Null Space Gradient Flows for Constrained Optimization with Applications to Shape Optimization

Florian Feppon
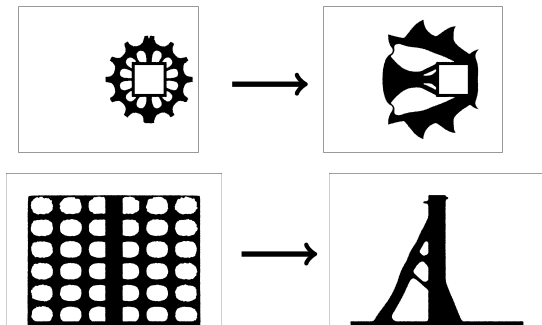
Grégoire Allaire, Charles Dapogny
Julien Cortial, Felipe Bordeu

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Multiphysics, non parametric, shape and topology optimization, in 2D. . .

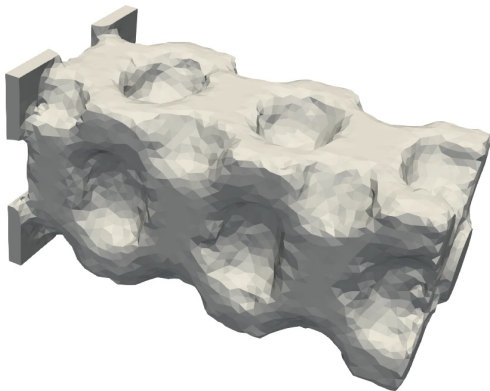# Shape optimization

And in 3D. . .

Figure: 3D shape optimization in linear elasticity
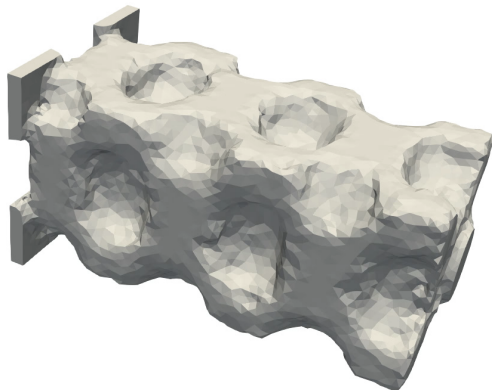
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...Nonlinear, non convex, infinite dimensional optimization problems featuring multiple and arbitrary constraints!

1. Gradient flows for equality and *inequality* constrained optimizations
2. Demonstration on topology optimization test cases

1. Constrained optimization

$$\min_{x \in \mathcal{X}} \quad J(x)$$

$$\text{s.t.} \begin{cases} \boldsymbol{g}(x) = 0 \\ \boldsymbol{h}(x) \leq 0, \end{cases}$$

with $J : \mathcal{X} \to \mathbb{R}$, $\boldsymbol{g} : \mathcal{X} \to \mathbb{R}^p$ and $\boldsymbol{h} : \mathcal{X} \to \mathbb{R}^q$ Fréchet differentiable.

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▶ a Hilbert space equipped with a scalar product $a(\cdot, \cdot)$, $\mathcal{X} = V$

▶ a "manifold", as in topology optimization:

$$\mathcal{X} = \{\Omega \subset D \,|\, \Omega \text{ Lipschitz} \}$$

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These methods suffer from:

- ▶ the need for tuning unintuitive parameters.
- ▶ "inconsistencies" when $\Delta t \to 0$: SLP, SQP, MFD subproblems may not have a solution if Δt too small. ALG does not guarantee reducing the objective function if constraints are satisfied.

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$\boldsymbol{g}(x(t)) = \boldsymbol{g}(x(0))e^{-\alpha_C t}$ and $J(x(t))$ is guaranteed to decrease if $\boldsymbol{g}(x(t)) = 0$.

