Shape optimisation for rigid objects in a Stokes flow

M2 Internship

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August 24, 2023

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Introduction

What is the shape optimisation ?

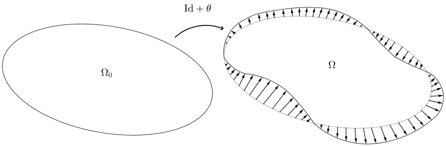

Figure 1: Geometric shape optimisation principle.

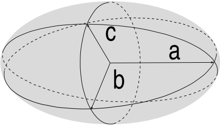

Figure 2: Ellipsoid parametrized.

- **Parametric optimisation** : Finite number of parameters.
- **Geometric optimisation** : Modification of the shape boundary while preserving the topology
- **Topology optimisation** : Modifying the shape by changing its topology

Setup

Shape Optimisation Setup

$$\inf_{\Omega \in \Omega_{ad}} J(\Omega, u(\Omega))$$

where

- Ω denotes a subset of $\mathbb{R}^N$
- Ω_{ad} the set of admissible forms.
- J is a cost function to be minimised
- u solution of a PDE defined on Ω

Geometric Shape Optimisation

Introduction

- Let Ω_0 be a reference domain (regular open set of $\mathbb{R}^N$).
- The deformation field θ :

$$\Omega = (\mathrm{Id} + \theta)(\Omega_0).$$

- Boundary of Ω :

$$\partial\Omega = \Gamma \cup \Gamma_{fixed}.$$

- Volume conservation and set of admissible forms :

$$\Omega_{ad} = \{\Omega \mid \Gamma_{fixed} \subset \partial\Omega,\ g(\Omega) = 0\} \quad \text{with} \quad g(\Omega) = |\Omega| - |\Omega_0|.$$

Céa's derivation method

The Lagrangian

We introduce the following Lagrangian

$$\begin{array}{rcl} \mathcal{L} : \Omega_{ad} \times V \times V & \rightarrow & \mathbb{R} \\ (\Omega, v, q) & \mapsto & J(\Omega, v(\Omega)) + E(v, q), \end{array}$$

where E is the weak formulation of the primal problem.

With $\nabla_{\Omega,v,q}\mathcal{L} = 0$, we can find :

1. primal problem.
2. dual problem.
3. the differential of the cost function.

Differentials

Some differentials w.r.t the domain Ω :

Differential of the cost function

Assume that the differential of the cost function is expressed as

$$DJ(\Omega)(\theta) = \int_\Gamma \theta \cdot n G(\Omega),$$

where $G(\Omega)$ is called **shape gradient**.

Differential of the volume constraint

The differential of $g(\Omega) = |\Omega| - |\Omega_0|$ is given by

$$Dg(\Omega)(\theta) = \int_\Gamma \theta \cdot n.$$

Minimisation via Gradient Descent (GD)

- $l \in \mathbb{R}$ such as $DJ(\Omega)(\theta) + lDg(\Omega)(\theta) = \int_\Gamma \theta \cdot n \, [l + G(\Omega)] = 0.$
- $(\Omega_k) : \partial\Omega_k = \Gamma_k \cup \Gamma_{fixed}.$
- $\Omega_{k+1} = (\mathrm{Id} + \theta_k)(\Omega_k)$ with

$$\begin{cases} -\Delta\theta_k = 0 & \text{in } \Omega_k \\ \theta_k = 0 & \text{on } \Gamma_{fixed} \\ \frac{\partial\theta_k}{\partial n} = -t\,[l_k + G(\Omega_k)]\, n_k & \text{on } \Gamma_k, \end{cases}$$

- $l_k(a,b,c) = al_{k-1} + b\frac{\int_{\Gamma_k} G(\Omega_k)}{|\Gamma_k|} + c\frac{|\Omega_k| - |\Omega_0|}{|\Omega_0|}.$

Minimisation via Null-space Gradient Flow (NSGF)

