Numerical solution of elliptic diffusion problems on random domains

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Overview

- Motivation
- Domain mapping approach
- Perturbation approach
- Thin layer approach
- Output functionals
- Numerical results
- Summary

Part 1. Motivation

Motivation

- elliptic boundary value problems can be solved with high accuracy, provided that the input data are known exactly
- practical significance of highly accurate numerical solutions is limited due to inexact input data

PDE on random domain:

$$-\Delta u(\omega) = f \text{ in } D(\omega), \quad u(\omega) = 0 \text{ on } \partial D(\omega)$$

Applications:

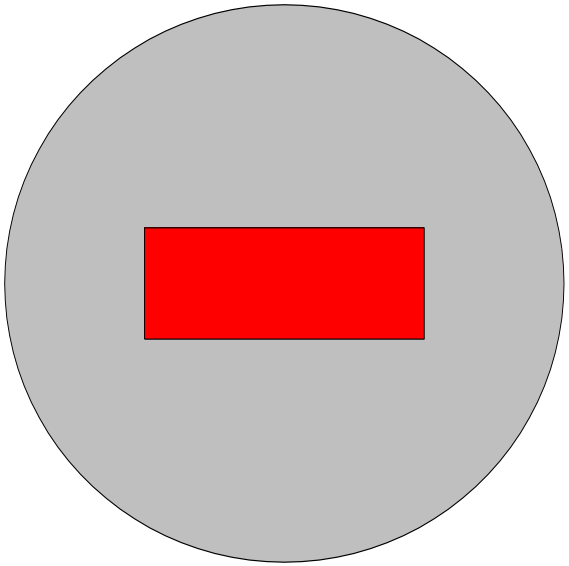
- tolerances in the shape of products fabricated by line production
- domains arising from inverse problems, e.g. tomography
- unsharp interfaces like cell membranes or molecular surfaces

Quantities of interest: $(\Omega, \Sigma, \mathbb{P})$ probability space

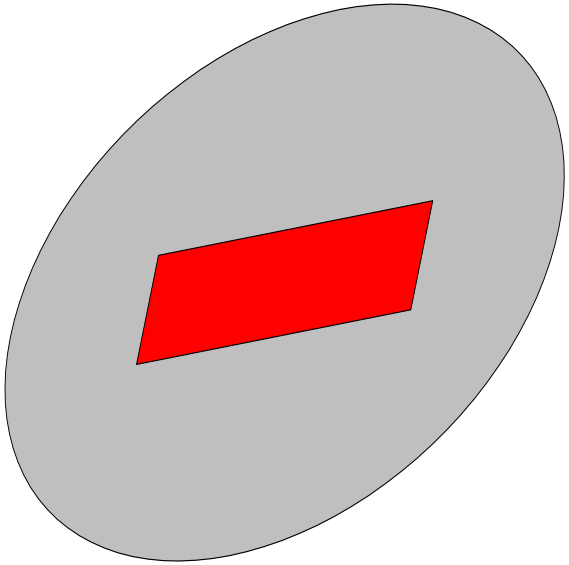
- expectation: $\mathbb{E}[u](\mathbf{x}) = \int_\Omega u(\mathbf{x}, \omega)\, \mathrm{d}\mathbb{P}(\omega)$
- two-point correlation: $\mathrm{Cor}[u](\mathbf{x}, \mathbf{x}') = \int_\Omega u(\mathbf{x}, \omega) u(\mathbf{x}', \omega)\, \mathrm{d}\mathbb{P}(\omega)$
- variance: $\mathbb{V}[u](\mathbf{x}) = \mathbb{E}[u^2](\mathbf{x}) - \mathbb{E}[u]^2(\mathbf{x}) = \mathrm{Cor}[u](\mathbf{x}, \mathbf{x}) - \mathbb{E}[u]^2(\mathbf{x})$

Goal: For given mean and two-point correlation of the domain perturbation field, compute the mean and the two-point correlation of the random solution of the PDE.

On domain perturbations

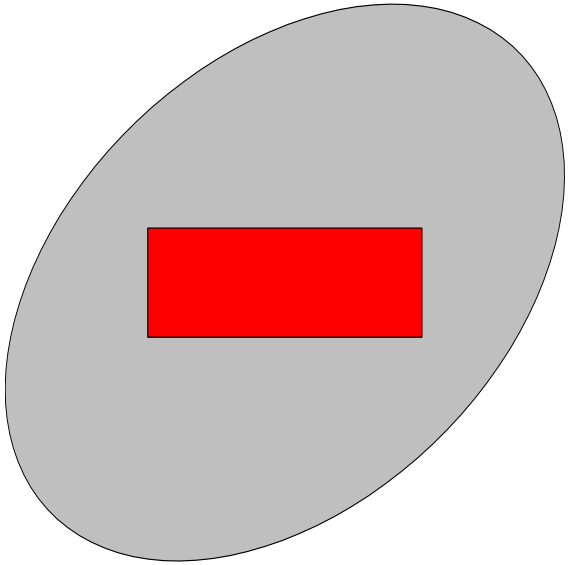


Nominal domain



Lagrangian specification

large deformations, but complete information on the domain perturbation has to be known



Eulerian specification

small deformations or point of interest far away from the boundary; requires only information on the boundary perturbation

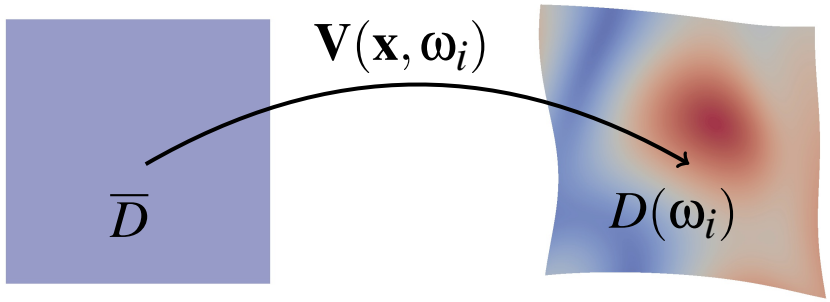
Part 2. Lagrangian specification

Lagrangian specification: Domain mapping approach

- Random domain variation: Random vector field $\mathbf{V}(\omega) : \overline{D} \to \mathbb{R}^d$ being invertible and bounded $\|\mathbf{V}(\omega)\|_{C^2(\overline{D};\mathbb{R}^d)} \leq C$ for all $\omega \in \Omega$ such that the singular values of the Jacobian $\mathbf{J}(\mathbf{x},\omega)$ satisfy

$$0 < \underline{\sigma} \leq \min\left\{\sigma\big(\mathbf{J}(\mathbf{x},\omega)\big)\right\} \leq \max\left\{\sigma\big(\mathbf{J}(\mathbf{x},\omega)\big)\right\} \leq \overline{\sigma} < \infty.$$

- Random domain: $D(\omega) := \{\mathbf{V}(\mathbf{x},\omega) : \mathbf{x} \in \overline{D}\}$



- In order to guarantee solvability for almost every $\omega \in \Omega$, we consider the right hand side $f(\mathbf{x})$ to be defined on the *hold-all* domain

$$\mathbb{D} := \bigcup_{\omega\in\Omega} D(\omega).$$

Variational formulation

- For given $\omega \in \Omega$, the variational formulation for the model problem is given as follows:

$$\text{Find } u(\omega) \in H_0^1\big(D(\omega)\big) \text{ such that}$$
$$\int_{D(\omega)} \langle \nabla u(\omega), \nabla v \rangle \, \mathrm{d}\mathbf{x} = \int_{D(\omega)} f v \, \mathrm{d}\mathbf{x} \quad \text{for all } v \in H_0^1\big(D(\omega)\big).$$

