UNCERTAINTIES IN SHAPE OPTIMIZATION: TWO DETERMINISTIC APPROACHES

Grégoire ALLAIRE
CMAP, Ecole Polytechnique

Joint work with Ch. Dapogny (LJK, Grenoble).

International workshop on calculus of variations and its applications,
On the occasion of Luisa Mascarenhas birthday,
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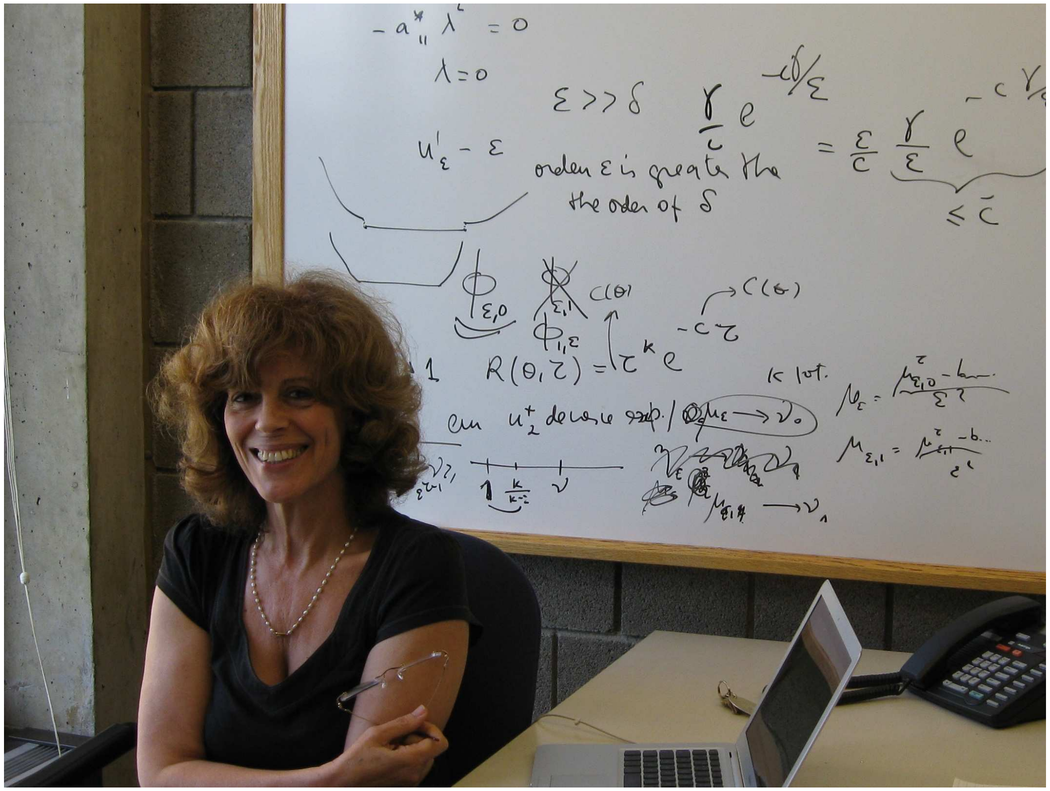
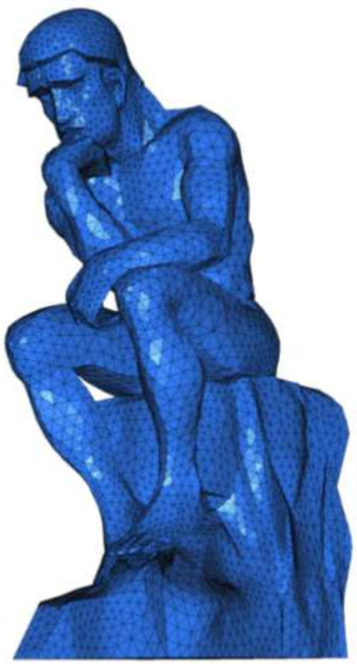


L. Mascarenhas, Γ-*limite d'une fonctionnelle liée à un phénomène de mémoire*, C. R. Acad. Sci. Paris. 313 (1991), pp. 67-70.

RODIN project



Ecole Polytechnique,

UPMC, INRIA,

Renault, Airbus,

Safran, ESI group, etc.

1. Introduction.
2. About uncertainties in optimal design.
3. Abstract setting for linearized worst-case design.
4. Applications in geometric optimization.
5. Abstract setting for a second-order averaged performance.
6. Applications in geometric optimization.

-I- INTRODUCTION

Shape optimization : minimize an objective function over a set of admissibles shapes Ω (including possible constraints)

$$\inf_{\Omega \in \mathcal{U}_{ad}} J(\Omega)$$

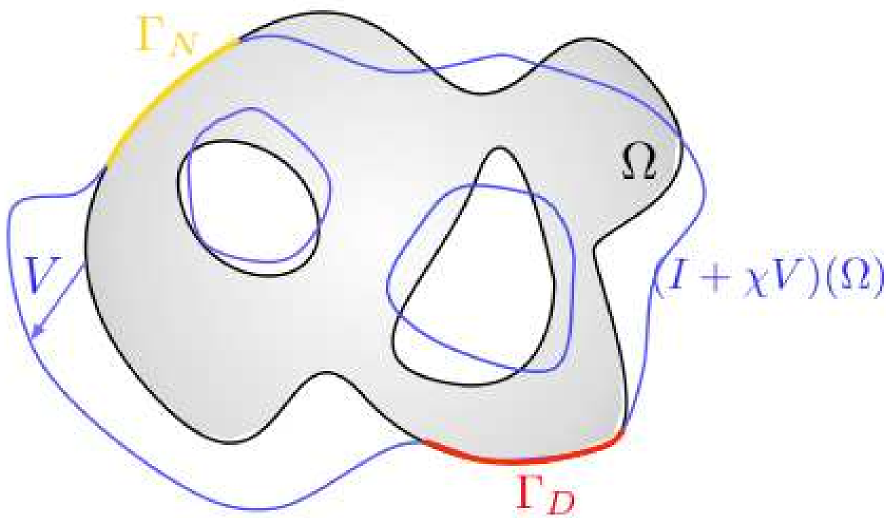
The objective function is evaluated through a partial differential equation (state equation)

$$J(\Omega) = \int_\Omega j(u_\Omega)\, dx$$

where u_Ω is the solution of

$$PDE(u_\Omega) = 0 \quad \text{in} \quad \Omega$$

Geometric optimization



Shape $\Omega \subset \mathbb{R}^d$ with boundary $\partial\Omega = \Gamma \cup \Gamma_N \cup \Gamma_D$, where Γ_D and Γ_N are fixed.
Only Γ is optimized (free boundary).

