Taking uncertainties into account in numerical shape optimization.

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joint works with Charles Dapogny (Grenoble), Helmut Harbrecht, Michael Peters (Basel) and Bénédicte Puig (Pau)

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Why should we consider uncertainties in shape optimization ?

- Mechanical systems rely on data, e.g. the loads, the properties of a constituent material, or the geometry of the system itself.

- In concrete situations, such data are plagued with uncertainties because:

    - they may be available only through (error-prone) measurements,
    - they may be altered with time (wear) and conditions of the ambient medium.

- The performances of structures are very sensitive to small perturbations of data.

Need to somehow anticipate uncertainties when designing and optimizing shape

Modelisation choice : uncertainties are seen as a random process.

$\rightsquigarrow$ we face a familly of shape functionals $(J(\omega, D))_{\omega \in \Omega}$ for domains D in an admissible class $\mathcal{A}$.

How to take these uncertainties into account in a viable numerical optimization strategy ?

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A priori two strategies can be explored in order to compute such a shape:

1. *solve* each problem

$$D^*(\omega) = \operatorname{Argmin}_{D \in \mathcal{A}} J(\omega, D)$$

   and take the *expectation* of D^*

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$$\mathbb{J}_\sigma(D) = \mathbb{E}\left[J(., D)\right] + \sigma \mathbb{V}ar\left[J(., D)\right]$$

   for $\sigma \geq 0$ and solve

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   difficulty: how to compute $\mathbb{J}_\sigma$ and its shape gradient ?

Exploring the first strategy: the Vorob'ev expectation.

Theory of random sets, I. Molchanov, Springer serie Probability and its applications, 2005

- Taking expectation of parametrizations leads to non intrinsic notions of expectation of random sets
- A convenient notion: Vorobe'v expectation.
  - first introduce the *coverage function* p of a random set $D(.)$

$$\forall \mathsf{x} \in \mathbb{R}^d, \quad p(\mathsf{x}) = \mathbb{E}\left[x \in D(.)\right].$$

  - idea: The Vorob'ev expectation $\mathbb{E}_{\mathcal{V}}[D]$ of $D(\omega)$ is then defined as a quantile of $D(\omega)$ such that its volume is $\mathbb{E}[\mathcal{L}^d(D)]$.

Definition (Vorob'ev expectation)

The Vorob'ev expectation $\mathbb{E}_{\mathcal{V}}[D]$ of $D(\omega)$ is defined as the set $\{\mathsf{x} \in \mathbb{R}^2 : p(\mathsf{x}) \geq \mu\}$ for $\mu \in [0,1]$ which is determined from the condition

$$\mathcal{L}^d(\{\mathsf{x} \in \mathbb{R}^d : p(\mathsf{x}) \geq \lambda\}) \leq \mathbb{E}[\mathcal{L}^d(D)] \leq \mathcal{L}^d(\{\mathsf{x} \in \mathbb{R}^d : p(\mathsf{x}) \geq \mu\})$$

for all $\lambda > \mu$.

- Drawback: there is no set-valued notion of correlation but notions of scalar deviation like:

$$\mathcal{D}_{\mathcal{V}}[D] = \mathbb{E}\left[\mathcal{L}^d(D(.)\Delta\mathbb{E}_{\mathcal{V}}[D]\right] \text{ or } \mathcal{D}_{\mathcal{H}}[D] = \mathbb{E}\left[d_{\mathcal{H}}(D(.),\mathbb{E}_{\mathcal{V}}[D])\right]$$

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- Advantage: this is computable. The idea is to build an estimator for p with i.i.d. copies D_i of D for $1 \leq i \leq M$, by the empirical mean

$$p_M(x) = \frac{1}{M}\sum_{i=1}^{M} \mathbb{1}_{D_i}(x).$$

  P. Heinrich, R. S. Stoica, and V. C. Tran. Level sets estimation and Vorob'ev expectation of random compact sets. Spatial Statistics, 2(1):47–61, 2012.