- Thus, with

$$\mathbf{A}(\mathbf{x}, \omega) := \big(\mathbf{J}(\mathbf{x}, \omega)^\intercal \mathbf{J}(\mathbf{x}, \omega)\big)^{-1} \det \mathbf{J}(\mathbf{x}, \omega)$$

and

$$\hat{u}(\mathbf{x}, \omega) := u\big(\mathbf{V}(\mathbf{x}, \omega)\big), \quad \hat{f}(\mathbf{x}, \omega) := f\big(\mathbf{V}(\mathbf{x}, \omega)\big) \det \mathbf{J}(\mathbf{x}, \omega),$$

we obtain the variational formulation with respect to the reference domain:

$$\text{Find } \hat{u}(\omega) \in H_0^1(\overline{D}) \text{ such that}$$
$$\int_{\overline{D}} \langle \mathbf{A}(\omega) \nabla \hat{u}(\omega), \nabla \hat{v} \rangle \, \mathrm{d}\mathbf{x} = \int_{\overline{D}} \hat{f}(\omega) \hat{v} \, \mathrm{d}\mathbf{x} \quad \text{for all } \hat{v} \in H_0^1(\overline{D}).$$

- Now, expectation and variance are well defined:

$$\mathbb{E}[u](\mathbf{x}) = \int_\Omega \hat{u}(\omega) \, \mathrm{d}\mathbb{P}(\omega) \in H_0^1(\overline{D}),$$
$$\mathbb{V}[u](\mathbf{x}) = \int_\Omega \big(\hat{u}(\omega) - \mathbb{E}[u]\big)^2 \, \mathrm{d}\mathbb{P}(\omega) \in W_0^{1,1}(\overline{D}).$$

Karhunen-Loève expansion

- Karhunen-Loève expansion: Assume that the domain perturbation field $\mathbf{V}(\mathbf{x},\omega)$ is given by a truncated Karhunen-Loève expansion

$$\mathbf{V}(\mathbf{x},\omega) = \mathbf{x} + \sum_{k=1}^{m} \sigma_k \varphi_k(\mathbf{x}) Y_k(\omega)$$

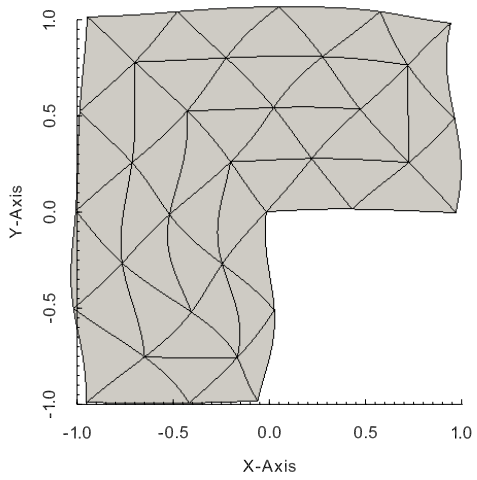
  where the random variables $\{Y_k(\omega)\}$ are independent and uniformly distributed in $[-1/2, 1/2]$ and the sequence $\{\gamma_k\}_k := \left\{ \|\sigma_k \varphi_k\|_{W^{1,\infty}(\overline{D};\mathbb{R}^d)} \right\}_k$ fulfills $\sum_{k=1}^{m} \gamma_k \leq c_\gamma < \infty$.
- Computation: It can be computed up to a prescribed precision by the pivoted Cholesky decomposition from the (matrix-valued) covariance function

$$\mathrm{Cov}[\mathbf{V}] : \overline{D} \times \overline{D} \to \mathbb{R}^{d \times d}, \quad \mathrm{Cov}[\mathbf{V}](\mathbf{x},\mathbf{x}') = [\mathrm{Cov}_{i,j}(\mathbf{x},\mathbf{x}')]_{i,j=1}^{d}.$$

- Illustration via some realizations:

$$\mathrm{Cov}[\mathbf{V}](\mathbf{x},\mathbf{x}') = \frac{1}{25} \begin{bmatrix} 2e^{-4\|\mathbf{x}-\mathbf{x}'\|_2^2} & 0 \\ 0 & e^{-\|\mathbf{x}-\mathbf{x}'\|_2^2} \end{bmatrix}$$

Length of the Karhunen-Loève expansion:
$M = 343$ for precision 10^{-6}



Parametric boundary value problem

- Parametrization: Introduce coordinates $\mathbf{y} \in \square := [-1/2, 1/2]^m$ and obtain the parameteric perturbation field

$$\mathbf{V}(\mathbf{x}, \omega) = \mathbf{x} + \sum_{k=1}^{m} \sigma_k \varphi_k(\mathbf{x}) Y_k(\omega) \quad \longrightarrow \quad \mathbf{V}(\mathbf{x}, \mathbf{y}) = \mathbf{x} + \sum_{k=1}^{m} \sigma_k \varphi_k(\mathbf{x}) y_k$$

- Parametric problem:

Find $\hat{u}(\mathbf{y}) \in H_0^1(\overline{D})$ such that

$$\int_{\overline{D}} \langle \mathbf{A}(\mathbf{y}) \nabla \hat{u}(\mathbf{y}), \nabla \hat{v} \rangle \, \mathrm{d}\mathbf{x} = \int_{\overline{D}} \hat{f}(\mathbf{y}) \hat{v} \, \mathrm{d}\mathbf{x} \quad \text{for all } \hat{v} \in H_0^1(\overline{D}).$$

where

$$\mathbf{A}(\mathbf{x}, \mathbf{y}) := \big(\mathbf{J}(\mathbf{x}, \mathbf{y})^\intercal \mathbf{J}(\mathbf{x}, \mathbf{y})\big)^{-1} \det \mathbf{J}(\mathbf{x}, \mathbf{y}),$$

$$\hat{f}(\mathbf{x}, \mathbf{y}) := f\big(\mathbf{V}(\mathbf{x}, \mathbf{y})\big) \det \mathbf{J}(\mathbf{x}, \mathbf{y}).$$

- Expectation and variance are high-dimensional integrals:

$$\mathbb{E}[u](\mathbf{x}) = \int_{\square} \hat{u}(\mathbf{y}) \, \mathrm{d}\mathbf{y} \in H_0^1(\overline{D}),$$

$$\mathbb{V}[u](\mathbf{x}) = \int_{\square} \big(\hat{u}(\mathbf{y}) - \mathbb{E}[u]\big)^2 \, \mathrm{d}\mathbf{y} \in W_0^{1,1}(\overline{D}).$$

Regularity of the solution

Theorem. Assume that the right hand side is analytic with respect to the spatial variable $\mathbf{x}$ and define the modified sequence

$$\{\mu_k\}_k := \left\{ \frac{8\overline{\sigma}^2}{\underline{\sigma}^d} C \max(1, c_D) \max\left(\frac{d}{\underline{\sigma}\rho \log 2}, \frac{2(1+c_\gamma)}{\underline{\sigma}^2 \log 2} \right) \gamma_k \right\}_k .$$

Then, the derivatives of the solution $\hat{u}(\mathbf{y})$ to the transported model problem satisfy

$$\left\| \partial_{\mathbf{y}}^{\alpha} \hat{u}(\mathbf{y}) \right\|_{H^1(\overline{D})} \lesssim |\alpha|! \mu^{\alpha}$$

with a constant which depends only on the right hand side f and the domain $\overline{D}$.

Remark.

This estimate implies that the solution $\hat{u}(\mathbf{y})$ depends analytically on the random input parameter $\mathbf{y}$. Especially, the k-th dimension is weighted by μ_k which means that higher the dimensions get less important.

Numerical realization

- Compute the Karhunen-Loève expansion with piecewise linear finite elements.
- Map the mesh of the nominal domain $\overline{D}$ to get the mesh on $D(\mathbf{y}_i)$.
- Compute the solution $u(\mathbf{x}, \mathbf{y}_i)$ on the perturbed domain with respect to the polygonal approximation of the mesh.
- The quadrature error of QMC based on N Halton points satisfies the dimension independent estimate

$$\left\| \mathbb{E}[u] - \frac{1}{N} \sum_{i=1}^{N} \hat{u}(\cdot, \mathbf{y}_i) \right\|_{H^1(\overline{D})} \leq C(\delta) N^{-1+\delta}$$

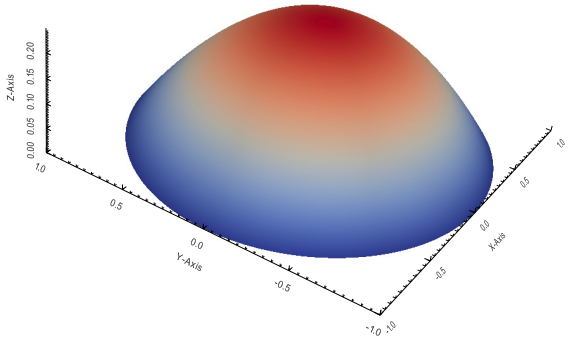
with a constant that satisfies $C(\delta) \to \infty$ as $\delta \to 0$ provided that $\gamma_k \lesssim k^{-3-\varepsilon}$.