Linearized elasticity setting

For given applied loads $g : \Gamma_N \to \mathbb{R}^d$, $f : \Omega \to \mathbb{R}^d$, the displacement $u : \Omega \to \mathbb{R}^d$ is the solution of

$$\begin{cases} -\operatorname{div}(A\,e(u)) = f & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \big(A\,e(u)\big)n = g & \text{on } \Gamma_N \\ \big(A\,e(u)\big)n = 0 & \text{on } \Gamma \end{cases}$$

Typical objective function: the compliance

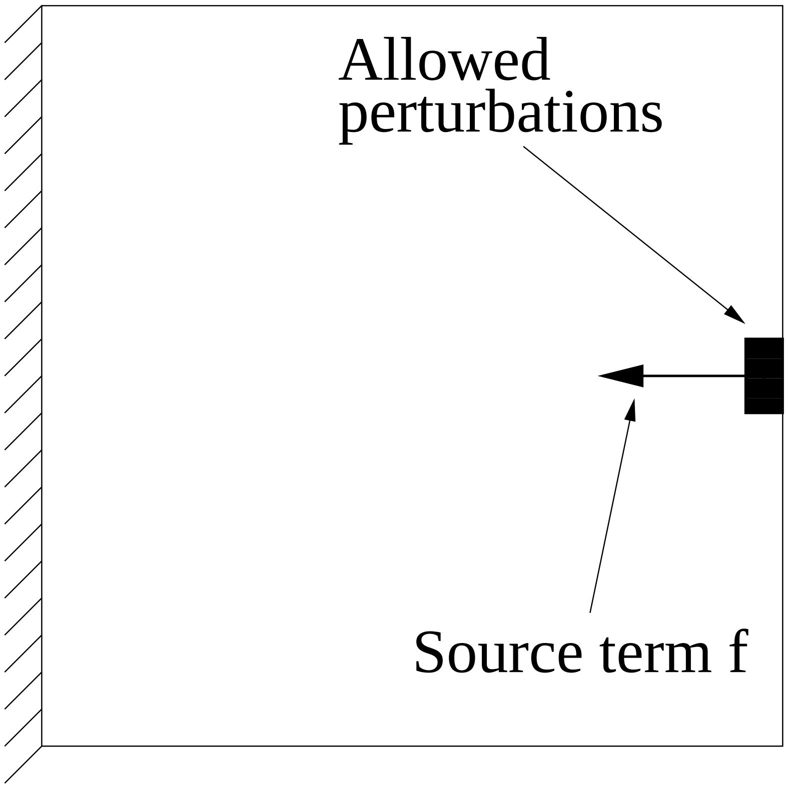
$$J(\Omega) = \int_\Omega f \cdot u\,dx + \int_{\Gamma_N} g \cdot u\,dx,$$

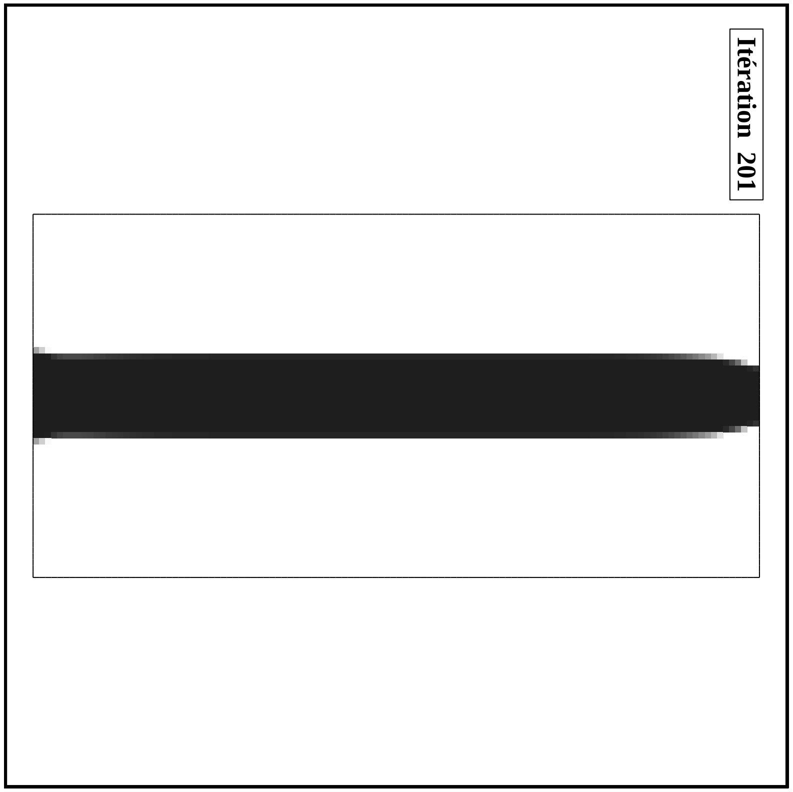
-II- ABOUT UNCERTAINTIES

- ☞ location, magnitude and orientation of the body forces or surface loads
- ☞ elastic material's properties
- ☞ geometry of the shape (thickness or boundary)

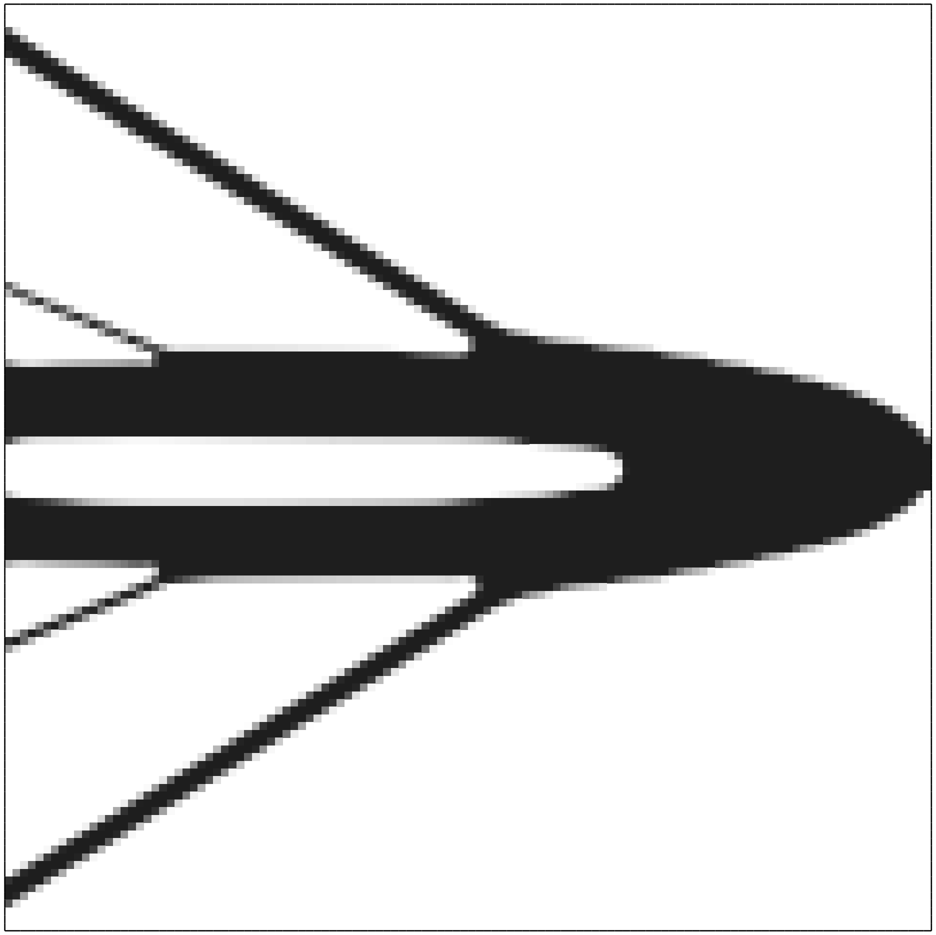
Crucial issue: optimal structures are so optimal for a given set of loads that they cannot sustain a different load !