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- Drawback : this is extremely costly, computing each D_i means *solving a shape optimization problem*

Illustration: exterior Bernoulli free boundary problem

Solution of a free boundary problem in presence of geometric uncertainties, M.D., H. Harbrecht, M.Peters and B. Puig, in redaction

We consider the free boundary problem

$$\begin{cases} \Delta u = 0 & \text{in } D, \\ \|\nabla u\| = f & \text{on } \Gamma, \\ u = 0 & \text{on } \Gamma, \\ u = 1 & \text{on } \Sigma, \end{cases}$$

in the case that the interior boundary is uncertain, i.e., if $\Sigma = \Sigma(\omega)$ with an additional parameter $\omega \in \Omega$.

First example: the setting

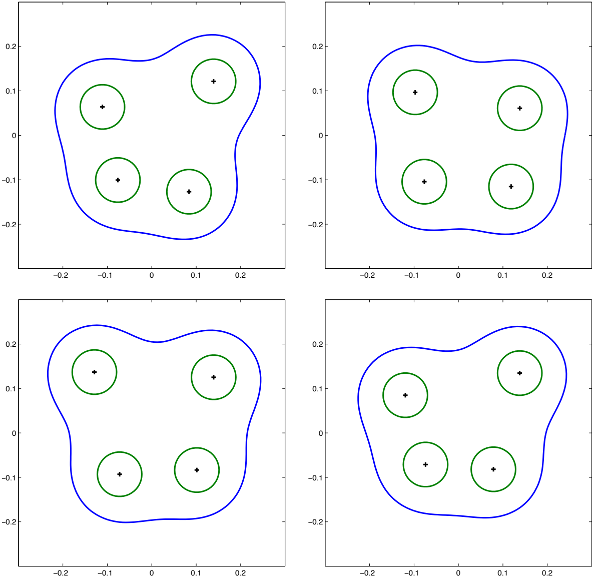
The inner boundary is the union of four circles of radius 0.05 and random centers

$$C_{i,j}(\omega) = \left(\frac{(-1)^i}{10} + 0.04 X_{2(2i+j)}(\omega), \frac{(-1)^i}{10} + 0.04 X_{2(2i+j)+1}(\omega) \right) \text{ for } i,j = 0,1.$$

The random variables $X_1, \ldots, X_8$ are independants, uniform on $[-1, 1]$

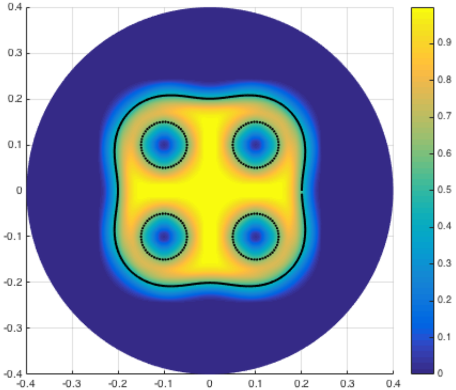
First example: some realisations

Simulations by Michael PETERS



First example: the coverage function and the Vorob'ev expectation

10^6 computations of a free boundary problem: around ten days of computation on a big laptop



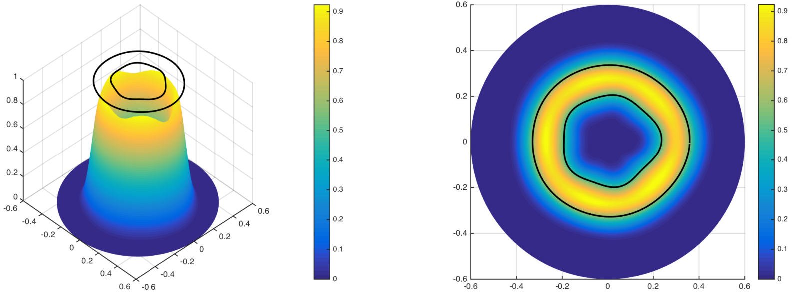
The inner boundary is the curve parametrized in polar coordinates by

$$r(\theta,\omega) = 0.2 + 0.01 f(\theta) + \sum_{k=1}^{10} \frac{\sqrt{2}}{k} \left[X_{2k-1} \cos k\theta + X_{2k} \sin k\theta\right]$$