- Transcribes the optimization process as an ODE in the space of admissible shapes Ω_{ad}

$$\dot{x} = F(x), \quad x \in \Omega_{ad}$$

- the vector field $F(x)$ is composed of two contributions:
    - a direction ξ_C responsible of constraint satisfaction
    - a direction ξ_J responsible of cost function minimization

$$\dot{x} = -\alpha_C \xi_C(x) - \alpha_J \xi_J(x) \quad x \in \Omega_{ad}$$

  with $\alpha_C, \alpha_J > 0$ constants depending on the discretization of the problem

- the two directions ξ_C, ξ_J depend on the differentials of cost and constraint functions

NSGF illustration

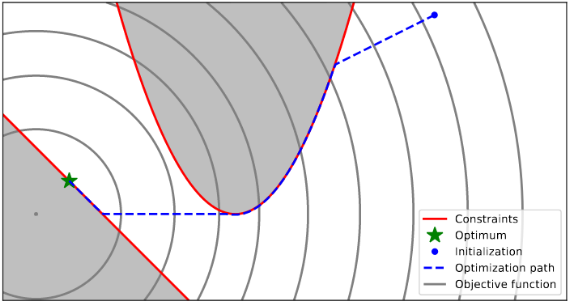

Figure 3: Illustration of the NSGF method taken from [Fep19].

NSGF for shape optimization

Let V be a Hilbert space. Consider the functions

$$\begin{aligned} g &: V \to \mathbb{R}^p, && \text{Constraint functions} \\ Dg &: V \to \mathbb{R}^p, && \text{Differential of constraint functions} \\ Dg^T &: \mathbb{R}^p \to V && \text{Transpose of } Dg \end{aligned}$$

such that

$$\left\langle Dg^T \mu, \xi \right\rangle_V = \mu^T Dg\xi \qquad \forall (\mu, \xi) \in \mathbb{R}^p \times V$$

Dg^T strong formulation

$$\begin{cases} -\gamma^2 \Delta (Dg^T(\Omega)(e_1)) + Dg^T(\Omega)(e_1) = 0 & \text{in } \Omega, \\ \frac{\partial Dg^T(\Omega)(e_1)}{\partial n} = \frac{1}{\gamma^2} n & \text{on } \Gamma \\ \frac{\partial Dg^T(\Omega)(e_1)}{\partial n} = 0 & \text{on } \Gamma_{fixed} \end{cases}$$

Numerical implementation

We define a domain sequence, Ω_k, such that

$$\Omega_{k+1} = (\mathrm{Id} + \theta_k)(\Omega_k).$$

Using the NSGF method, we define the displacement field θ_k over all Ω_k such that

$$\begin{cases} -\Delta\theta_k = 0 & \text{in } \Omega_k \\ \theta_k = 0 & \text{on } \Gamma_{fixed} \\ \frac{\partial\theta_k}{\partial n} = -\alpha_{C,k}\xi_C(\Omega_k) - \alpha_{J,k}\xi_J(\Omega_k) & \text{on } \Gamma_k. \end{cases}$$

Null space and range space directions

$\xi_J(\Omega) : \mathbb{R}^N \to \mathbb{R}^N$ and $\xi_C(\Omega) : \mathbb{R}^N \to \mathbb{R}^N$ are defined by :

$$\begin{cases} \xi_J(\Omega)(X) = \nabla J(\Omega)(X) - Dg^T(\Omega)\left[(Dg(\Omega)Dg^T(\Omega))^{-1}Dg(\Omega)\nabla J(\Omega)\right](X), \\ \xi_C(\Omega)(X) = Dg^T(\Omega)\left[(Dg(\Omega)Dg^T(\Omega))^{-1}g(\Omega)\right](X). \end{cases}$$

Choice of $\alpha_{J,k}$ and $\alpha_{C,k}$

Let $n_0 > 0$ the n_0-th iteration.

