Computing quantities of interest on random domains

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60th anniversary of C. CONCA
Our motivations: about tolerances

Realistic geometries of mechanical devices differ from the nominal one but are close of it:
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Realistic geometries of mechanical devices differ from the nominal one but are close of it:
Tolerances: true geometries are graphs over the nominal boundary

The real domain boundary $\partial D_{true}$ can be defined thanks to a real valued random field $X$ over $\partial D_{nominal}$ according to

$$\partial D_{true} = \{ x + X(x)n(x); \ x \in \partial D_{nominal} \}$$

where $n(x)$ denotes the outer unit normal field at a point $x$ in $\partial D_{nominal}$. 
Tolerances: true geometries are graphs over the nominal boundary

The real domain boundary $\partial D_{true}$ can be defined thanks to a real valued random field $X$ over $\partial D_{nominal}$ according to

$$\partial D_{true} = \{x + \varepsilon X(x)\mathbf{n}(x); \; x \in \partial D_{nominal}\}$$

where $\mathbf{n}(x)$ denotes the outer unit normal field at a point $x$ in $\partial D_{nominal}$, where the small parameter $\varepsilon > 0$ models the tolerancy range.
Tolerancies: true geometries are graphs over the nominal boundary

The real domain boundary $\partial D_{true}$ can be defined thanks to a real valued random field $X$ over $\partial D_{nominal}$ according to

$$\partial D_{true}(\omega) = \{ x + \varepsilon X(x, \omega) n(x); x \in \partial D_{nominal} \}$$

where $n(x)$ denotes the outer unit normal field at a point $x$ in $\partial D_{nominal}$, where the small parameter $\varepsilon > 0$ models the tolerancy range.
Our objective

In order to take the question of uncertain geometrical definition into account in numerical simulations, we have to incorporate the randomness of the computational domain to the underlying model equations. Thus, the quantities of engineering interest are also random.

We address the following question: given a complete probabilistic description of the random perturbation of the nominal boundary, compute as much information as possible on the distribution of the quantity of interest.
An academic example to illustrate the question

- Random perturbations of the disk:
  \( \alpha_i \) are i.i.d. following the uniform distribution on \([-1/2, 1/2]\)
  \( f_i \) the Fourier modes

\[
D_\varepsilon(\omega) = \left\{ (r, \theta) : 0 \leq r < 1 + \varepsilon f(\theta, \omega) \text{ and } f(\theta) = \sum_{i=1}^{N} \alpha_i(\omega) f_i(\theta) \right\}
\]
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Consider the Dirichlet energy \( E(D) \) defined as

\[
E(D) = -\frac{1}{2} \int_{\partial D} |\nabla u_D|^2,
\]

where \( u_D \) is the solution of \(-\Delta u = 1 \) in \( H_0^1(D) \).
Monte-Carlo simulations: first moments of the output
Our contribution

Given a complete probabilistic description of the random perturbation of the nominal boundary, we obtain

1. **deterministic expressions** for the coefficients of the power (in the small parameter $\varepsilon$) expansion of the moments of the output distribution

2. a **efficient numerical method** to compute these coefficients
We use Murat-Simon shape calculus based on a parametrization based on
diffeomorphisms $T = Id + \theta$ with $\theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ and one
differentiate $\theta \mapsto J((Id + \theta)(\Omega))$ at $\theta = 0$. 
A purely deterministic tool: shape sensitivity analysis

We use Murat-Simon shape calculus based on a parametrization based on diffeomorphisms $T = Id + \theta$ with $\theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ and one differentiate $\theta \mapsto J((Id + \theta)(\Omega))$ at $\theta = 0$.