- the random variables $X_1, \ldots, X_8$ are independants, uniform on $[-1, 1]$
- f is the trigonometric polynomial of coefficients

  $$[a_5, \ldots, a_0, b_1, \ldots, b_4] = [0.33, 0.26, 0.51, 0.70, 0.89, 0.48, 0.55, 0.14, 0.15, 0.26]$$

Second example: the coverage function and the Vorob'ev expectation



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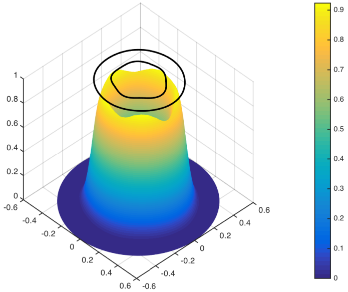

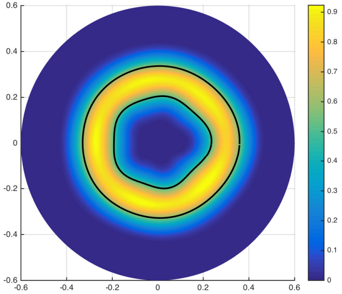

the problem is extremely stable $\rightsquigarrow$ it will be interesting to perform similar simulation for a less stable problem but computational cost increases

Exploring the second strategy: using an averaged objective.

Our objective: derive a deterministic expression for $\mathbb{J}$ and its shape gradient to avoid Monte-Carlo method to obtain reasonable computational times

there is one significant case where we know how to do that.

Shape optimization for quadratic functionals and states with random right-hand sides M.D, C. Dapogny and H. Harbrecht. SIAM Control and Optimization 53 (2015), no. 5, 3081–3103

A non trivial case.

- Consider an linear elliptic state equation with random right-hand side. For example, the equations of linear elasticity with random forcing

$$\begin{cases} -\mathrm{div}(Ae(u)) = 0 & \text{in } D, \\ u = 0 & \text{on } \Gamma_D, \\ Ae(u)n = g & \text{on } \Gamma_N, \\ Ae(u)n = 0 & \text{on } \Gamma, \end{cases}$$

where $e(u) = (\nabla u + \nabla u^T)/2$ and with Hooke's law A given by

$$\forall e \in \mathcal{S}(\mathbb{R}^d), \ \ Ae = 2\mu e + \lambda \, \mathrm{Tr} e \, I.$$

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- Consider a quadratic functional in the state: for example *compliance* of shapes

$$\mathcal{C}(D, \omega) = \int_D Ae(u_D)(x, \omega) : e(u_D)(x, \omega)\, dx = \int_D g(x, \omega) \cdot u_D(x, \omega)\, ds(x),$$

The idea in finite dimension: the setting.

- Consider a finite dimensional space $\mathcal{H}$ of designs h. The cost function is

$$C(h,\omega) =< Bu(h,\omega), u(h,\omega) >$$

where the state $u(h,\omega)$ is defined as the solution of the linear system with random right-hand side

$$A(h)u(h,\omega) = f(\omega)$$

- The averaged objective is

$$\mathcal{M}(h) = \mathbb{E}[C(h,.)] = \int_\Omega \mathcal{C}(h,\omega)\mathbb{P}(d\omega)$$

The idea in finite dimension: doubling the variables to transform quadratic quantities in linear ones.

Sparse finite elements for elliptic problems with stochastic loading, Numerische Mathematik, C. Schwab, R.Todor, 95/4 (2003), pp. 707-734

- Rewrite cost function as

$$C(h,\omega) =< Bu(h,\omega), u(h,\omega) >= \mathcal{B} : (u(h,\omega) \otimes u(h,\omega))$$

$v \otimes w$ of two vectors $v, w \in \mathbb{R}^N$ is the $(N \times N)$-matrix with entries $(v \otimes w)_{i,j} = v_i w_j$, $i, j = 1, \ldots, N$,

: stands for the Frobenius inner product over matrices.