Example: minimal weight and minimal compliance





Optimal design with load uncertainties



State of the art: many works !

☞ Probabilistic approach (Ben-Tal et al. 97, Choi et al. 2007, Frangopol-Maute 2003, Kalsi et al. 2001...)

- Monte-Carlo methods
- Polynomial chaos, Karhunen-Loève expansions...
- First-Order Reliability-based Methods (FORM)

☞ Various objectives or goals:

- Minimization of expected value or mean
- Worst case design
- Minimal failure probability

☞ Special cases with simplifications:

- Robust compliance: Cherkaev-Cherkaeva (1999, 2003), de Gournay-Allaire-Jouve (2008).
- Mean expectation of compliance: Alvarez-Carrasco 2005, Dunning-Kim 2013...

Present work: two approaches

☞ Linearized worst-case approach.

- worst case optimization (min-max problem),
- linearization for small uncertainties (similar idea for control in Nagy-Braatz 2004, for p.d.e. in Babuska-Nobile-Tempone 2005 and for optimization in Diehl-Bock-Kostina 2006).

☞ A second-order averaged approach.

- optimization of averaged performance (mean, variance, failure probability),
- second-order Taylor expansion for small uncertainties.

The goal is to obtain a computationally cheap deterministic setting.

Worst case design

Example in the case of force uncertainties.

The force is the sum $f + \xi$ where f is known and ξ is unknown.

The only information is the location of ξ and its maximal magnitude $m > 0$ such that $\|\xi\| \leq m$.

We replace the standard objective function $J(\Omega, f + \xi)$ by its worst case version $\mathcal{J}(\Omega, f)$.

Worst case design optimization problem:

$$\min_{\Omega} \mathcal{J}(\Omega, f) = \min_{\Omega} \max_{\|\xi\| \leq m} J(\Omega, f + \xi)$$

Averaged performance

Example in the case of force uncertainties.

The force is the sum $f(x) + \xi(x,\omega)$ where f is known and ξ is random.

We assume that ξ is small and finite-dimensional in the sense that

$$\xi(x,\omega) = \sum_{i=1}^{N} f_i(x)\xi_i(\omega)$$

where ξ_i are normalized, uncorrelated random variables:

$$\int_{\mathcal{O}} \xi_i(\omega)\mathbb{P}(d\omega) = 0, \quad \int_{\mathcal{O}} \xi_i(\omega)\xi_j(\omega)\,\mathbb{P}(d\omega) = \delta_{ij}.$$

We replace the standard objective function $J(\Omega, f + \xi)$ by its mean value.

Averaged performance optimization problem:

$$\min_{\Omega} \left\{ \mathcal{J}(\Omega, f) = \int_{\mathcal{O}} J(\Omega, f + \xi)\,\mathbb{P}(d\omega) \right\}$$

-III- ABSTRACT WORST-CASE SETTING

- ☞ Designs $h \in \mathcal{H}$
- ☞ State equation $\mathcal{A}(h)u(h) = b$ with a linear operator $\mathcal{A}(h)$
- ☞ Perturbations $\delta \in \mathcal{P}$ in a Banach space $\mathcal{P}$
- ☞ Assume for simplicity that only b (not $\mathcal{A}$) depends on δ
- ☞ Perturbed state equation $\mathcal{A}(h)u(h, \delta) = b(\delta)$
- ☞ Worst case objective function

$$\mathcal{J}(h) = \sup_{\substack{\delta \in \mathcal{P} \\ ||\delta||_{\mathcal{P}} \le m}} J(u(h, \delta))$$

- ☞ Goal

$$\inf_{h \in \mathcal{H}} \mathcal{J}(h)$$

Linearization

Assume that the perturbations are small, i.e., $m << 1$.

☞ Unperturbed case $\delta = 0$, $u(h) = u(h, 0)$

☞ Derivative of the state equation

$$\mathcal{A}(h) \frac{\partial u}{\partial \delta}(h, 0) = \frac{db}{d\delta}(0)$$

☞ Linearization of the worst-case objective function

$$\mathcal{J}(h) \approx \widetilde{\mathcal{J}}(h) = \sup_{\substack{\delta \in \mathcal{P} \\ ||\delta||_{\mathcal{P}} \leq m}} \left(J(u(h)) + \frac{dJ}{du}(u(h)) \frac{\partial u}{\partial \delta}(h, 0)(\delta) \right)$$

Since the right hand side is linear in δ we deduce

$$\widetilde{\mathcal{J}}(h) = J(u(h)) + m \left|\left| \frac{dJ}{du}(u(h)) \frac{\partial u}{\partial \delta}(h, 0) \right|\right|_{\mathcal{P}^*}$$

Adjoint approach

The previous formula for $\widetilde{\mathcal{J}}(h)$ is not fully explicit:

$$\widetilde{\mathcal{J}}(h) = J(u(h)) + m \left|\left| \frac{dJ}{du}(u(h)) \frac{\partial u}{\partial \delta}(h,0) \right|\right|_{\mathcal{P}^*}$$

Introduce an adjoint state

$$\mathcal{A}(h)^T p(h) = \frac{dJ}{du}(u(h)),$$

from which we deduce

$$\mathcal{A}(h)^T p(h) \cdot \frac{\partial u}{\partial \delta}(h,0) = \mathcal{A}(h) \frac{\partial u}{\partial \delta}(h,0) \cdot p(h) = \frac{dJ}{du}(u(h)) \cdot \frac{\partial u}{\partial \delta}(h,0) = \frac{db}{d\delta}(0) \cdot p(h)$$

Conclusion:

$$\widetilde{\mathcal{J}}(h) = J(u(h)) + m \left|\left| \frac{db}{d\delta}(0) \cdot p(h) \right|\right|_{\mathcal{P}^*}$$

Linearized worst-case design

We add to the usual objective function a perturbation term which is proportional to m and to the standard adjoint p:

$$\widetilde{\mathcal{J}}(h) = J(u(h)) + m \left|\left| \frac{db}{d\delta}(0) \cdot p(h) \right|\right|_{\mathcal{P}^*}$$

☞ Classical sensitivity approach can be applied to $\widetilde{\mathcal{J}}(h)$

☞ The appearance of the adjoint is not a surprise: it is known to measure the sensitivity of the optimal value with respect to the constraint level (or right hand side in the state equation).