Numerical results I

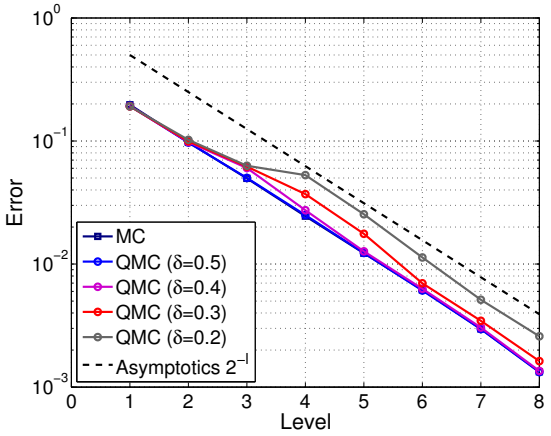
Problem. Poisson equation on a randomly perturbed unit disk:

$$\mathrm{Cov}[\mathbf{V}](\mathbf{x},\mathbf{y}) = \frac{1}{100}\begin{bmatrix} 5e^{-4\|\mathbf{x}-\mathbf{y}\|_2^2} & e^{-0.1\|2\mathbf{x}-\mathbf{y}\|_2^2} \\ e^{-0.1\|\mathbf{x}-2\mathbf{y}\|_2^2} & 5e^{-\|\mathbf{x}-\mathbf{y}\|_2^2} \end{bmatrix}, \quad f(\mathbf{x}) = 1.$$

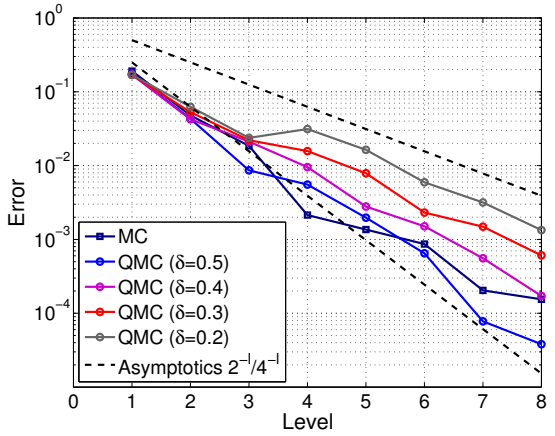
Mean



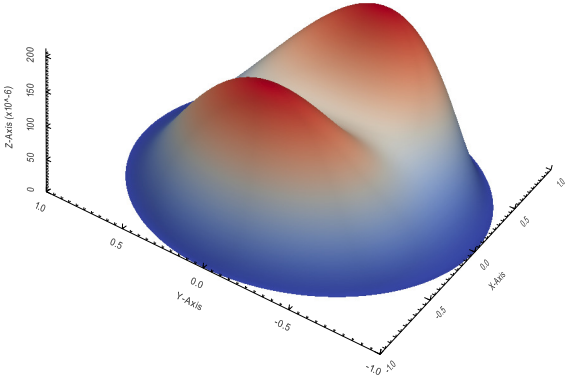
H^1-error



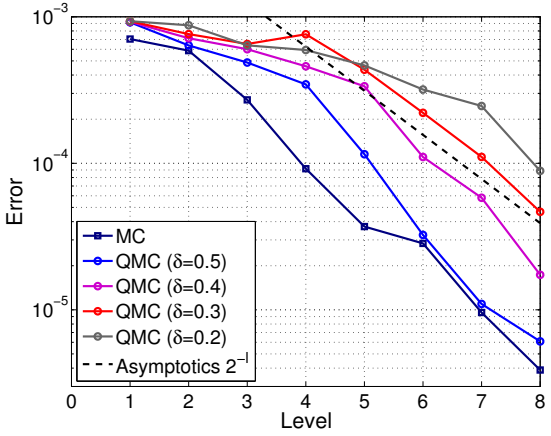
L^2-error



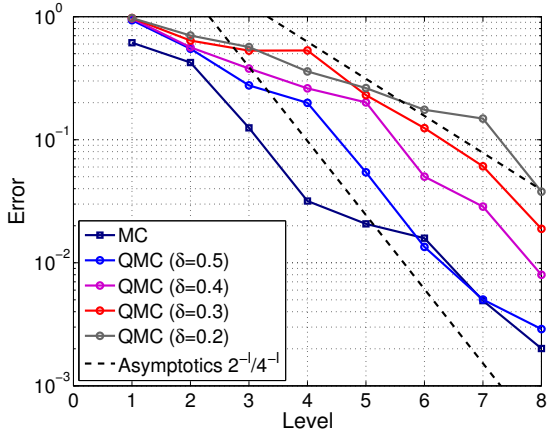
Variance



$W^{1,1}$-error



L^2-error

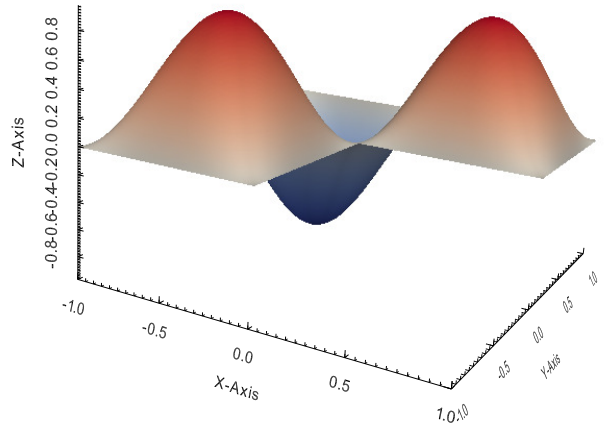


Numerical results II

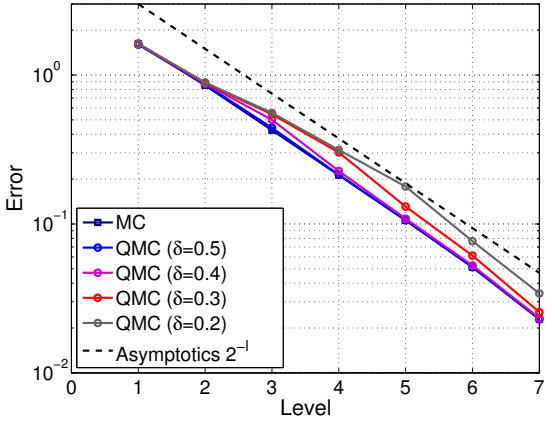
Problem. Poisson equation on a randomly perturbed L-shape:

$$\mathrm{Cov}[\mathbf{V}](\mathbf{x},\mathbf{x}') = \frac{1}{25}\begin{bmatrix} e^{-4\|\mathbf{x}-\mathbf{x}'\|_2^2} & 0 \\ 0 & e^{-\|\mathbf{x}-\mathbf{x}'\|_2^2} \end{bmatrix}, \quad f(\mathbf{x}) = 2\pi^2 \sin(\pi x_1)\sin(\pi x_2).$$