$\alpha_{J,n}$ and $\alpha_{C,n}$

$$\alpha_{J,n} = \begin{cases} \frac{\texttt{hmin}}{\|\xi_J(\Omega_n)\|_{L^\infty}} & n < n_0 \\ \frac{\texttt{hmin}}{\max\{\|\xi_J(\Omega_n)\|_{L^\infty}, \|\xi_J(\Omega_{n_0})\|_{L^\infty}\}} & n \geq n_0 \end{cases}$$

$$\alpha_{C,n} = \min\left\{0.9, \frac{\texttt{hmin}}{\max\{\texttt{1e-9}, \|\xi_C(\Omega_n)\|_{L^\infty}\}}\right\}$$

Consequences

$$\forall n \geq 0 \quad \|\alpha_{J,n}\xi_J(\Omega_n)\|_{L^\infty} \leq \texttt{hmin}$$

$$\forall n \geq 0 \quad \|\alpha_{C,n}\xi_C(\Omega_n)\|_{L^\infty} \leq \min\{\texttt{0.9}, \texttt{hmin}\}$$

A rigid body in a Stokes flow

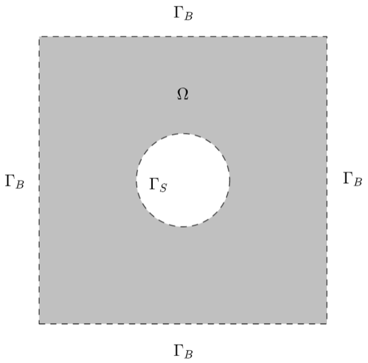

Figure 4: 2D representation of the Stokes problem.

PDE of the Stokes problem

Let's consider a linear flow U^∞ and U the translastion velocity of the body. The fluid velocity $u : \mathbb{R}^N \to \mathbb{R}^N$ and the pressure field $p : \mathbb{R}^N \to \mathbb{R}$ are solutions of the Stokes equation

$$\begin{cases} -\mu \Delta u + \nabla p = 0 & \text{in } \Omega, \\ \nabla \cdot u = 0 & \text{in } \Omega, \\ u = U & \text{on } \Gamma_S, \\ u = U^\infty & \text{on } \Gamma_B. \end{cases}$$

A rigid body in a Stokes flow

We want to solve the following problem

$$\inf_{\Omega \in \Omega_{ad}} \left\{ J_\alpha(\Omega) = \int_{\Gamma_S} \sigma(u,p)n \cdot \alpha \right\}$$

with n the unit normal outside Ω and σ the stress tensor defined by

$$\sigma(u,p) = -pI + 2\mu e(u).$$

J_α	U	α	U^∞
K_{ij}	e_j	e_i	0
Q_{ij}	$e_j \wedge (x,y,z)^T$	$e_i \wedge (x,y,z)^T$	0
C_{ij}	$e_j \wedge (x,y,z)^T$	e_i	0

Table 1: Cost function J_α associated with the entries of the large strength tensor (see [MIP22]) as a function of the choice of U, α and U^∞.

Examples of different resistance problems

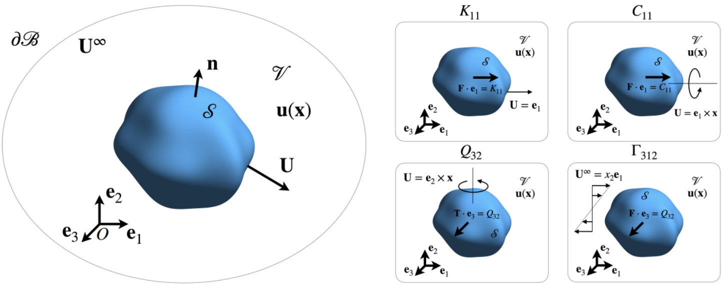

Figure 5: Setup of the problem, image taken from [MIP22]

Results

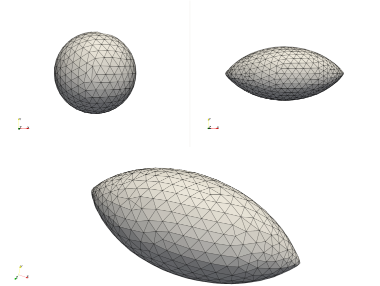

Figure 6: Optimum shape for K_{11}

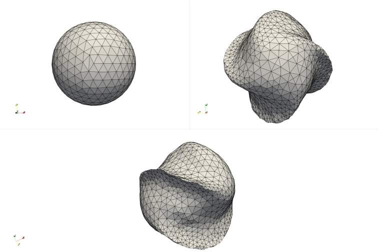

Figure 7: Optimum shape for C_{11}

Parametric Shape Optimisation

Constrained minimisation problem

Setup

Let $c : \mathbb{R}^d \to \mathbb{R}^m$ be m inequality constraints, which can be written as $c(x) = (c^1(x), ..., c^m(x))$. We seek to solve the following problem:

$$\inf_{x \in C} f(x)$$

where $C = \left\{x \in \Omega \subset \mathbb{R}^d \mid c(x) \leq 0\right\}$.