☞ The entire argument needs to be made rigorous in each specific case.

☞ We don't say anything about the existence of optimal designs.

☞ We don't prove that optimal designs for $\widetilde{\mathcal{J}}(h)$ are close to those of $\mathcal{J}(h)$.

What remains to be done (in this talk)

Linearized worst-case design optimization:

$$\inf_{h\in\mathcal{H}} \left\{ \widetilde{\mathcal{J}}(h) = J(u(h)) + m \left\| \frac{db}{d\delta}(0) \cdot p(h) \right\|_{\mathcal{P}^*} \right\}$$

where

$$\mathcal{A}(h)u(h) = b(0) \quad \text{and} \quad \mathcal{A}(h)^T p(h) = \frac{dJ}{du}(u(h)),$$

☞ We compute a derivative of $\widetilde{\mathcal{J}}(h)$: it requires two additional adjoints !

☞ We build a gradient-based algorithm.

☞ We test it on various objective functions.

-IV- GEOMETRIC OPTIMIZATION

(Worst case design)

First case: loading uncertainties.

Given load $f \in L^2(\mathbb{R}^d)^d$. Unknown load $\xi \in L^2(\mathbb{R}^d)^d$ with small norm $\|\xi\|_{L^2(\mathbb{R}^d)^d} \leq m$. Solution $u_{\Omega,\xi}$ of

$$\begin{cases} -\operatorname{div}\left(A\, e(u_{\Omega,\xi})\right) = f + \xi & \text{in } \Omega \\ u_{\Omega,\xi} = 0 & \text{on } \Gamma_D \\ \big(A\, e(u_{\Omega,\xi})\big)n = g & \text{on } \Gamma_N \\ \big(A\, e(u_{\Omega,\xi})\big)n = 0 & \text{on } \Gamma \end{cases}$$

Many variants are possible (ξ may be localized, or parallel to a fixed vector, or on Γ_N, etc.)

Theorem.

$$\widetilde{\mathcal{J}}(\Omega) = \int_\Omega j(0, u_\Omega)\, dx + m||\nabla_f j(0, u_\Omega) - p_\Omega||_{L^2(\Omega)^d},$$

where p_Ω is the first adjoint state, defined by

$$\left\{ \begin{array}{rcll} -\text{div}(Ae(p_\Omega)) & = & -\nabla_u j(0, u_\Omega) & \text{in } \Omega, \\ p_\Omega & = & 0 & \text{on } \Gamma_D, \\ Ae(p_\Omega)n & = & 0 & \text{on } \Gamma \cup \Gamma_N. \end{array} \right.$$

If $\nabla_f j(0, u_\Omega) - p_\Omega \neq 0$ in $L^2(\Omega)^d$, then $\widetilde{\mathcal{J}}$ is shape differentiable

$$\begin{array}{rl} \widetilde{\mathcal{J}}'(\Omega)(\theta) = & \displaystyle\int_\Gamma \Big(j(0, u_\Omega) + Ae(u_\Omega) : e(p_\Omega) - p_\Omega \cdot f \Big) \theta \cdot n\, ds \\ + & \frac{m}{2||\nabla_f j(0,u_\Omega) - p_\Omega||_{L^2(\Omega)^d}} \displaystyle\int_\Gamma \theta \cdot n \Big(|\nabla_f j(0, u_\Omega) - p_\Omega|^2 - z_\Omega \cdot f \\ & + \nabla_u j(0, u_\Omega) \cdot q_\Omega + Ae(u_\Omega) : e(z_\Omega) + Ae(p_\Omega) : e(q_\Omega) \Big)\, ds, \end{array}$$

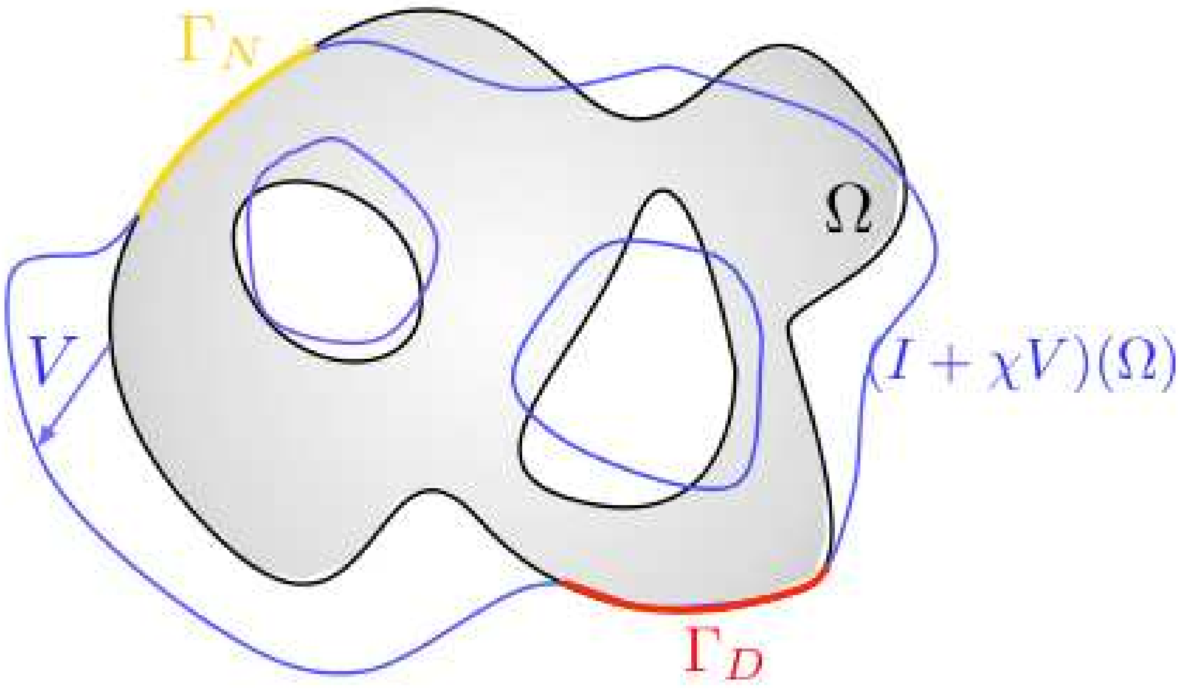
The second and third adjoint states q_Ω, z_Ω are defined by