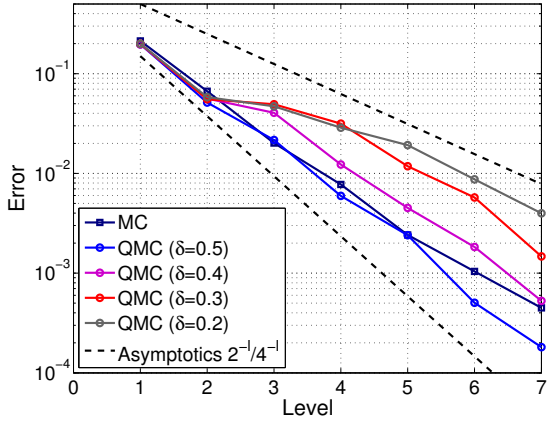
Mean



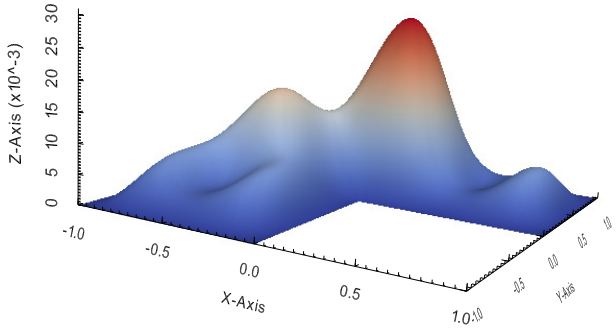
H^1-error



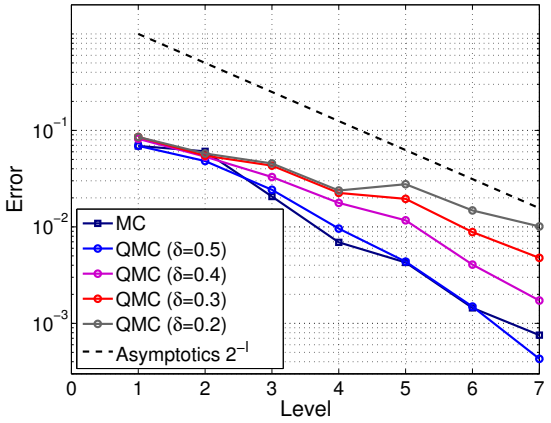
L^2-error



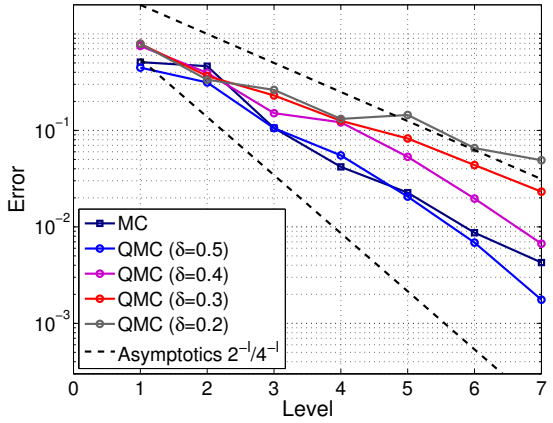
Variance



$W^{1,1}$-error



L^2-error



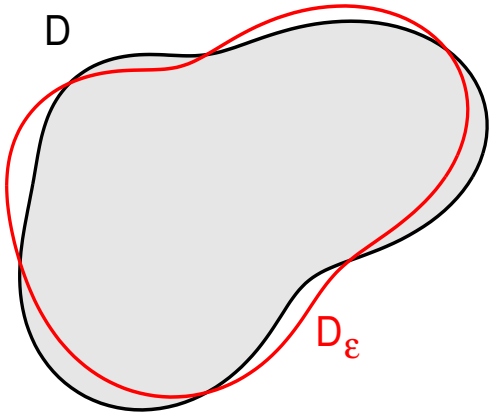
Part 3. Eulerian specification: Shape derivative approach

Eulerian specification: Shape sensitivity analysis

- Boundary variation: $\mathbf{V}(\mathbf{x}) := \mathbf{x} + \varepsilon\kappa(\mathbf{x})\mathbf{n}$ where $\kappa \in C^{1,1}(\partial D)$ satisfies $\|\kappa\|_{C^{1,1}(\partial D)} \leq 1$
- Perturbed domain: $\partial D_\varepsilon := \{\mathbf{V}(\mathbf{x}) : \mathbf{x} \in \Gamma\} \subset C^{1,1}$
- Local shape derivative: (Eppler/Kirsch/Potthast)

Consider the boundary value problems

$$-\Delta u_\varepsilon = f \quad \text{in } D_\varepsilon, \qquad u_\varepsilon = 0 \quad \text{on } \partial D_\varepsilon.$$



The local shape derivative $\delta u = \delta u[\mathbf{V}]$, defined pointwise by

$$\delta u(\mathbf{x}) = \lim_{\varepsilon \to 0} \frac{u_\varepsilon(\mathbf{x}) - u(\mathbf{x})}{\varepsilon}, \quad \mathbf{x} \in D \cap D_\varepsilon$$

reads as

$$\Delta \delta u[\mathbf{V}] = 0 \text{ in } D, \quad \delta u[\mathbf{V}] = -\kappa \frac{\partial u}{\partial \mathbf{n}} \text{ on } \partial D$$

$\rightsquigarrow$ **shape Taylor expansion:** $u_\varepsilon(\mathbf{x}) = u(\mathbf{x}) + \varepsilon \delta u[\mathbf{V}](\mathbf{x}) + O(\varepsilon^2), \quad \mathbf{x} \in K \Subset D \setminus \Gamma$

Derivative of a boundary value problem

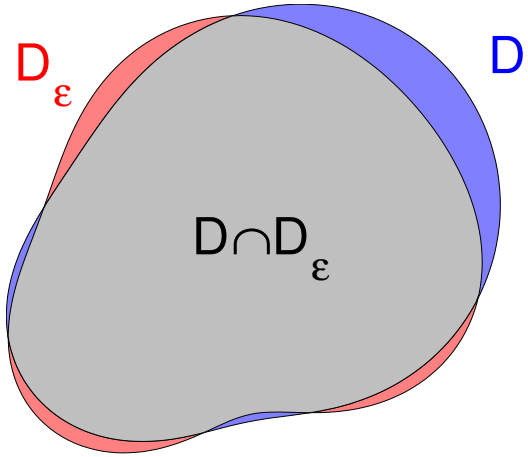
Sketch of the proof: It obviously holds $\Delta\delta u = 0$ since $u_\varepsilon - u$ is harmonic in $D \cap D_\varepsilon$.
Let $\delta u \in C(\overline{D})$ and

$$\Gamma_+ := \{\mathbf{x} \in \Gamma : \mathbf{x} \in D_\varepsilon\} \qquad \Gamma_- := \{\mathbf{x} \in \Gamma : \mathbf{x} \notin D_\varepsilon\} \qquad \Gamma_0 := \Gamma \setminus (\Gamma_+ \cup \Gamma_-)$$

For $\mathbf{x} \in \Gamma$ and $\mathbf{y} := \mathbf{x} + \varepsilon \mathbf{V}(\mathbf{x}) \in \Gamma_\varepsilon$, there holds

- if $\mathbf{x} \in \Gamma_+ \subset D_\varepsilon$, then

$$\delta u(\mathbf{x})\big|_{\Gamma_+} = \lim_{\varepsilon\to 0} \frac{u_\varepsilon(\mathbf{x}) - u(\mathbf{x})}{\varepsilon} = \lim_{\varepsilon\to 0} \frac{u_\varepsilon(\mathbf{x}) - u_\varepsilon(\mathbf{y}) + \overbrace{u_\varepsilon(\mathbf{y})}^{=0} - \overbrace{u(\mathbf{x})}^{=0}}{\varepsilon}$$
$$= -\langle \nabla u, \mathbf{V}\rangle = -\langle \mathbf{V}, \mathbf{n}\rangle \frac{\partial u}{\partial \mathbf{n}} - \langle \mathbf{V}, \mathbf{t}\rangle \underbrace{\frac{\partial u}{\partial \mathbf{t}}}_{=0}$$



- if $\mathbf{x} \in \Gamma_- \not\subset D_\varepsilon$, then

$$\delta u(\mathbf{x})\big|_{\Gamma_-} = \lim_{\varepsilon\to 0} \frac{u_\varepsilon(\mathbf{y}) - u(\mathbf{y})}{\varepsilon} = \lim_{\varepsilon\to 0} \frac{\overbrace{u_\varepsilon(\mathbf{y})}^{=0} - \overbrace{u(\mathbf{x})}^{=0} + u(\mathbf{x}) - u(\mathbf{y})}{\varepsilon}$$
$$= -\langle \nabla u, \mathbf{V}\rangle = -\langle \mathbf{V}, \mathbf{n}\rangle \frac{\partial u}{\partial \mathbf{n}} - \langle \mathbf{V}, \mathbf{t}\rangle \underbrace{\frac{\partial u}{\partial \mathbf{t}}}_{=0}$$

