k\rangle = \int_\Omega k \nabla u \cdot \nabla p \, dx \qquad \forall\, k \in \mathcal{U}_{ad}.$$

Main idea: we change the scalar product !
Previously we identified $\mathcal{U}_{ad}$ to a subspace of $L^2(\Omega)$, thus

$$\langle J'(h), k\rangle = \int_\Omega J'(h)\, k \, dx \qquad \Rightarrow \qquad J'(h) = \nabla u \cdot \nabla p \, .$$

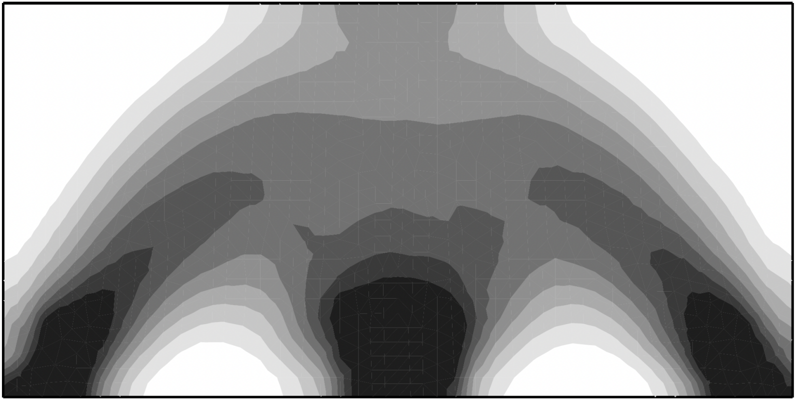
Now, we identify $\mathcal{U}_{ad}$ to a subspace $H^1(\Omega)$, thus

$$\langle J'(h), k\rangle = \int_\Omega \big(\nabla J'(h) \cdot \nabla k + J'(h) k\big) \, dx \, ,$$

and we deduce a new formula for the gradient

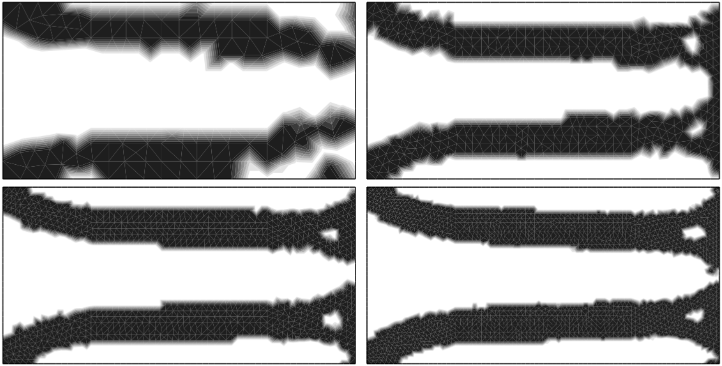
$$\begin{cases} -\Delta J'(h) + J'(h) = \nabla u \cdot \nabla p & \text{in } \Omega, \\ \dfrac{\partial J'(h)}{\partial n} = 0 & \text{on } \partial\Omega. \end{cases}$$

Regularized optimal design



Finite elements P_1-P_0. Compliance minimization. Alternate directions algorithm.

Regularized optimal shapes



Same case as the "numerical counter-examples" (meshes 448, 947, 3992, 7186).

Conclusion on regularization

- Regularization works !
- It has a tendency to smooth the geometric details.
- It costs a bit more (solving an additional Laplacian to compute the gradient).
- Difficulty in choosing the regularization parameter $\epsilon > 0$ (which can be interpreted as a lengthscale)

$$-\epsilon^2 \Delta J'(h) + J'(h) = \nabla u \cdot \nabla p \quad \text{in } \Omega$$

- Another possibility: H^1 penalization of the thickness

$$\tilde{J}(h) = J(h) + \frac{\epsilon^2}{2} \int_\Omega |\nabla h|^2 \, dx$$

  and use of an H^1 gradient.
- One can use filters, considering for instance

$$\tilde{J}(h) = J(\phi * h)$$

  for some convolution kernel ϕ.