Scalable Constrained Bayesian Optimisation (SCBO)

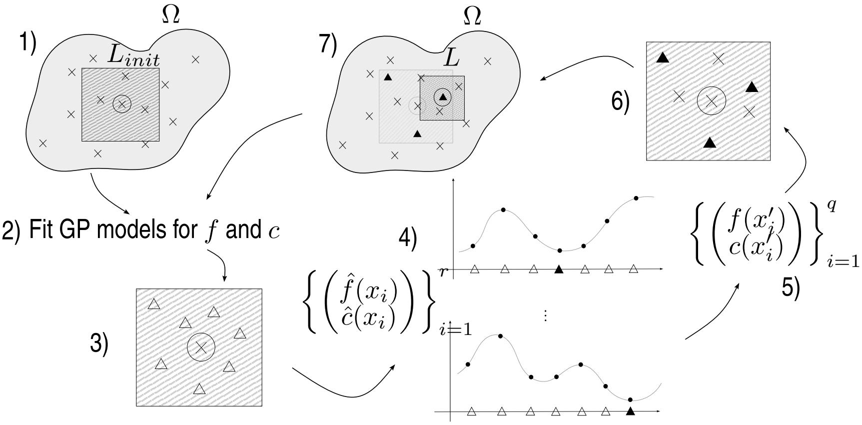

Figure 8: SCBO algorithm.

Free-Form-Deformation (FFD)

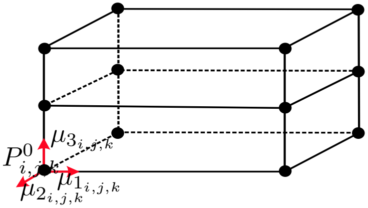

Figure 9: Uniformly distributed control points with $I = 2$, $J = 2$ and $K = 3$.

- Diffeomorphism :

$$\begin{array}{rcl} \psi : D_0 & \to & [0,1]^3 \\ (x,y,z) & \mapsto & (s,t,p). \end{array}$$

- Control points :

$$P^0_{i,j,k} = \begin{pmatrix} i/I \\ j/J \\ k/K \end{pmatrix}.$$

- Deformation : $\nu_{i,j,k} \in \mathbb{R}^3$ such as

$$P_{i,j,k} = P^0_{i,j,k} + \nu_{i,j,k}.$$

FFD

- The map of deformation :

$$T(x,y,z,\nu) = \psi^{-1}\left(\sum_{i=0}^{J}\sum_{j=0}^{J}\sum_{k=0}^{K} b_{i,j,k}^{I,J,K}\left(\psi(x,y,z)\right)P_{i,j,k}(\nu)\right).$$

- Bernstein polynomials :

$$b_l^M(\gamma) = \binom{M}{l}(1-\gamma)^{M-l}\gamma^l$$

with $M \in \mathbb{N}^*$, $l \in 0, M$ and $\gamma \in [0,1]$.

- Products of Bernstein polynomials :

$$b_{i,j,k}^{I,J,K}(s,t,p) = b_i^J(s)b_j^J(t)b_k^K(p).$$

A rigid body in a Stokes flow

PDE of the Stokes problem

The fluid occupies an infinite domain Ω within $\mathbb{R}^N$. The fluid velocity field $u : \mathbb{R}^N \to \mathbb{R}^N$ and the pressure field $p : \mathbb{R}^N \to \mathbb{R}$ are solutions to the Stokes equations:

$$\begin{cases} -\mu\Delta u + \nabla p = 0 & \text{in } \Omega, \\ \nabla \cdot u = 0 & \text{in } \Omega, \\ u = U & \text{on } \Gamma_S, \\ \|u\|, p \to 0 & \text{as } \|x\| \to +\infty. \end{cases}$$

The set of admissible shapes is defined as follows:

$$\Omega_{ad} = \left\{ P \in \mathbb{R}^{N\times M} \mid g(P) = 0 \right\}$$

with $g(P) = |S(P)| - |S_0|$. For S_0, we will consider the unit sphere.