- if $\mathbf{x} \in \Gamma_0$, then $\delta u(\mathbf{x}) = 0$, which is consistent with $\langle \mathbf{V}(\mathbf{x}), \mathbf{n}(\mathbf{x})\rangle = 0$

Random domains

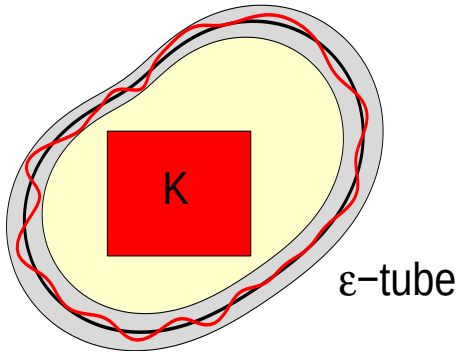
Consider a random boundary variation $\mathbf{V}(\mathbf{x},\omega) = \mathbf{x} + \varepsilon\kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x})$ where

$$\kappa \in L^2_{\mathbb{P}}\big(\Omega, C^{2,1}(\partial\overline{D})\big), \quad \mathbb{E}[\kappa] = 0 \quad \text{and} \quad \|\kappa(\omega)\|_{C^{2,1}(\partial\overline{D})} \leq 1 \quad \text{for } \mathbb{P}\text{-a.e.} \quad \omega \in \Omega.$$

The random domain is described via its boundary

$$\partial D(\omega) := \{\mathbf{x} + \varepsilon\kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x}) : \mathbf{x} \in \partial\overline{D}\}$$

where $\varepsilon > 0$ is a sufficiently small parameter.



Random Poisson equation:

$$-\Delta u(\omega) = f \text{ in } D(\omega), \quad u(\omega) = 0 \text{ on } \partial D(\omega)$$

Random shape Taylor expansion:

$$u(\mathbf{x},\omega) = \overline{u}(\mathbf{x}) + \varepsilon\delta u[\kappa(\omega)](\mathbf{x}) + O(\varepsilon^2), \quad \mathbf{x} \in K \Subset \bigcap_{\omega\in\Omega} D(\omega)$$

where $\overline{u} \in H^1(\overline{D})$ is the solution of the unperturbed Poisson problem and $\delta u[\kappa(\omega)]$ is the associated shape derivative.

Expectation and covariance of the random solution

Theorem: There holds

$$\mathbb{E}[u] = \overline{u} + O(\varepsilon^2) \quad \text{in } K,$$

$$\mathrm{Cov}[u] = \varepsilon^2 \mathbb{E}\big(\delta u[\kappa(\omega)] \otimes \delta u[\kappa(\omega)]\big) + O(\varepsilon^3) \quad \text{in } K \times K.$$

Proof: Use the random Taylor expansion:

$$\mathbb{E}\big(u_\varepsilon(\omega)\big) = \mathbb{E}\big(\overline{u} + \varepsilon \delta u[\kappa(\omega)] + O(\varepsilon^2)\big) = \overline{u} + \varepsilon \mathbb{E}\big(\delta u[\kappa(\omega)]\big) + O(\varepsilon^2).$$

There holds $\mathbb{E}[\delta u] := \mathbb{E}\big(\delta u[\kappa(\omega)]\big) = 0$ due to

$$\Delta \mathbb{E}[\delta u] = 0 \text{ in } \overline{D}, \qquad \mathbb{E}[\delta u] = -\underbrace{\mathbb{E}[\kappa]}_{\equiv 0} \frac{\partial \overline{u}}{\partial \mathbf{n}} \text{ on } \partial \overline{D}.$$

The second assertion follows finally from

$$\begin{aligned}
\mathrm{Cov}[u] &= \mathbb{E}\Big(\big(u(\omega) - \mathbb{E}[u]\big) \otimes \big(u(\omega) - \mathbb{E}[u]\big) \Big) \\
&= \mathbb{E}\Big(\big(\varepsilon \delta u[\kappa(\omega)] + O(\varepsilon^2)\big) \otimes \big(\varepsilon \delta u[\kappa(\omega)] + O(\varepsilon^2)\big) \Big) \\
&= \varepsilon^2 \mathbb{E}\big(\delta u[\kappa(\omega)] \otimes \delta u[\kappa(\omega)]\big) + O(\varepsilon^3). \qquad \square
\end{aligned}$$

Computing the covariance

Theorem. The two-point correlation

$$\mathrm{Cor}[\delta u](\mathbf{x},\mathbf{x}') := \mathbb{E}\big(\delta u[\kappa(\omega)](\mathbf{x}) \cdot \delta u[\kappa(\omega)](\mathbf{x}')\big)$$

is the unique solution in $H^{1,1}_{\mathrm{mix}}(\overline{D}\times\overline{D})$ of the tensor product boundary value problem

$$\begin{aligned}
(\Delta_{\mathbf{x}} \otimes \Delta_{\mathbf{x}'})\,\mathrm{Cor}[\delta u](\mathbf{x},\mathbf{x}') &= 0, \qquad \mathbf{x},\mathbf{x}' \in \overline{D},\\
\Delta_{\mathbf{x}}\,\mathrm{Cor}[\delta u](\mathbf{x},\mathbf{x}') &= 0, \qquad \mathbf{x} \in \overline{D},\ \mathbf{x}' \in \partial\overline{D},\\
\Delta_{\mathbf{x}'}\,\mathrm{Cor}[\delta u](\mathbf{x},\mathbf{x}') &= 0, \qquad \mathbf{x} \in \partial\overline{D},\ \mathbf{x}' \in \overline{D},\\
\mathrm{Cor}[\delta u](\mathbf{x},\mathbf{x}') &= \mathrm{Cor}[\kappa](\mathbf{x},\mathbf{x}')\left[\frac{\partial\overline{u}}{\partial\mathbf{n}}(\mathbf{x}) \otimes \frac{\partial\overline{u}}{\partial\mathbf{n}}(\mathbf{x}')\right], \qquad \mathbf{x},\mathbf{x}' \in \partial\overline{D}.
\end{aligned}$$

$\mathrm{Cor}[\delta u] \in H^{s+1/2,s+1/2}_{\mathrm{mix}}(\overline{D}\times\overline{D})$ provided that $\partial\overline{u}/\partial\mathbf{n} \in H^s(\partial\overline{D})$ for some $s \geq 1/2$.

Remark. Efficient solution via

- sparse grid combination technique
- low-rank approximation
- adaptive low-rank approximation / $\mathcal{H}$-matrix approach

Interface problem I

Problem: Let $D = (-1,1)^2$ and $\overline{\Gamma} = \{\mathbf{x} \in \mathbb{R}^2 : \|\mathbf{x}\| = 1/2\}$. Define the random interface $\Gamma_\varepsilon(\omega)$ via parametrization

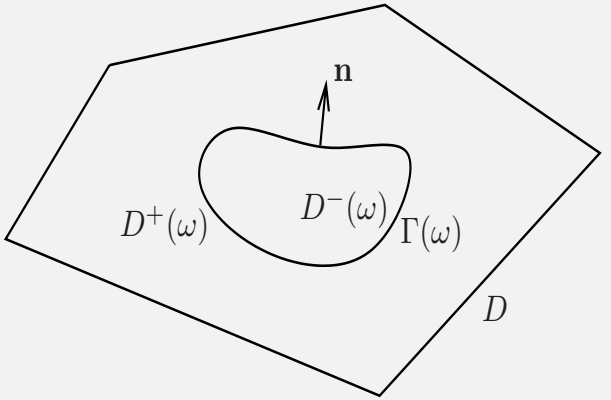
$$\gamma : [0, 2\pi] \times \Omega \to \Gamma_\varepsilon(\omega), \quad \gamma(s,\omega) := \left(\frac{1}{2} + \varepsilon\kappa(s,\omega)\right) \begin{bmatrix} \cos(s) \\ \sin(s) \end{bmatrix}$$

where the random perturbation is given by

$$\kappa(s,\omega) := \sum_{k=0}^{5} a_k(\omega)\cos(ks) + b_k(\omega)\sin(ks)$$

with $a_k(\omega), b_k(\omega) \in [-1,1]$ being uniformly distributed and independent. This leads to the two-point correlation function

$$\mathrm{Cor}[\kappa](s,t) = \frac{1}{3}\sum_{k=0}^{5} \cos(ks)\cos(kt) + \sin(ks)\sin(kt).$$