- The averaged objective becomes

$$\mathcal{M}(h) = \mathbb{E}[C(h,.)] = \int_\Omega \mathcal{C}(h,\omega)\mathbb{P}(d\omega) = \mathcal{B} : \mathrm{Cov}(u,u)(h)$$

$\mathsf{Cov}(u,v)(h)$ is the *covariance matrix* (of size N^2) of $u(h,\omega)$, whose entries read

$$\mathsf{Cov}(u,v)(h)_{i,j} = \int_\Omega u_i(h,\omega)v_j(h,\omega)\,\mathbb{P}(d\omega), \quad i,j = 1,\ldots,N.$$

Notation: $\mathsf{Cov}(u) = \mathsf{Cov}(u,u)$

- $\mathrm{Cov}(u)(h)$ can be directly computed: it solves the (N^2)-dimensional system
$$(\mathcal{A}(h) \otimes \mathcal{A}(h))\,\mathrm{Cov}(u)(h) = \mathrm{Cov}(f).$$
- we can derive with respect to h in the direction $\widehat{h}$:
$$\mathcal{M}'(h)(\widehat{h}) = \left(\mathcal{A}'(h)(\widehat{h}) \otimes I\right)\mathrm{Cov}(u,p)(h).$$
where $\mathrm{Cov}(u,p)(h)$ solves
$$\left(\mathcal{A}(h) \otimes \mathcal{A}(h)^T\right)\mathrm{Cov}(u,p)(h) = -\,(\mathcal{A}(h) \otimes \mathcal{B})\,\mathrm{Cov}(u)(h).$$

Conclusion

Both, the objective function $\mathcal{M}(h)$ and its gradient, can be exactly calculated from the sole datum of the covariance matrix of f (and not of its law!).

Going back to the compliance case

Following the previous idea, $\mathcal{M}(D)$ can be rewritten

$$\mathcal{M}(D) = \int_D ((Ae_x : e_y)\mathrm{Cov}(u))(x,x)\,dx,$$

$(Ae_x : e_y) : [H^1_{\Gamma_D}(D)]^d \otimes [H^1_{\Gamma_D}(D)]^d \to L^2(D) \otimes L^2(D)$ is the linear operator induced from the bilinear mapping

$$(u,v) \mapsto Ae(u) : e(v).$$

its derivative reads

$$\forall \theta \in \Theta_{ad},\ \ \mathcal{M}'(D)(\theta) = -\int_\Gamma ((Ae_x : e_y)\mathrm{Cov}(u))(x,x)(\theta \cdot n)(x)\,ds(x).$$

It remains to compute $\mathrm{Cov}(u)$

$\mathrm{Cov}(u) \in [H^1_{\Gamma_D}(D)]^d \otimes [H^1_{\Gamma_D}(D)]^d$ is the unique solution to the following boundary value problem:

$$(\mathrm{div}_x \otimes \mathrm{div}_y)(Ae_x \otimes Ae_y)\,\mathrm{Cov}(u) = 0 \text{ in } D \times D,$$

with boundary conditions

$$\begin{cases} \mathrm{Cov}(u) = 0 & \text{on } \Gamma_D \times \Gamma_D, \\ (\mathrm{div}_x \otimes I_y)(Ae_x \otimes I_y)\,\mathrm{Cov}(u) = 0 & \text{on } D \times \Gamma_D, \\ (I_x \otimes \mathrm{div}_y)(I_x \otimes Ae_y)\,\mathrm{Cov}(u) = 0 & \text{on } \Gamma_D \times D, \\ (Ae_x \otimes Ae_y)\,\mathrm{Cov}(u)(n_x \otimes n_y) = \mathrm{Cov}(g) & \text{on } \Gamma_N \times \Gamma_N, \\ (\mathrm{div}_x \otimes I_y)(Ae_x \otimes Ae_y)\,\mathrm{Cov}(u)(I_x \otimes n_y) = 0 & \text{on } D \times (\Gamma_N \cup \Gamma), \\ (I_x \otimes \mathrm{div}_y)(Ae_x \otimes Ae_y)\,\mathrm{Cov}(u)(n_x \otimes I_y) = 0 & \text{on } (\Gamma_N \cup \Gamma_N) \times D, \\ (Ae_x \otimes Ae_y)\,\mathrm{Cov}(u)(n_x \otimes n_y) = 0 & \text{on } \big((\Gamma_N \cup \Gamma) \times (\Gamma_N \cup \Gamma)\big) \setminus (\Gamma_N \times \Gamma_N), \\ (Ae_x \otimes I_y)\,\mathrm{Cov}(u)(n_x \otimes I_y) = 0 & \text{on } (\Gamma_N \times \Gamma) \times \Gamma_D, \\ (I_x \otimes Ae_y)\,\mathrm{Cov}(u)(I_x \otimes n_y) = 0 & \text{on } \Gamma_D \times (\Gamma_N \times \Gamma). \end{cases}$$