Shape derivative exist also at second order so that a second order Taylor formula holds for $\theta = I + X\mathbf{n}$

$$J(D(X)) = J(D_0) + L[J](D_0)X + \frac{1}{2}B[J](D_0)(X, X) + R_2(X),$$

where
- $L[J](D_0)$ is the shape gradient,
- $B[J](D_0)$ is the shape hessian,
- $R_2$ is (uniformly in $X$) negligible with respect to $\|X\|^2_{W^{1,\infty}}$. 
Structure of shape derivatives

Let $k \geq 1$ be an integer and $J$ a real valued shape function defined on the open bounded domains of $\mathbb{R}^d$ with a $C^k$ boundary. Let us define the function $\mathcal{J}$ on $C^{k,1}(\mathbb{R}^d, \mathbb{R}^d)$ by

$$\mathcal{J}(\theta) = J((I + \theta)(D)).$$

- **Shape gradient:** If $D \in \mathcal{O}_{k+1}$ and $\mathcal{J}$ is differentiable at $0$, then there exists a continuous linear form $L$ on $C^k(\partial D)$ such that:

  $$D\mathcal{J}(0)\xi = L(\xi \cdot n) \text{ for all } \xi \in C^{k,1}(\mathbb{R}^d, \mathbb{R}^d).$$
Structure of shape derivatives

Let \( k \geq 1 \) be an integer and \( J \) a real valued shape function defined \( \mathcal{O}_k \) the open bounded domains of \( \mathbb{R}^d \) with a \( C^k \) boundary. Let us define the function \( \mathcal{J} \) on \( C^{k,1}(\mathbb{R}^d, \mathbb{R}^d) \) by

\[
\mathcal{J}(\theta) = J((I + \theta)(D)).
\]

\textbf{Shape hessian:} If \( D \in \mathcal{O}_{k+2} \) and \( \mathcal{J} \) is twice differentiable at 0, then there exists a continuous symmetric bilinear form \( B \) on \( C^k(\partial D) \times C^k(\partial D) \) such that for all \( (\xi, \zeta) \in C^{k,1}(\mathbb{R}^d, \mathbb{R}^d)^2 \)

\[
D^2 \mathcal{J}(0)(\xi, \zeta) = B(\xi \cdot n, \zeta \cdot n) + L(Z),
\]

where

\[
Z = (D_\tau n \zeta_\tau) \cdot \xi_\tau - \nabla_\tau (\zeta \cdot n) \cdot \xi_\tau - \nabla_\tau (\xi \cdot n) \cdot \zeta_\tau.
\]
Example of shape derivatives

Consider the Dirichlet energy $E(D)$ defined as $E(D) = -\frac{1}{2} \int_{\partial D} |\nabla u_D|^2$, where $u_D$ is the solution of $-\Delta u = 1$ in $H^1_0(D)$. 
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where $u_D$ is the solution of $-\Delta u = 1$ in $H^1_0(D)$.

$$L[E](D).X = -\frac{1}{2} \int_{\partial D} (\partial_n u)^2 X;$$

$$B[E](D).(X, X) = \langle -\partial_n u X, \Lambda(-\partial_n u X) \rangle_{H^{1/2} \times H^{-1/2}}$$

$$+ \int_{\partial D} \left[ \partial_n u + \frac{1}{2} H(\partial_n u)^2 \right] X^2;$$

where $\Lambda : H^{1/2}(\partial D) \rightarrow H^{-1/2}(\partial D)$ is the Dirichlet-to-Neumann map for the domain $D$ defined as $\Lambda(X) = -\partial_n V(X)$ with $V(X)$ being the solution of

$$-\Delta V(X) = 0 \text{ in } D, \quad V(X) = X \text{ on } \partial D,$$
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$$L[E](D).X = -\frac{1}{2} \int_{\partial D} (\partial_n u)^2 X;$$

$$B[E](D).(X, X) = \int_D |\nabla V(-\partial_n u X)|^2$$

$$+ \int_{\partial D} \left[ \partial_n u + \frac{1}{2} H(\partial_n u)^2 \right] X^2;$$

with $V(X)$ being the solution of

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Example of shape derivatives

Consider the Dirichlet energy $E(D)$ defined as $E(D) = -\frac{1}{2} \int_{\partial D} |\nabla u_D|^2$, where $u_D$ is the solution of $-\Delta u = 1$ in $H^1_0(D)$.