Solve

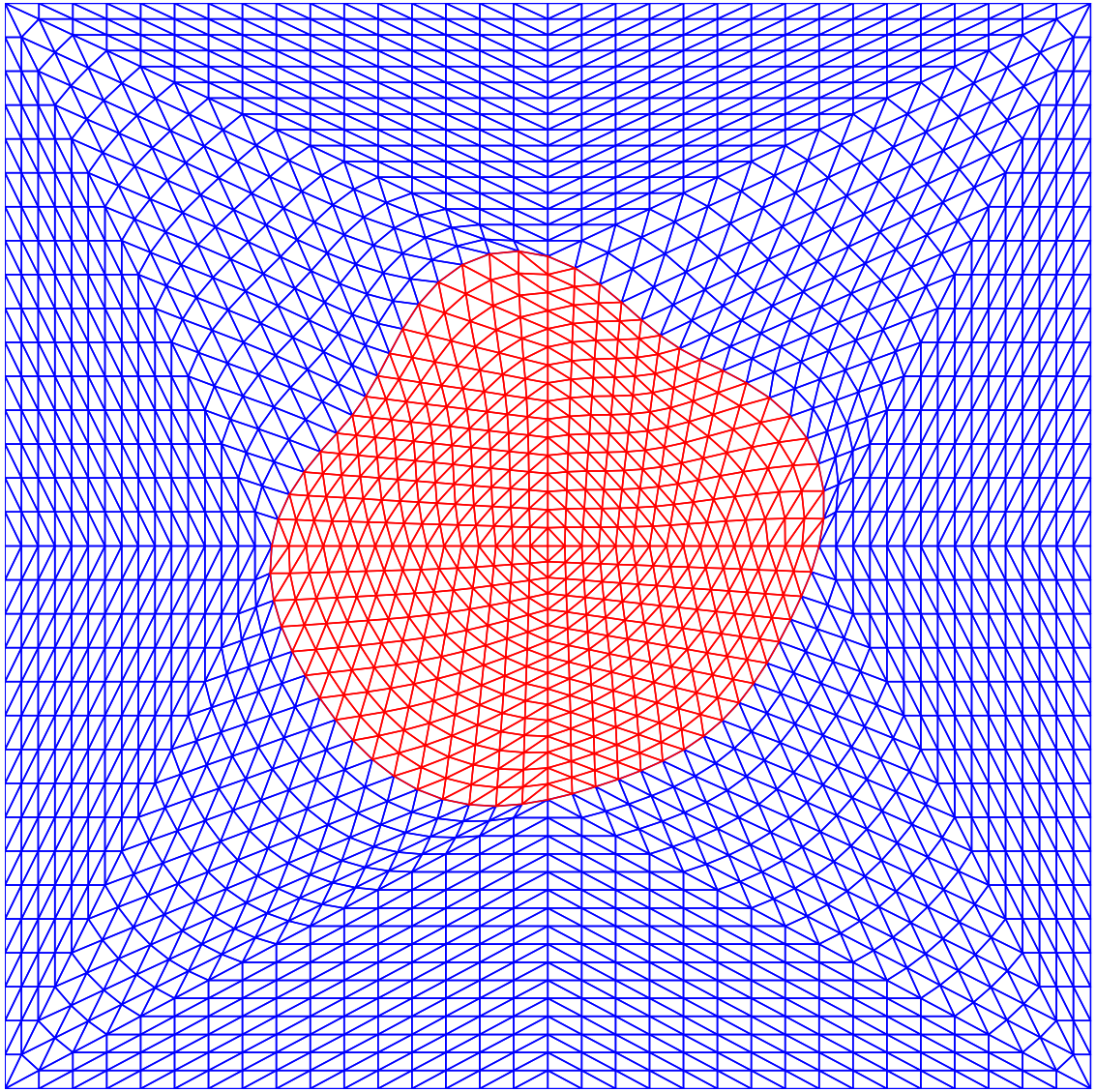
$$-\nabla \cdot \big(\alpha(\omega)\nabla u(\omega)\big) = 1 \quad \text{in } D^-(\omega) \cup D^+(\omega)$$

$$[u(\omega)] = 0, \ \left[\alpha(\omega)\frac{\partial u}{\partial \mathbf{n}}(\omega)\right] = 0 \quad \text{on} \Gamma(\omega)$$

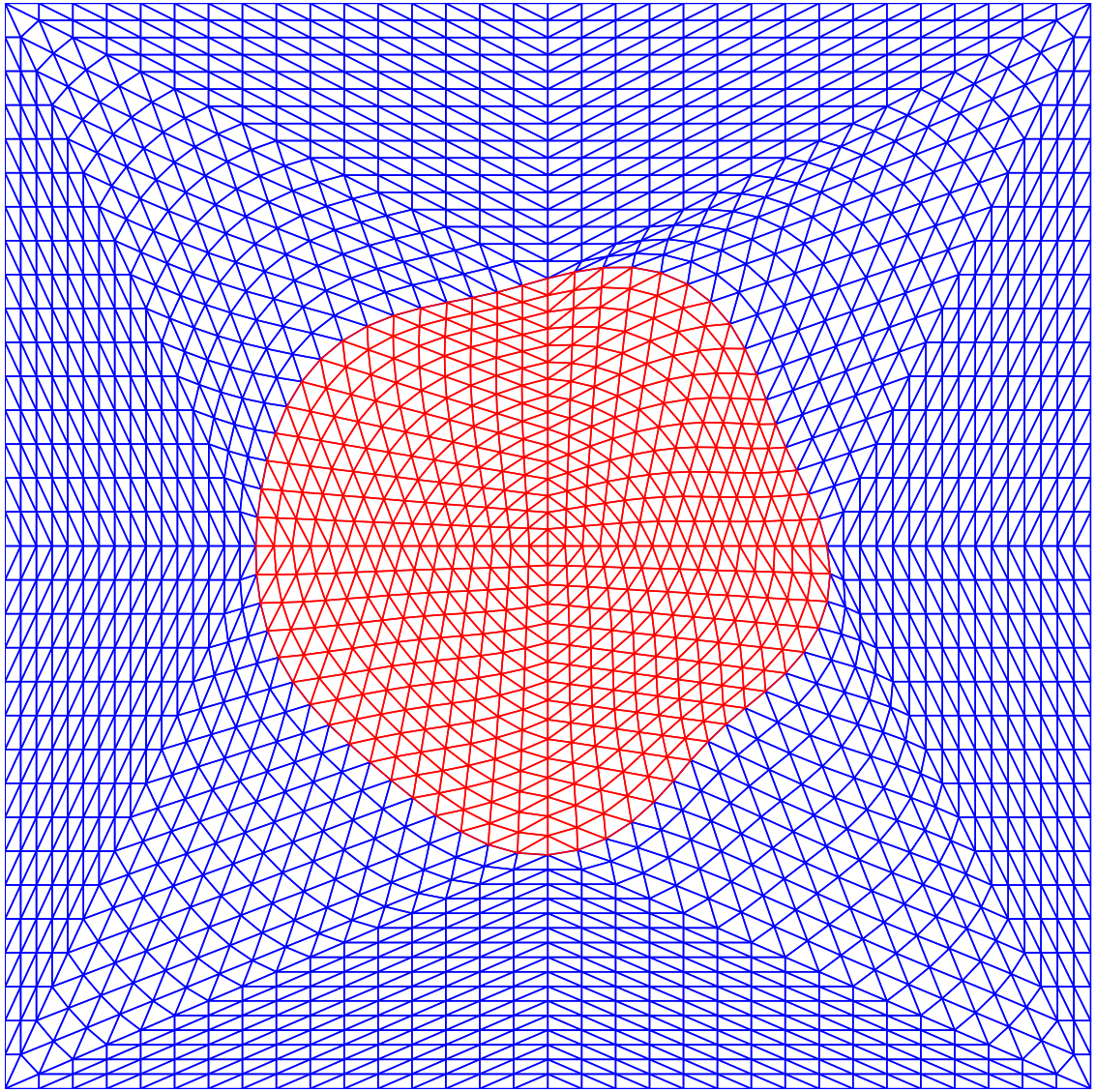
$$u(\omega) = 0 \quad \text{on } \partial D$$

where the coefficient $\alpha(\omega)$ satisfies $\alpha^+(\omega) = 1$ and $\alpha^-(\omega) = const$.