$$\begin{cases} -\mathrm{div}(Ae(q_\Omega)) & = & -2\left(p_\Omega - \nabla_f j(0,u_\Omega)\right) & \text{in } \Omega, \\ q_\Omega & = & 0 & \text{on } \Gamma_D, \\ Ae(q_\Omega)n & = & 0 & \text{on } \Gamma_N, \end{cases}$$

$$\begin{cases} -\mathrm{div}(Ae(z_\Omega)) = & -\nabla_u^2 j(u_\Omega) q_\Omega - 2\nabla_f \nabla_u j(u_\Omega)^T (\nabla_f j(u_\Omega) - p_\Omega) & \text{in } \Omega, \\ z_\Omega = & 0 & \text{on } \Gamma_D, \\ Ae(z_\Omega)n = & 0 & \text{on } \Gamma_N. \end{cases}$$

Second case: geometric uncertainties.

Perturbed shapes $(I + \chi V)(\Omega)$, $\quad V \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$, $||V||_{L^\infty(\mathbb{R}^d)^d} \leq m$.



χ is a smooth localizing function such that $\chi \equiv 0$ on $\Gamma_D \cup \Gamma_N$.

Theorem.

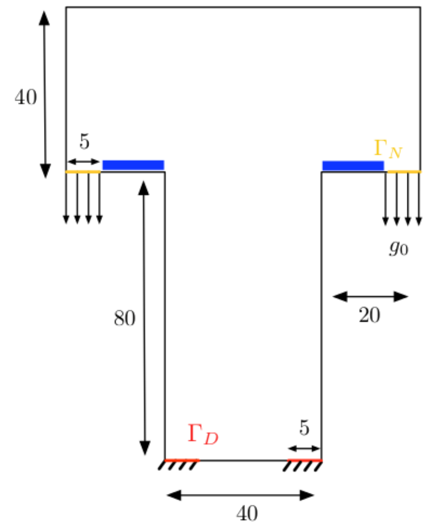
The linearized worst-case design objective function is

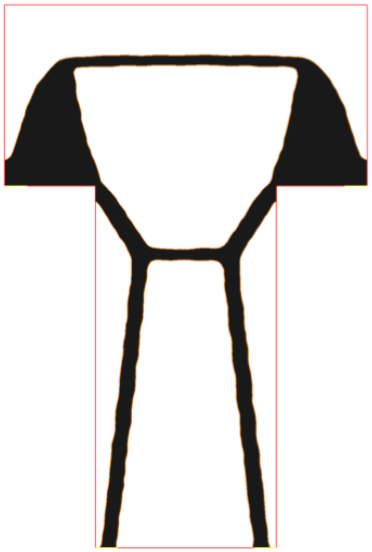
$$\widetilde{\mathcal{J}}(\Omega) = \int_\Omega j(u_\Omega)\, dx + m \int_\Gamma \chi \Big| j(u_\Omega) + Ae(u_\Omega) : e(p_\Omega) - f \cdot p_\Omega \Big|\, ds,$$

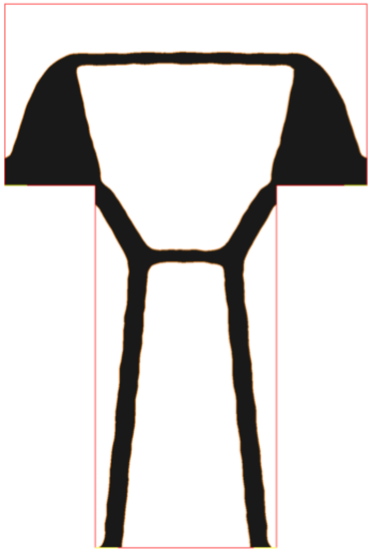
where p_Ω is the (previous) adjoint state.

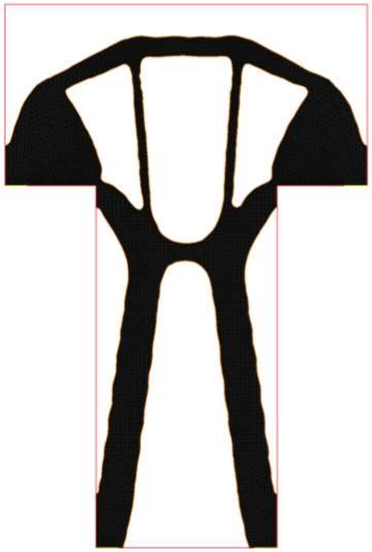
If $E_\Gamma := \{x \in \Gamma,\ \left(j(u_\Omega) + Ae(u_\Omega) : e(p_\Omega) - f \cdot p_\Omega\right)(x) = 0\}$ has zero Lebesgue measure, then it admits a (hugly) shape derivative $\widetilde{\mathcal{J}}'(\Omega)(\theta)$ involving two (new) additional adjoints q_Ω, z_Ω.

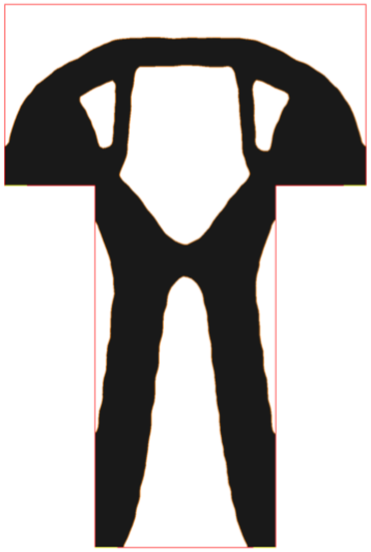
Load uncertainties in geometric optimization (compliance)