Minimisation problem

$$\inf_{\Omega\in\Omega_{ad}} \left\{ J_\alpha(\Omega) = \int_{\Gamma_S} \sigma(u,p)n \cdot \alpha \right\},$$

where n denotes the normal vector to Γ_S and $\alpha \in \mathbb{R}^N$.

Case studies

n°	Sym.	Sphere	Bounds
1	Yes	No	$[-2, 2]^{39}$
2	Yes	Yes	$[-2, 2]^{39}$
3	No	Yes	$[-2, 2]^{81}$
4	Yes	No	$[-4, 4]^{39}$
5	Yes	Yes	$[-4, 4]^{39}$

Table 2: Case studies.

Results : K_{11}

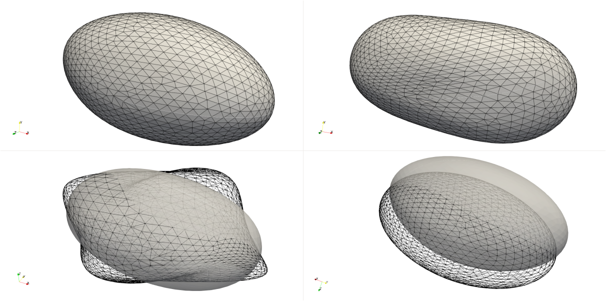

Figure 10: K_{11} shapes : case n°2 (upper left), case n°1 (upper right), case n°2 in gray surface with case n°4 in black wireframe (bottom left) and, case n°2 in gray surface with case n°3 in balck wireframe.

Results : C_{11}

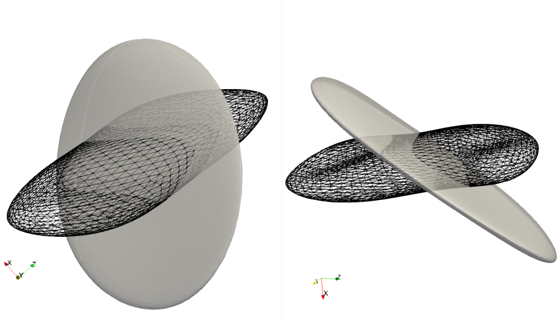

Figure 11: C_{11} shapes : case n°1 in black wireframe and case n°2 in grey surface.

Conclusion and Perspectives

Conclusion Perspectives

- Geometric shape Optimisation :
  - Regularity of the displacement field
  - Code parallelization
- Parametric shape Optimisation :
  - Number of control points
  - Space shapes
  - Code parallelization
- Swimming robots with flagella

References

References i

Grégoire Allaire, *Conception optimale de structures*, Mathématiques & applications, vol. 58, Springer Berlin Heidelberg, 2006 (fr).

Luca Berti, *Numerical methods and optimization for micro-swimming*, These de doctorat, Strasbourg, December 2021.

Maximilian Balandat, Brian Karrer, Daniel R. Jiang, Samuel Daulton, Benjamin Letham, Andrew Gordon Wilson, and Eytan Bakshy, *BoTorch: A Framework for Efficient Monte-Carlo Bayesian Optimization*, Advances in Neural Information Processing Systems 33, 2020.

Jean Cea, *Conception optimale ou identification de formes, calcul rapide de la dérivée directionnelle de la fonction coût*, M2AN - Modélisation mathématique et analyse numérique **20** (1986), no. 3, 371–402 (fr).

References ii

Charles Dapogny, Pascal Frey, Florian Omnès, and Yannick Privat, *Geometrical shape optimization in fluid mechanics using FreeFem++*, Structural and Multidisciplinary Optimization **58** (2018), no. 6, 2761–2788 (en).