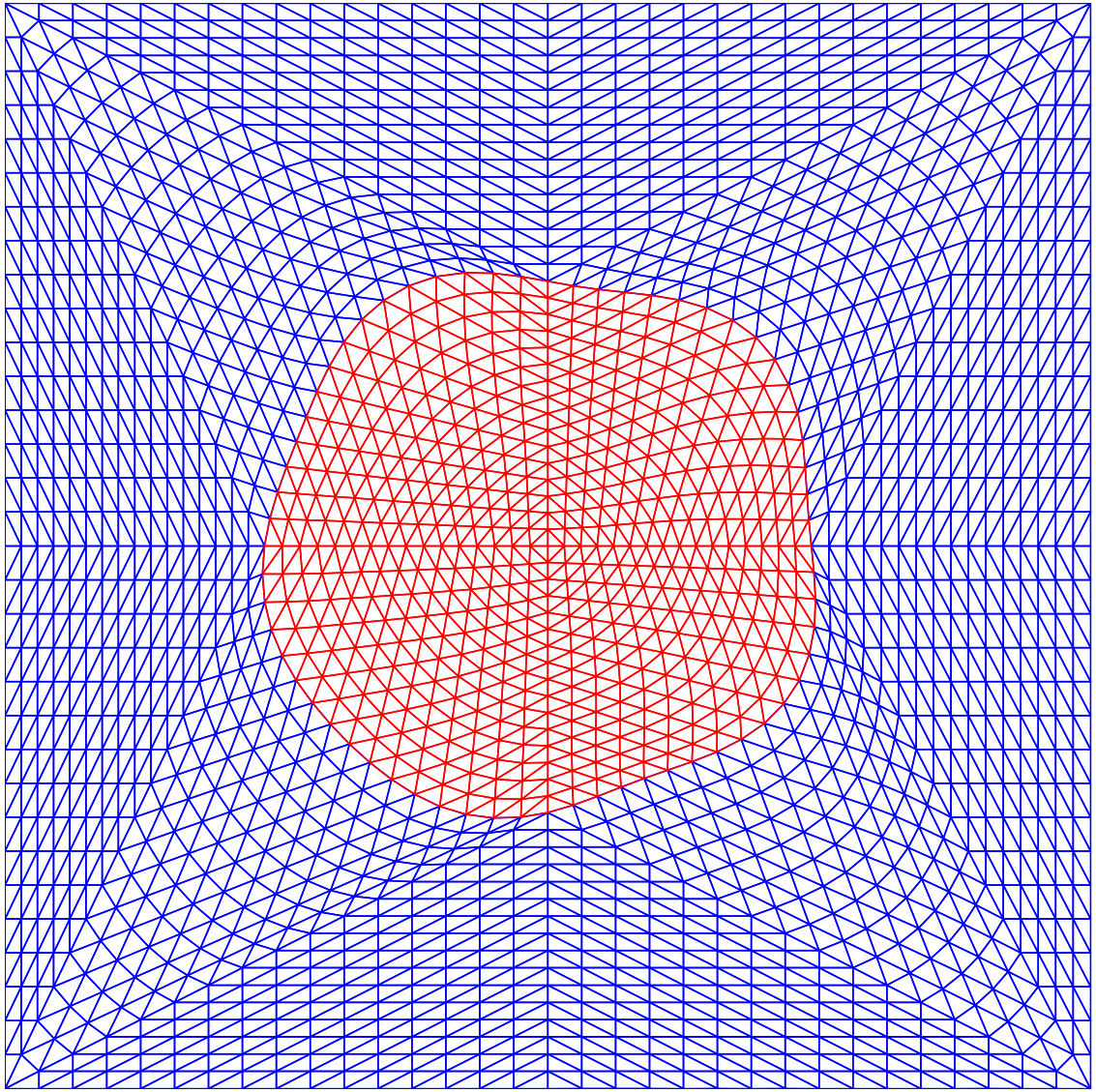
Sample ($\varepsilon = 0.02$)



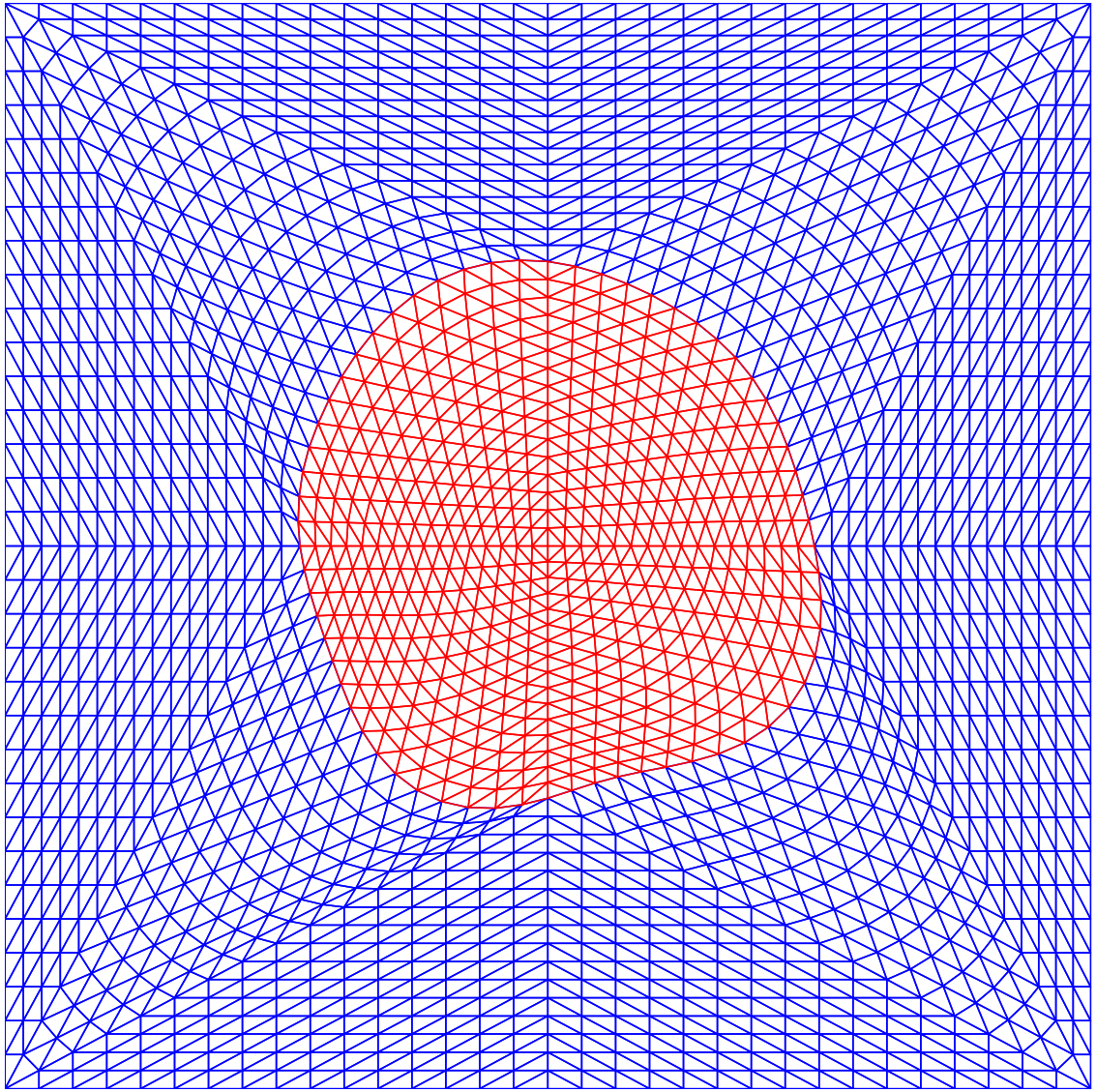
Sample ($\varepsilon = 0.02$)