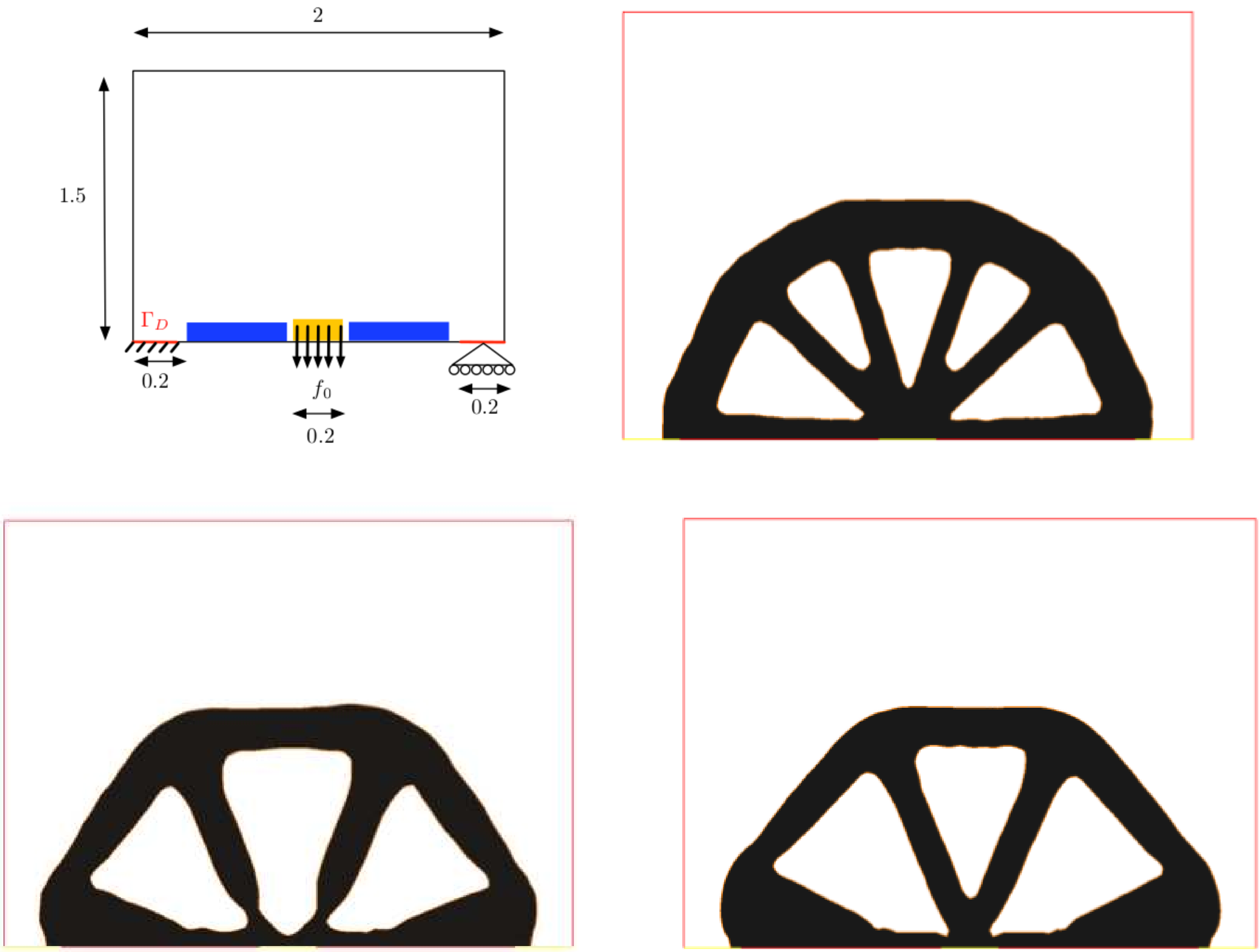




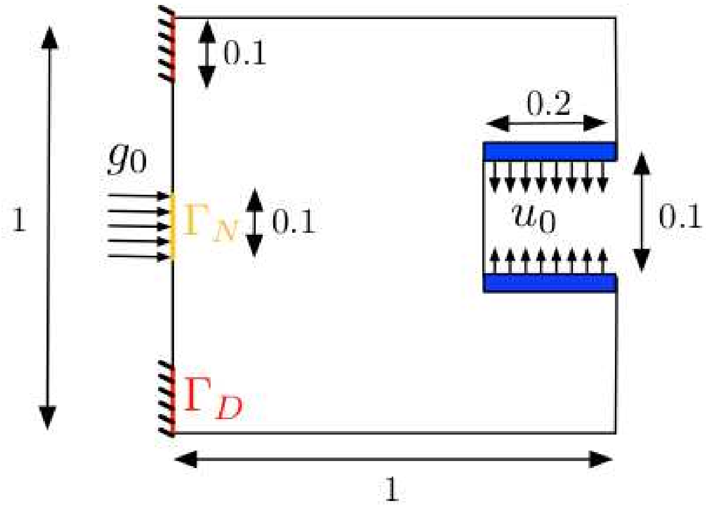


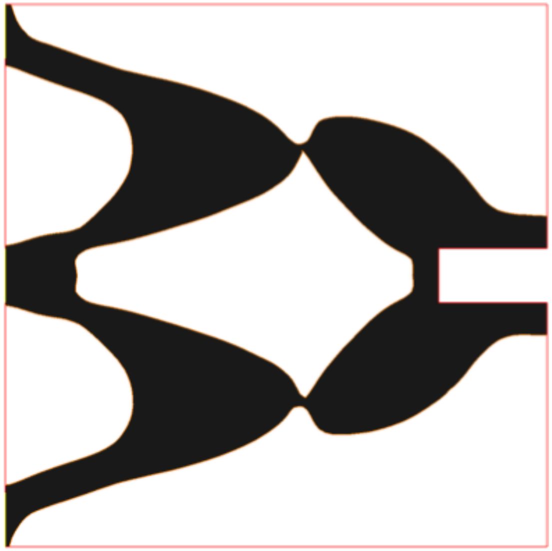


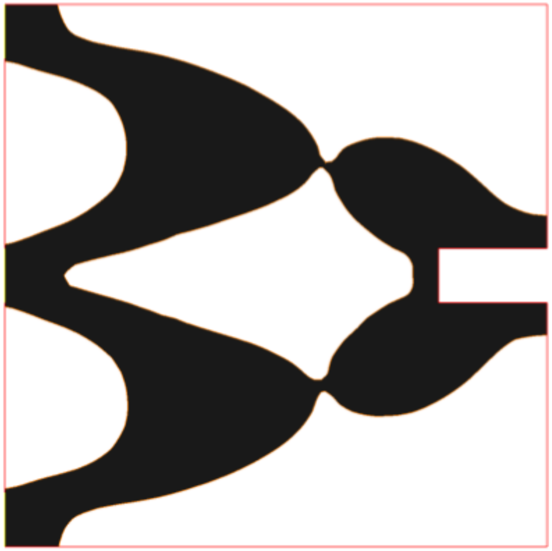
Load uncertainties in geometric optimization (compliance)