On the unit ball, when one expand any function $X$ in $L^2(\partial B_1)$ as the Fourier series:

$$X(x) = \sum_{k=0}^{\infty} \sum_{l=1}^{d_k} \alpha_{k,l}(X) Y_{k,l}(x), \quad \text{for } |x| = 1.$$ 

one gets

$$B[E](B_1). (X, X) = \sum_{k=0}^{\infty} \sum_{l=1}^{d_k} \left[ \frac{1}{d^2} k^2 - \frac{d + 1}{2d^2} \right] \alpha_{k,l}(X)^2,$$
The idea

If the random process $X$ satisfies

**Uniform regularity**: $X \in L^2_p(\Omega, \mathcal{C}^{2,1}(\partial D_0))$.

**Uniform boundedness**: $\exists h_{\text{max}} > 0$, $\forall \omega \in \Omega$, $\|X(\omega, \cdot)\|_{\mathcal{C}^{2,1}} \leq h_{\text{max}}$
The idea

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then the second order Taylor formula

$$ J(D(\varepsilon X(\omega))) = J(D_0) + L[J](D_0) \varepsilon X(\omega) + \frac{1}{2} B[J](D_0)(\varepsilon X(\omega), \varepsilon X(\omega)) + o(\varepsilon^2), $$

holds over the probability space $\Omega$ and can be integrated over $\Omega$ then ...
The expectation and variance of $J(D(\omega))$ admit the asymptotic expansions

$$\mathbb{E}(J(D)) = J(D_0) + \mathbb{E}(L(X)) \, \varepsilon + \frac{1}{2} \mathbb{E}(B(X, X)) \, \varepsilon^2 + o(\varepsilon^2)$$

$$\text{var}(J(D)) = \mathbb{E} \left( [L(X) - \mathbb{E}(L(X))]^2 \right) \varepsilon^2$$

$$+ \mathbb{E} \left( [L(X) - \mathbb{E}(L(X))] [B(X, X) - \mathbb{E}(B(X, X))] \right) \varepsilon^3$$

$$+ o(\varepsilon^3).$$
For all $k \geq 2$, the centered normalized moment of $J(D(\omega))$ admits the asymptotic expansion

$$
M_k(J(D)) := \mathbb{E}\left( \frac{[J(D) - \mathbb{E}(J(D))]^k}{\sqrt{\text{var}(J(D))}} \right) = a_k + b_k \varepsilon + o(\varepsilon), \quad (1)
$$

where the deterministic coefficients $a_k$ and $b_k$ are

$$
a_k = \gamma_k \mathbb{E}\left( [L(X) - \mathbb{E}(L(X))]^k \right) \mathbb{E}\left( [L(X) - \mathbb{E}(L(X))]^2 \right),
$$

$$
b_k = \gamma_k \frac{k}{2} \left\{ \mathbb{E}\left( [L(X) - \mathbb{E}(L(X))]^{k-1} [B(X,X) - \mathbb{E}(B(X,X))] \right) \mathbb{E}\left( [L(X) - \mathbb{E}(L(X))]^2 \right) \right.
$$

$$
- \mathbb{E}\left( [L(X) - \mathbb{E}(L(X))] [B(X,X) - \mathbb{E}(B(X,X))] \right) \mathbb{E}\left( [L(X) - \mathbb{E}(L(X))]^k \right) \left\} ,
$$

and the normalization constant $\gamma_k$ is

$$
\gamma_k = \mathbb{E}\left( [L(X) - \mathbb{E}(L(X))]^2 \right)^{-1 - k/2}.
$$
The assumptions on the random field