1. Gradient flows for inequality constraints

For *both* equality constraints $\boldsymbol{g}(x) = 0$ and inequality constraints $\boldsymbol{h}(x) \leq 0$, consider $\widetilde{I}(x)$ the set of violated constraints:

$$\widetilde{I}(x) = \{i \in \{1, \ldots, q\} \,|\, h_i(x) \geqslant 0\}.$$

$$\boldsymbol{C}_{\widetilde{I}(x)} = \left[\boldsymbol{g}(x) \quad | \quad (h_i(x))_{i \in \widetilde{I}(x)}\right]^T$$

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We propose

$$\dot{x} = -\alpha_J \boldsymbol{\xi}_J(x(t)) - \alpha_C \boldsymbol{\xi}_C(x(t))$$

with

$$-\boldsymbol{\xi}_J(x) := \begin{cases} \text{the ``best'' descent direction} \\ \text{with respect to the constraints } \widetilde{I}(x) \end{cases}$$

$$-\boldsymbol{\xi}_C(x) := \begin{cases} \text{the Gauss-Newton direction} \\ -\mathrm{D}\boldsymbol{C}_{\widetilde{I}(x)}^{\mathcal{T}} (\mathrm{D}\boldsymbol{C}_{\widetilde{I}(x)} \mathrm{D}\boldsymbol{C}_{\widetilde{I}(x)}^{\mathcal{T}})^{-1} \boldsymbol{C}_{\widetilde{I}(x)}(x) \end{cases}$$

1. Gradient flows for inequality constraints

$$\min_{(x_1, x_2) \in \mathbb{R}^2} \quad J(x_1, x_2) = x_1^2 + (x_2 + 3)^2$$

$$\text{s.t.} \quad \begin{cases} h_1(x_1, x_2) = -x_1^2 + x_2 & \leq 0 \\ h_2(x_1, x_2) = -x_1 - x_2 - 2 & \leq 0 \end{cases}$$

We propose:
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with

$$\boldsymbol{\xi}_J(x) := (I - \mathrm{D}\boldsymbol{C}_{\widehat{I}(x)}^{\mathcal{T}}(\mathrm{D}\boldsymbol{C}_{\widehat{I}(x)}\mathrm{D}\boldsymbol{C}_{\widehat{I}(x)}^{\mathcal{T}})^{-1}\mathrm{D}\boldsymbol{C}_{\widehat{I}(x)})(\nabla J(x))$$

$$\boldsymbol{\xi}_C(x) := \mathrm{D}\boldsymbol{C}_{\widetilde{I}(x)}^{\mathcal{T}}(\mathrm{D}\boldsymbol{C}_{\widetilde{I}(x)}\mathrm{D}\boldsymbol{C}_{\widetilde{I}(x)}^{\mathcal{T}})^{-1}\boldsymbol{C}_{\widetilde{I}(x)}(x).$$

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$\widehat{I}(x) \subset \widetilde{I}(x)$ is a subset of the active or violated constraints which can be computed by mean of a dual subproblem.

1. Gradient flows for inequality constraints

The best descent direction $-\boldsymbol{\xi}_J(x)$ must be proportional to

$$\boldsymbol{\xi}^* = \underset{\boldsymbol{\xi} \in V}{\arg\min} \quad \mathrm{D}J(x)\boldsymbol{\xi}$$

$$\text{s.t.} \begin{cases} \mathrm{D}\boldsymbol{g}(x)\boldsymbol{\xi} = 0 \\ \mathrm{D}\boldsymbol{h}_{\widetilde{I}(x)}(x)\boldsymbol{\xi} \leq 0 \\ \|\boldsymbol{\xi}\|_V \leq 1. \end{cases}$$

where $\boldsymbol{h}_{\widetilde{I}(x)}(x) = (h_i(x))_{i \in \widetilde{I}(x)}$

1. Gradient flows for inequality constraints

Proposition

Let $(\boldsymbol{\lambda}^*(x), \boldsymbol{\mu}^*(x)) \in \mathbb{R}^p \times \mathbb{R}^{\mathrm{Card}\widetilde{I}(x)}$ the solutions of the following dual minimization problem:

$$(\boldsymbol{\lambda}^*(x), \boldsymbol{\mu}^*(x)) := \arg \min_{\substack{\boldsymbol{\lambda} \in \mathbb{R}^p \\ \boldsymbol{\mu} \in \mathbb{R}^{\widetilde{q}(x)}, \, \boldsymbol{\mu} \geqslant 0}} ||\nabla J(x) + \mathrm{D}\boldsymbol{g}(x)^{\mathcal{T}}\boldsymbol{\lambda} + \mathrm{D}\boldsymbol{h}_{\widetilde{I}(x)}(x)^{\mathcal{T}}\boldsymbol{\mu}||_V.$$