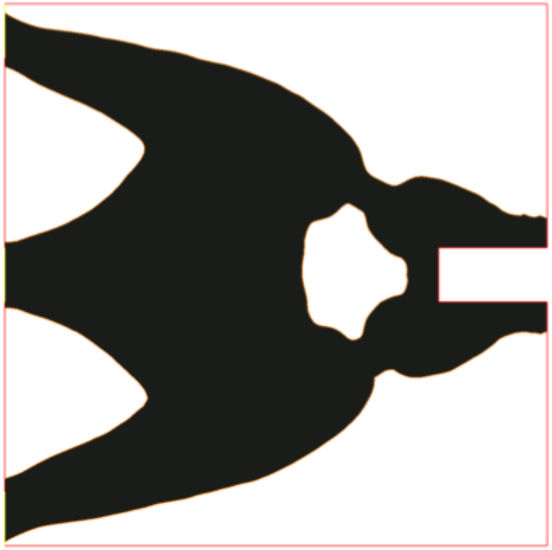


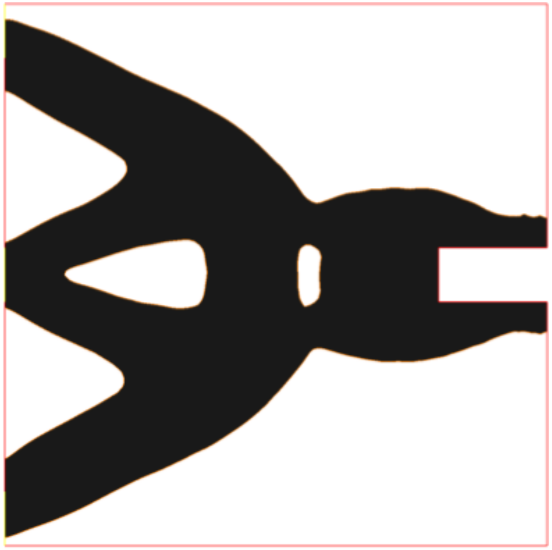
Geometric uncertainties in geometric optimization



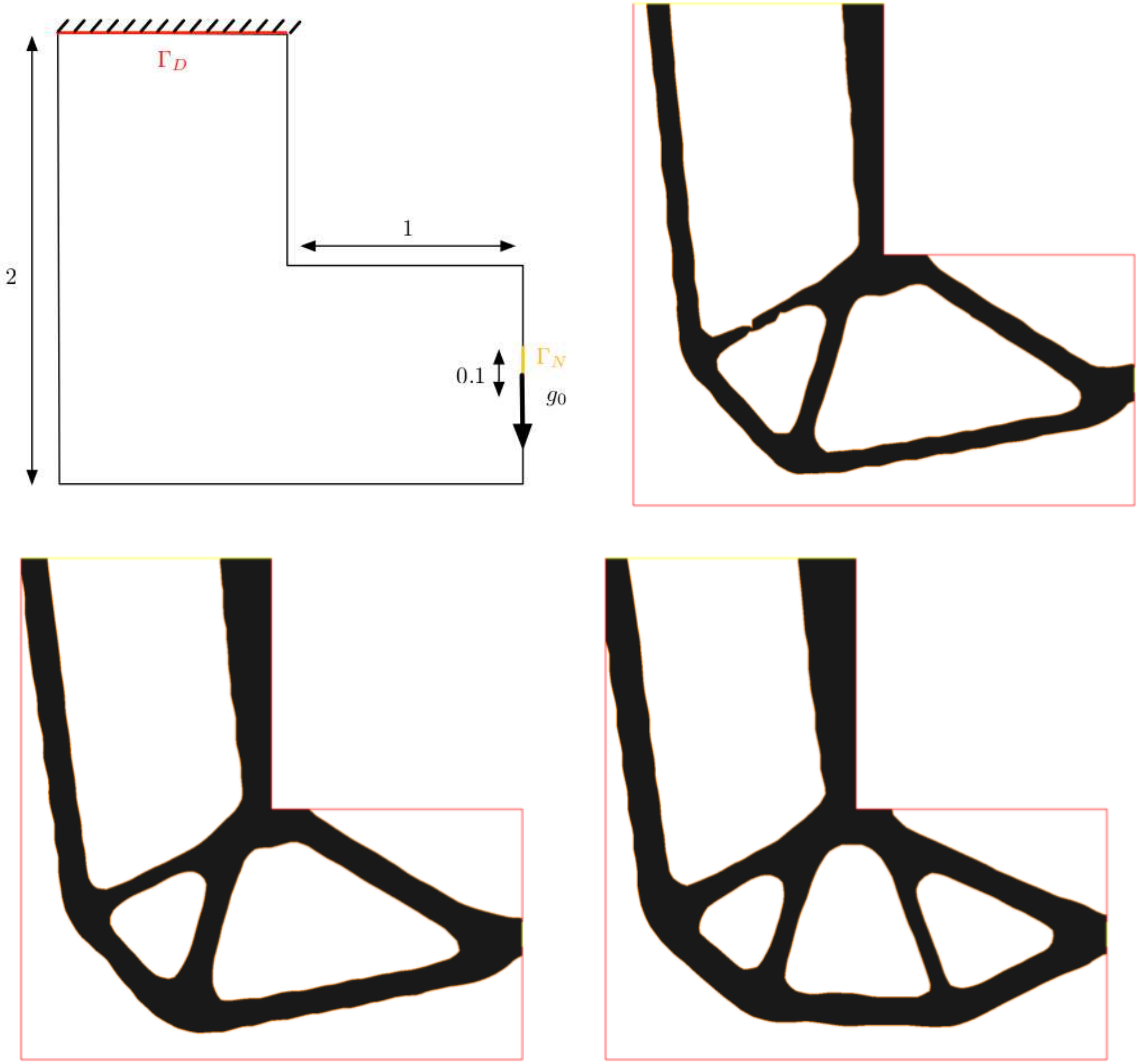








Geometric uncertainties (stress minimization)



-V- A SECOND-ORDER AVERAGED OPTIMIZATION

- One limitation of the linearization process: the worst perturbation is always symmetric.
- Worst-case design is pessimistic.
- Another approach: optimization of the mean and/or variance of an objective function under a random distribution of uncertainties.
  - Assumption of small uncertainties: second-order Taylor expansion.
  - Only the mean and variance of the random distribution are required.
  - Higher CPU cost (proportional to the number of uncorrelated random variables).

Abstract framework

- The performance of a design h is evaluated by a cost $\mathcal{C} \equiv \mathcal{C}(f, u_{h,f})$,
- which involves a state $u_{h,f}$, solution to a physical system:

$$\mathcal{A}(h)u_{h,f} = b(f),$$

- where, for simplicity, the uncertain data f acts on the right-hand side

$$f(x,\omega) = f_0(x) + \widehat{f}(x,\omega)$$

where f_0 is known and $\widehat{f}$ is random.