We have to compute terms of the type

$$\mathbb{E}([L(X) - \mathbb{E}(L(X))]) \text{ or } \mathbb{E}([B(X, X) - \mathbb{E}(B(X, X))])$$

where $L$ is linear continuous and $B$ bilinear continuous.
The assumptions on the random field

Let us compute the leading coefficient in the expansion of the variance

\[
\mathbb{E} (L(X)^2) = \mathbb{E} \left[ \left( \int_{\partial D} \ell(x)X(x, \omega) d\sigma(x) \right)^2 \right]
\]

\[
= \mathbb{E} \left[ \int_{\partial D} \int_{\partial D} X(x, \omega)X(y, \omega)\ell(x)\ell(y) d\sigma(x) d\sigma(y) \right]
\]

\[
= \int_{\partial D} \int_{\partial D} \mathbb{E}[X(x, .)X(y, .)]\ell(x)\ell(y) d\sigma(x) d\sigma(y)
\]

\[
= \int_{\partial D} \int_{\partial D} \text{Cov}_X(x, y)\ell(x)\ell(y) d\sigma(x) d\sigma(y).
\]

**Hint:** One can think of the Karhunen-Loève decomposition of the process \( X \)
The assumptions on the random field

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where $L$ is linear continuous and $B$ bilinear continuous.

To obtain simple algebra, we take $X(x, \omega) = \sum_{i=1}^{\infty} \alpha_i(\omega)f_i(x)$

$\alpha_i$ are either uncorrelated or i.i.d. following the same centered distribution $\mathcal{L}$ of a random variable $\alpha$ with finite second order moment.

Technical assumption: the series $\sum_{i \in \mathbb{N}} \|f_i\|_{C^{2,1}}$ is convergent
A useful result for numerical computations

- if \((\alpha_i)\) are uncorrelated, then

\[
\mathbb{E}(J(D)) = J(D_0) + \frac{\varepsilon^2}{2} \mathbb{E}(\alpha^2) \sum_{i=1}^{\infty} B(f_i, f_i) + o(\varepsilon^2).
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\]

- If \((\alpha_i)\) are independent and \(\alpha\) has finite moments up to the order 3, then

\[
\text{var}(J(D)) = \varepsilon^2 \mathbb{E}(\alpha^2) \sum_{i=1}^{\infty} (L(f_i))^2 \\
+ \varepsilon^3 \mathbb{E}(\alpha^3) \sum_{i=1}^{\infty} L(f_i) B(f_i, f_i) + \mathcal{O}(\varepsilon^3).
\]
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+ \varepsilon^3 \mathbb{E}(\alpha^3) \sum_{i=1}^{\infty} L(f_i) B(f_i, f_i) + \mathcal{O}(\varepsilon^3).
\]
A useful result for numerical computations

It suffices to evaluate the derivatives $L(f_i)$ and $B(f_i, f_i)$ for a truncated series

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

In the example of Dirichlet energy:

$$L(f_i) = -\frac{1}{2} \int_{\partial D} (\partial_n u)^2 f_i$$
A useful result for numerical computations

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In the example of Dirichlet energy:

$$B(f_i, f_i) = \int_D |\nabla V(-\partial_n u f_i)|^2 + \int_{\partial D} \left[ \partial_n u + \frac{1}{2} H(\partial_n u)^2 \right] f_i^2$$

with $V(X)$ being the solution of

$$-\Delta V(X) = 0 \text{ in } D, \quad V(X) = X \text{ on } \partial D,$$

it costs $N + 1$ resolutions of linear systems with the same matrix and various right hand side. There is a single mesh, a single rigidity matrix,...we work only on the nominal domain.
Comparaison with Monte-Carlo \((N = 11)\)

**Expectation - uniform law**

**Variance - uniform law**

**Expectation - beta law**

**Variance - beta law**
Thanks for your attention . . .
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Happy birthday Carlos !!!!