Then, unless x is a KKT point, the best descent direction $\boldsymbol{\xi}^*(x)$ is given by

$$\boldsymbol{\xi}^*(x) = -\frac{\nabla J(x) + \mathrm{D}\boldsymbol{g}(x)^{\mathcal{T}}\boldsymbol{\lambda}^*(x) + \mathrm{D}\boldsymbol{h}_{\widetilde{I}(x)}(x)^{\mathcal{T}}\boldsymbol{\mu}^*(x)}{||\nabla J(x) + \mathrm{D}\boldsymbol{g}(x)^{\mathcal{T}}\boldsymbol{\lambda}^*(x) + \mathrm{D}\boldsymbol{h}_{\widetilde{I}(x)}(x)^{\mathcal{T}}\boldsymbol{\mu}^*(x)||_V}.$$

Proposition

Let $\widehat{I}(x)$ the set obtained by collecting the non zero components of $\boldsymbol{\mu}^*(x)$:

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Then $\boldsymbol{\xi}^*(x)$ is explicitly given by:

$$\boldsymbol{\xi}^*(x) = -\frac{\Pi_{C_{\widehat{I}(x)}}(\nabla J(x))}{\|\Pi_{C_{\widehat{I}(x)}}(\nabla J(x))\|_V},$$

with

$$\Pi_{C_{\widehat{I}(x)}}(\nabla J(x)) = (I - \mathrm{D}\boldsymbol{C}_{\widehat{I}(x)}^{\mathcal{T}}(\mathrm{D}\boldsymbol{C}_{\widehat{I}(x)}\mathrm{D}\boldsymbol{C}_{\widehat{I}(x)}^{\mathcal{T}})^{-1}\mathrm{D}\boldsymbol{C}_{\widehat{I}(x)})(\nabla J(x))$$

We can prove:

1. Constraints are asymptotically satisfied:

$$\boldsymbol{g}(x(t)) = e^{-\alpha_c t}\boldsymbol{g}(x(0)) \text{ and } \boldsymbol{h}_{\widetilde{I}(x(t))} \leq e^{-\alpha_c t}\boldsymbol{h}(x(0))$$

2. J decreases as soon as the violation $\boldsymbol{C}_{\widetilde{I}(x(t))}$ is sufficiently small

3. All stationary points x^* of the ODE are KKT points

2. Applications to shape optimization

A multiple load case.
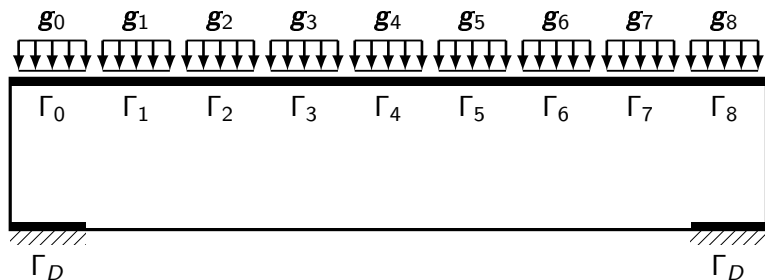
$$\begin{cases} -\operatorname{div}(Ae(\boldsymbol{u}_i)) = 0 & \text{in } \Omega \\ Ae(\boldsymbol{u}_i)\boldsymbol{n} = 0 & \text{on } \Gamma \\ Ae(\boldsymbol{u}_i)\boldsymbol{n} = \boldsymbol{g}_i & \text{on } \Gamma_i \\ Ae(\boldsymbol{u}_i)\boldsymbol{n} = 0 & \text{on } \Gamma_j \text{ for } j \neq i \\ \boldsymbol{u}_i = 0 & \text{on } \Gamma_D, \end{cases}$$