- We replace the standard cost function $\mathcal{C}(f, u_{h,f})$ by its mean value: the averaged performance optimization problem:

$$\mathcal{M}(h) = \int_{\mathcal{O}} \mathcal{C}(f_0 + \widehat{f}(\omega), u_{h,f_0+\widehat{f}(\omega)})\, \mathbb{P}(d\omega)$$

Working hypotheses

- Perturbations are small: depending on the context, this may mean:
  - $\widehat{f} \in L^\infty(\mathcal{O}, \mathcal{P})$: all the realizations $\widehat{f}(\omega) \in \mathcal{P}$ are small.
  - $\widehat{f} \in L^p(\mathcal{O}, \mathcal{P})$, for $p < \infty$: $\widehat{f}$ may have unprobably large realizations.
- Perturbations are finite-dimensional:

$$\boxed{\widehat{f}(x, \omega) = \sum_{i=1}^{N} f_i(x) \xi_i(\omega),}$$

where $f_i \in \mathcal{P}$, and the ξ_i are normalized, uncorrelated random variables:

$$\int_{\mathcal{O}} \xi_i(\omega) \mathbb{P}(d\omega) = 0, \quad \int_{\mathcal{O}} \xi_i(\omega) \xi_j(\omega) \, \mathbb{P}(d\omega) = \delta_{i,j}.$$

Example: $\widehat{f}$ is obtained as a truncated Karhunen-Loève expansion.

Strategy

- Calculate approximate functionals $\widetilde{\mathcal{M}}(h)$ which are
  - deterministic: no random variable or probabilistic integral is involved.
  - consistent with their exact counterparts, i.e. the differences $|\mathcal{M}(h) - \widetilde{\mathcal{M}}(h)|$ are 'small'.
- Calculate their derivatives $\widetilde{\mathcal{M}}'(h)(\widehat{h})$,
- Minimize the approximate functionals $\widetilde{\mathcal{M}}(h)$ (under constraints), by using gradient algorithms.

2nd order Taylor expansion

Use the smallness of perturbations to perform a second-order Taylor expansion of the mappings $f \mapsto u_{h,f}$ and $f \mapsto \mathcal{C}(f, u_{h,f})$ around f_0:

$$\boxed{u_{h,f_0+\widehat{f}} \approx u_h + u_h^1(\widehat{f}) + \frac{1}{2} u_h^2(\widehat{f},\widehat{f}),}$$

$$\text{where} \quad \mathcal{A}(h) u_h^1(\widehat{f}) = \frac{\partial b}{\partial f}(f_0)(\widehat{f}), \text{ and } \mathcal{A}(h) u_h^2(\widehat{f},\widehat{f}) = \frac{\partial^2 b}{\partial f^2}(f_0)(\widehat{f},\widehat{f}).$$

$$\boxed{\mathcal{C}(f_0+\widehat{f}, u_{h,f_0+\widehat{f}}) \approx \mathcal{C}(f_0, u_h) + \mathcal{L}_h(\widehat{f}) + \frac{1}{2}\mathcal{B}_h(\widehat{f},\widehat{f}),}$$

where the linear and bilinear forms $\mathcal{L}_h$ and $\mathcal{B}_h$ read:

$$\mathcal{L}_h(\widehat{f}) = \frac{\partial \mathcal{C}}{\partial f}(f_0, u_h)(\widehat{f}) + \frac{\partial \mathcal{C}}{\partial u}(f_0, u_h)(u_h^1(\widehat{f})),$$

$$\mathcal{B}_h(\widehat{f},\widehat{f}) = \frac{\partial^2 \mathcal{C}}{\partial f^2}(f_0, u_h)(\widehat{f},\widehat{f}) + 2\frac{\partial^2 \mathcal{C}}{\partial f \partial u}(f_0, u_h)(\widehat{f}, u_h^1(\widehat{f}))$$
$$+ \frac{\partial^2 \mathcal{C}}{\partial u^2}(f_0, u_h)(u_h^1(\widehat{f}), u_h^1(\widehat{f})) + \frac{\partial \mathcal{C}}{\partial u}(f_0, u_h)(u_h^2(\widehat{f},\widehat{f})).$$

Approximation of moment functionals

- Replacing the cost with its second-order expansion gives rise to the approximate mean-value functional:

$$\widetilde{\mathcal{M}}(h) = \mathcal{C}(f_0, u_h) + \int_{\mathcal{O}} \mathcal{L}_h(\widehat{f}(\omega))\, \mathbb{P}(d\omega) + \frac{1}{2}\int_{\mathcal{O}} \mathcal{B}_h(\widehat{f}(\omega), \widehat{f}(\omega))\, \mathbb{P}(d\omega).$$

- Using the structure of perturbations $\widehat{f}(\omega) = \sum_{i=1}^{N} f_i \xi_i(\omega)$, it comes:

$$\boxed{\widetilde{\mathcal{M}}(h) = \mathcal{C}(f_0, u_h) + \tfrac{1}{2}\textstyle\sum_{i=1}^{N} \mathcal{B}_h(f_i, f_i),}$$

a formula which involves the calculation of the $N+2$ 'reduced states':

$$u_h,\ \ u_{h,i} := u_h^1(f_i),\ (i = 1, ..., N),\ \text{and}\ u_h^2 := \sum_{i=1}^{N} u_h^2(f_i, f_i).$$

- This approach can be applied to other moments of $\mathcal{C}$, e.g. its variance:

$$\mathcal{V}(h) = \int_{\mathcal{O}} \Big(\mathcal{C}(f_0 + \widehat{f}(\omega), u_{h, f_0 + \widehat{f}(\omega)}) - \mathcal{M}(h)\Big)^2\, \mathbb{P}(d\omega).$$

What remains to be done (in this talk)

2nd-order averaged optimization:

$$\inf_{h\in\mathcal{H}} \left\{ \widetilde{\mathcal{M}}(h) = \mathcal{C}(f_0, u_h) + \frac{1}{2}\sum_{i=1}^{N} \mathcal{B}_h(f_i, f_i) \right\}$$

☞ Similar (in CPU cost) to a $(N+2)$-multiple loads optimization.

☞ Prove that $\widetilde{\mathcal{M}}(h)$ is closed to $\mathcal{M}(h)$.

☞ Compute a derivative of $\widetilde{\mathcal{M}}(h)$: it requires $(N+2)$ adjoints.

☞ Build a gradient-based algorithm.

☞ Test it on various objective functions.

-VI- GEOMETRIC OPTIMIZATION

☞ Random loads.

☞ Uncertainties in the material properties.

☞ Geometric uncertainties.