David Eriksson and Matthias Poloczek, *Scalable Constrained Bayesian Optimization*, February 2021, arXiv:2002.08526 [cs, stat].

Florian Feppon, *Shape and topology optimization of multiphysics systems*, These de doctorat, Université Paris-Saclay (ComUE), December 2019.

David Field, *Qualitative measures for initial meshes*, International Journal for Numerical Methods in Engineering **47** (2000), 887–906.

References iii

- Robert B. Gramacy, *Surrogates: Gaussian process modeling, design and optimization for the applied sciences*, Chapman Hall/CRC, Boca Raton, Florida, 2020, `http://bobby.gramacy.com/surrogates/`.
- Anwar Koshakji, Alfio Quarteroni, and Gianluigi Rozza, *Free form deformation techniques applied to 3d shape optimization problems*.
- matthieuaussal, *matthieuaussal/gypsilab*, March 2023, original-date: 2017-07-10T12:22:09Z.
- Clement Moreau, Kenta Ishimoto, and Yannick Privat, *Shapes optimising grand resistance tensor entries for a rigid body in a Stokes flow*, July 2022.

References iv

Christophe Prud'homme, Vincent Chabannes, Thibaut Metivet, Thomas Saigre, Lorenzo Sala, Christophe Trophime, Abdoulaye SAMAKE, Luca Berti, and Céline Van Landeghem, *feelpp/feelpp: Feel++ v111 alpha.1*, March 2023.

Calcul de Dg^T

On a

$$\left\langle Dg^T(\Omega)\mu, \phi \right\rangle_V = \mu^T Dg(\Omega)\phi \qquad \forall(\mu, \phi) \in \mathbb{R} \times V.$$

Or, en notant $e = e_1 = 1$ la base canonique de $\mathbb{R}$, on obtient

$$Dg^T(\Omega)\mu = \sum_{i=1}^{p} \mu_i Dg^T(\Omega)(e_i) = \mu_1 Dg^T(\Omega)(e_1).$$

De plus, on prenant $\mu = e_1$, on a pour tout ϕ dans V

$$\begin{aligned} \left\langle Dg^T(\Omega)e_1, \phi \right\rangle_V &= e_1 Dg(\Omega)\phi = Dg(\Omega)\phi \\ &= \int_\Omega \gamma^2 \nabla \left(Dg^T(\Omega)(e_1) \right) : \nabla\phi + Dg^T(\Omega)(e_1) \cdot \phi = \int_{\Gamma_S} \phi \cdot n. \end{aligned}$$

Résolution

On souhaite résoudre

$$\int_\Omega \gamma^2 \nabla U : \nabla \phi + U \cdot \phi = \int_{\Gamma_S} \phi \cdot n,$$

pour tout ϕ dans V avec $U = Dg^T(\Omega)(e_1)$. En appliquant une intégration par partie, on a

$$\int_\Omega \left(-\gamma^2 \Delta U + U\right) \cdot \phi = \int_{\Gamma_S} \left(I - \gamma^2 \nabla U\right) n \cdot \phi - \int_{\Gamma_B} \gamma^2 \nabla U n \cdot \phi.$$

En prenant $\nabla U n = I \frac{n}{\gamma^2}$ sur Γ_S et $\nabla U n = 0$ sur Γ_B, on se ramène donc à résoudre le problème suivant

Formulation forte

$$\begin{cases} -\gamma^2 \Delta(Dg^T(\Omega)(e_1)) + Dg^T(\Omega)(e_1) = 0 & \text{dans } \Omega, \\ \frac{\partial Dg^T(\Omega)(e_1)}{\partial n} = \frac{1}{\gamma^2} n & \text{sur } \Gamma_S \\ \frac{\partial Dg^T(\Omega)(e_1)}{\partial n} = 0 & \text{sur } \Gamma_B \end{cases}$$