Volume minimization subject to multiple load rigidity constraints

$$\min_{\Omega} \quad \int_{\Omega} \mathrm{d}x$$
$$s.t. \int_{\Omega} Ae(\boldsymbol{u}_i) : e(\boldsymbol{u}_i)\mathrm{d}x \leq C, \quad \forall i = 1\ldots 9$$

Demonstration on shape optimization test cases

(a) One load (only g_4 is considered).

(b) Three loads (only g_0, g_4, g_8 are considered).

(c) All nine loads.
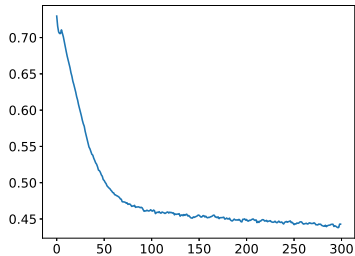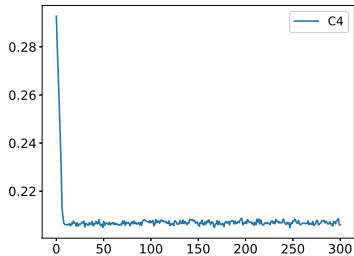
(a) $J(\Omega) = \mathrm{Vol}(\Omega)$.

(b) Constraints C_i.

Figure: Single load case.
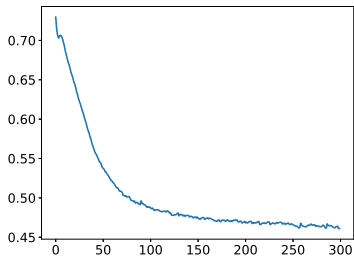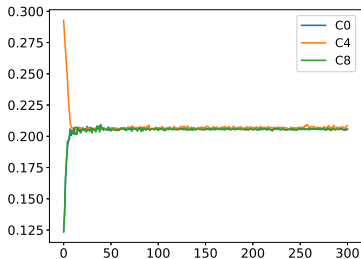
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Figure: Three load case.
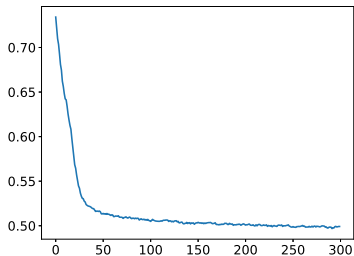
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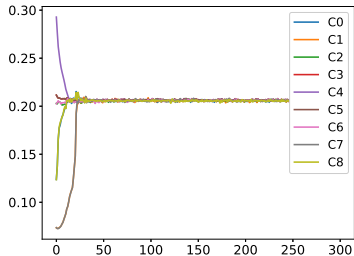
(b) Constraints C_i.

Figure: Nine load case.

Thermal heat minimization:

$$\max_{\Omega_f \subset D} \quad \int_D T \mathrm{d}x$$

$$s.t. \quad \int_{\Omega_f} \mathrm{d}x = V_0$$

Figure: Thermal conduction.

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Lift maximization subject to maximum drag constraint:

$$\max_{\Omega_f \subset D} \int_{\partial \Omega_s} \boldsymbol{e}_y \cdot \sigma_f(\boldsymbol{v}, p) \cdot \boldsymbol{n} \mathrm{d}\boldsymbol{s}$$

$$s.t. \begin{cases} \int_{\Omega_f} 2\nu e(\boldsymbol{v}) : e(\boldsymbol{v}) \mathrm{d}x \leq C_0 \\ \int_{\Omega_f} \mathrm{d}x = V_0 \\ \int_{\Omega_s} x \mathrm{d}x = x_0 \end{cases}$$

Figure: Lift maximization (Navier Stokes flow).