Computing $\mathrm{Cov}(u)(h)$*: low-rank approximation of* $\mathrm{Cov}(f)$*.*

The idea in finite dimension

If

$$\mathrm{Cov}(f) \approx \sum_{i=1}^{m} f_i \otimes f_i,$$

Then,

$$\mathrm{Cov}(u)(h) \approx \sum_{i=1}^{m} u_i(h) \otimes u_i(h), \text{ and } \mathrm{Cov}(u,p)(h) \approx \sum_{i=1}^{m} u_i(h) \otimes p_i(h)$$

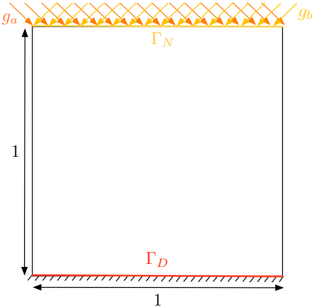
where $u_i(h)$ (resp. $p_i(h)$) solves

$$\mathcal{A}(h) u_i(h) = f_i \text{ resp. } \mathcal{A}(h)^T p_i(h) = -\mathcal{B}^T u_i(h).$$

Cost of the computation

Computing and its gradient cost m usual systems for the state and m for the adjoint.

Example: a robust bridge



The loadings are

$$g(x,\omega) = \xi_1(\omega) g_a(x) + \xi_2(\omega) g_b(x),$$

with

$g_a = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$, $g_b = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$,

ξ_1 and ξ_2 are centered of variance 1.

Our goal: minimize the averaged compliance under the volume constraint $Vol(D) = 0.35$ enforced owing to a standard Augmented Lagrangian procedure.

Simulations obtained by C. Dapogny - each 12 min on a MacBook air

Set $\alpha := \int_\Omega \xi_1 \xi_2 \, \mathbb{P}(d\omega)$ so that

$$\mathrm{Cor}(g) = g_a \otimes g_a + g_b \otimes g_b + \alpha \left(g_a \otimes g_b + g_b \otimes g_a \right).$$

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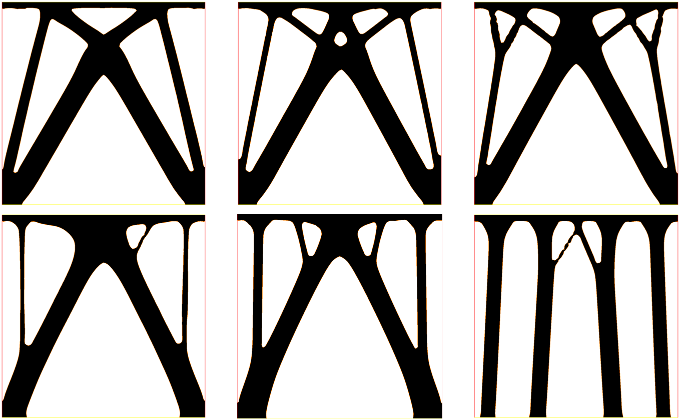

Optimal shapes obtained associated to degrees of correlation $\alpha = -1, -0.7, 0, 0.5, 0.8, 1$ (from left to right, top to bottom).