Calcul de ξ_C

Par linéarité de $Dg(\Omega)$ et $Dg^T(\Omega)$, on obtient les résultats suivants :

$$g(\Omega) = \int_\Omega dx - |\Omega_0| \in \mathbb{R},$$

$$Dg(\Omega)Dg^T(\Omega) : \mathbb{R} \to \mathbb{R},$$

$$(Dg(\Omega)Dg^T(\Omega))^{-1}g(\Omega) = \frac{g(\Omega)}{\int_{\partial\Omega} Dg^T(\Omega)(e_1)\cdot n}.$$

ξ_C dans le cas de Stokes

$$\xi_C(\Omega)(X) = \left(\frac{g(\Omega)}{\int_{\partial\Omega} Dg^T(\Omega)(e_1)\cdot n}\right) Dg^T(\Omega)\,(e_1)\,(X)$$

Calcul de $\xi_J(\Omega)$

Pareil que ξ_C mais avec $g(\Omega) = Dg(\Omega)(\nabla J(\Omega))$.

ξ_J

$$\xi_J(\Omega)(X) = \nabla J(\Omega)(X) - Dg^T(DgDg^T)^{-1}Dg\nabla J(\Omega)(X).$$

ξ_J dans le cas de Stokes

$$\xi_J(\Omega)(X) = \nabla J(\Omega)(X) - \frac{\left(\int_{\partial\Omega} \nabla J(\Omega) \cdot n\right) Dg^T(e_1)(X)}{\int_\Omega Dg^T(\Omega)\,(e_1) \cdot n}.$$

Cantilever

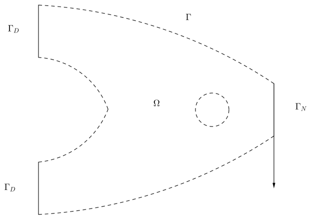

Figure 12: 2D representation of the elastic cantilever problem.

We want to solve the following problem

$$\inf_{\Omega \in \Omega_{ad}} \left\{ J(\Omega) = \int_{\Gamma_N} f \cdot u \right\}.$$

PDE of the cantilever problem

Let $u : \mathbb{R}^N \to \mathbb{R}^N$ the displacement solution of

$$\begin{cases} -\nabla \cdot \sigma = 0 & \text{in } \Omega \\ \sigma = 2\mu e(u) + \lambda tr(e(u))I & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \sigma n = f & \text{on } \Gamma_N \\ \sigma n = 0 & \text{on } \Gamma \end{cases}$$

with $\sigma(u) \in M_N(\mathbb{R})$, $\lambda, \mu > 0$ and $e(u) = \frac{1}{2}\left(\nabla u + \nabla u^T\right) \in M_N(\mathbb{R})$.

Results

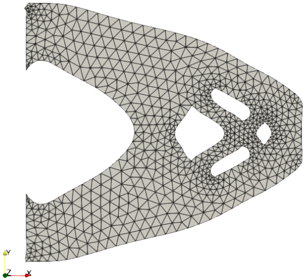

Figure 13: Optimum shape found for 2D cantilever with 4 holes.

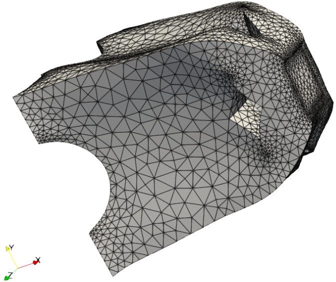

Figure 14: Optimum shape found for 3D cantilever with one hole.

Gaussian Process Formulation

- A Gaussian Process is fully specified by its mean function $\mu(x)$ and covariance function (kernel) $K(x, x')$.
- Given observations $D_n = (X_n, Y_n)$, where X_n is the input matrix and Y_n is the target vector, we have

$$F(x) \mid D_n \sim \mathcal{N}\left(\mu(x), \sigma^2(x)\right)$$

with

$$\begin{cases} \mu(x) = \Sigma\left(x, X_n\right) \Sigma_n^{-1} Y_n \, \sigma^2(x) \\ \sigma^2(x) = \Sigma(x, x) - \Sigma\left(x, X_n\right) \Sigma_n^{-1} \Sigma\left(X_n, x\right) \end{cases}$$

where $\Sigma_n = \Sigma(X_n, X_n)$ and $\Sigma(x, x') = K(x, x') + \sigma_n^2 \mathrm{I}$.