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Heat exchange subject to maximal pressure drop (with Dirichlet boundary condition on Γ):

$$\max_{\Omega_f \subset D} \quad \int_{\Omega_f} \rho c_p \boldsymbol{v} \cdot \nabla T \mathrm{d}x$$

$$s.t. \quad \int_{\partial \Omega_{f,out}} p \mathrm{d}\boldsymbol{s} - \int_{\partial \Omega_{f,in}} p \mathrm{d}\boldsymbol{s} \leq \mathrm{DP}_0,$$

$$T = T_0 \text{ on } \Gamma$$

Figure: Single pipe heat exchanger.

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397.5
375.1
352.8
330.4
308.1

Figure: Single pipe heat exchanger.

Figure: 3D shape optimization in heat conduction

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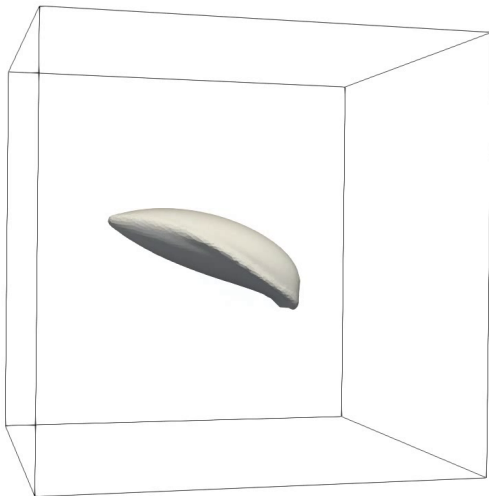Figure: 3D lift maximization for a Navier Stokes flow

Figure: 3D lift maximization for a Navier Stokes flow

References

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HAL preprint hal-01879571 (2019).

Many thanks!

Constrained optimization
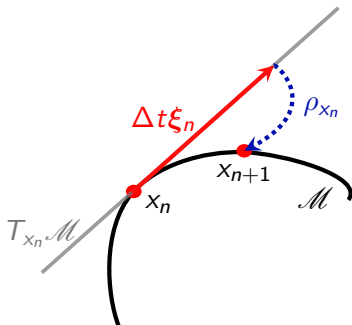
▶ For a vector space $\mathcal{X} = V$, a sequence of updates will be of the form

$$x_{n+1} = x_n - \Delta t \boldsymbol{\xi}_n$$

where $-\boldsymbol{\xi}_n$ is the current descent direction.

▶ For a manifold, this becomes

$$x_{n+1} = \rho_{x_n}(-\Delta t \boldsymbol{\xi}_n)$$

Warning: $\nabla J(x)$ and the transpose ^{T} must be computed with respect to the scalar product a of the Hilbert space V or T_{x_n}. In practice this means solving

$$\forall \boldsymbol{\xi} \in V, \ a(\nabla J(x), \boldsymbol{\xi}) = \mathrm{D}J(x)\boldsymbol{\xi}$$

$$\forall \boldsymbol{\xi} \in V, \ a(\nabla g_i(x), \boldsymbol{\xi}) = \mathrm{D}g_i(x)\boldsymbol{\xi}$$

$$\forall \boldsymbol{\xi} \in V, \ a(\nabla h_i(x), \boldsymbol{\xi}) = \mathrm{D}h_i(x)\boldsymbol{\xi}$$

Then

$$\mathrm{D}\boldsymbol{g}^T(x) = \begin{bmatrix} \nabla g_0(x) & \cdots & \nabla g_p(x) \end{bmatrix}^T$$

$$\mathrm{D}\boldsymbol{h}^T(x) = \begin{bmatrix} \nabla h_0(x) & \cdots & \nabla h_q(x) \end{bmatrix}^T$$

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3. Scalar product a for identifying these derivatives

2. Applications to shape optimization

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3. Scalar product a for identifying these derivatives
4. Typical length scale Δt (e.g. the mesh size)
5. α_J and α_C for tuning the relative magnitude of $\boldsymbol{\xi}_J$ and $\boldsymbol{\xi}_C$, i.e. the speed at which violated constraints become satisfied.