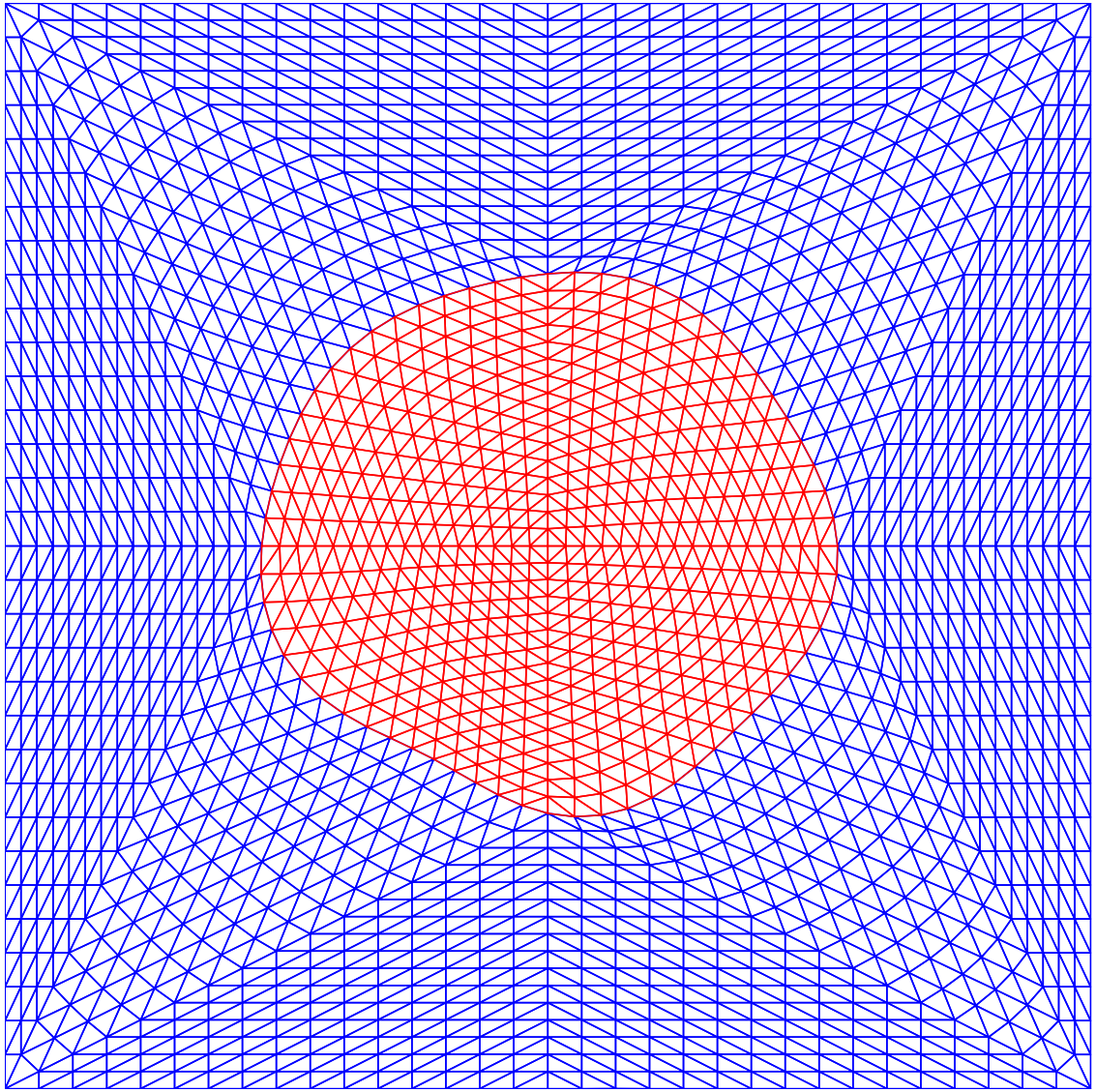
Sample ($\varepsilon = 0.02$)



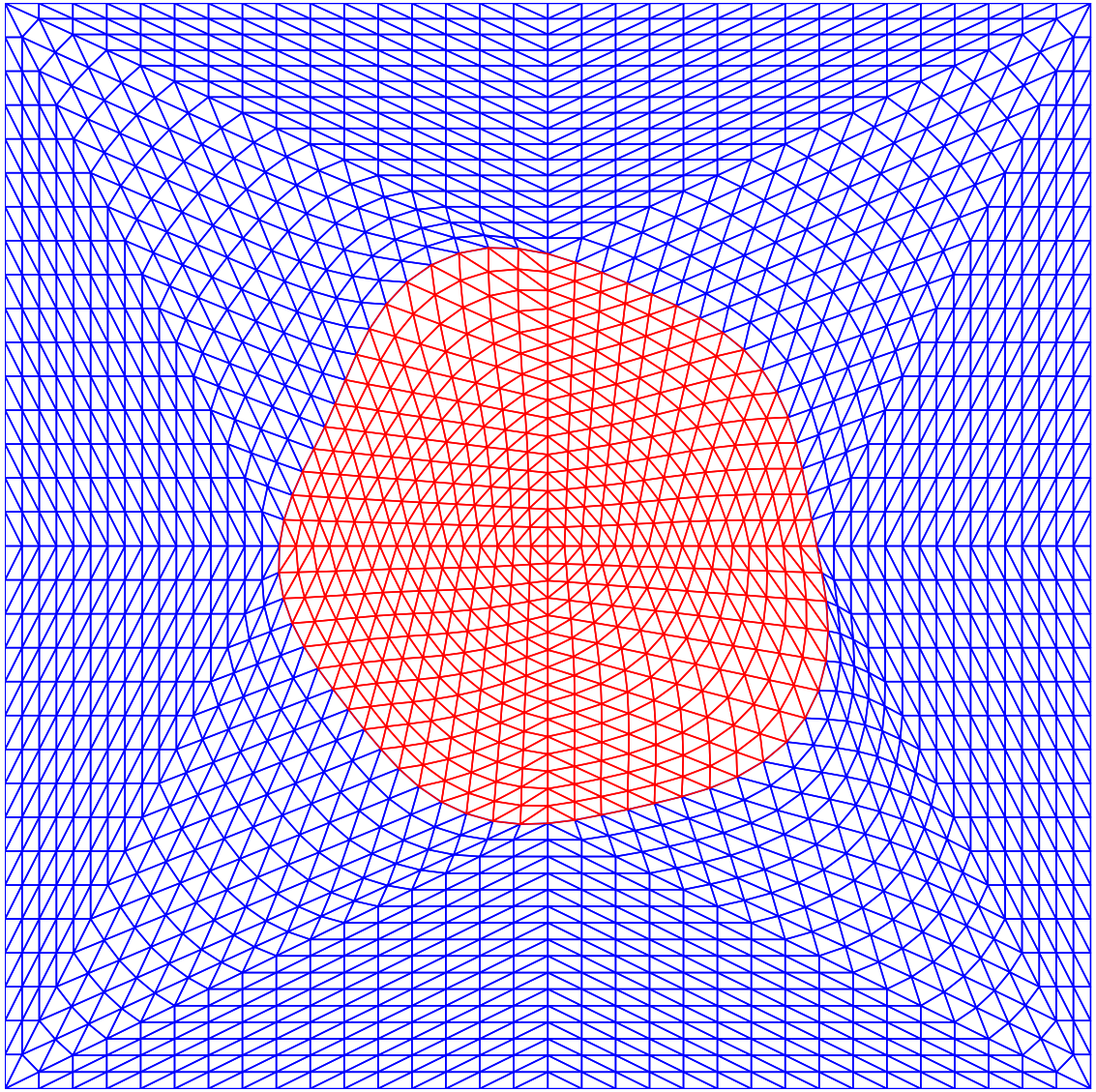
Sample ($\varepsilon = 0.02$)



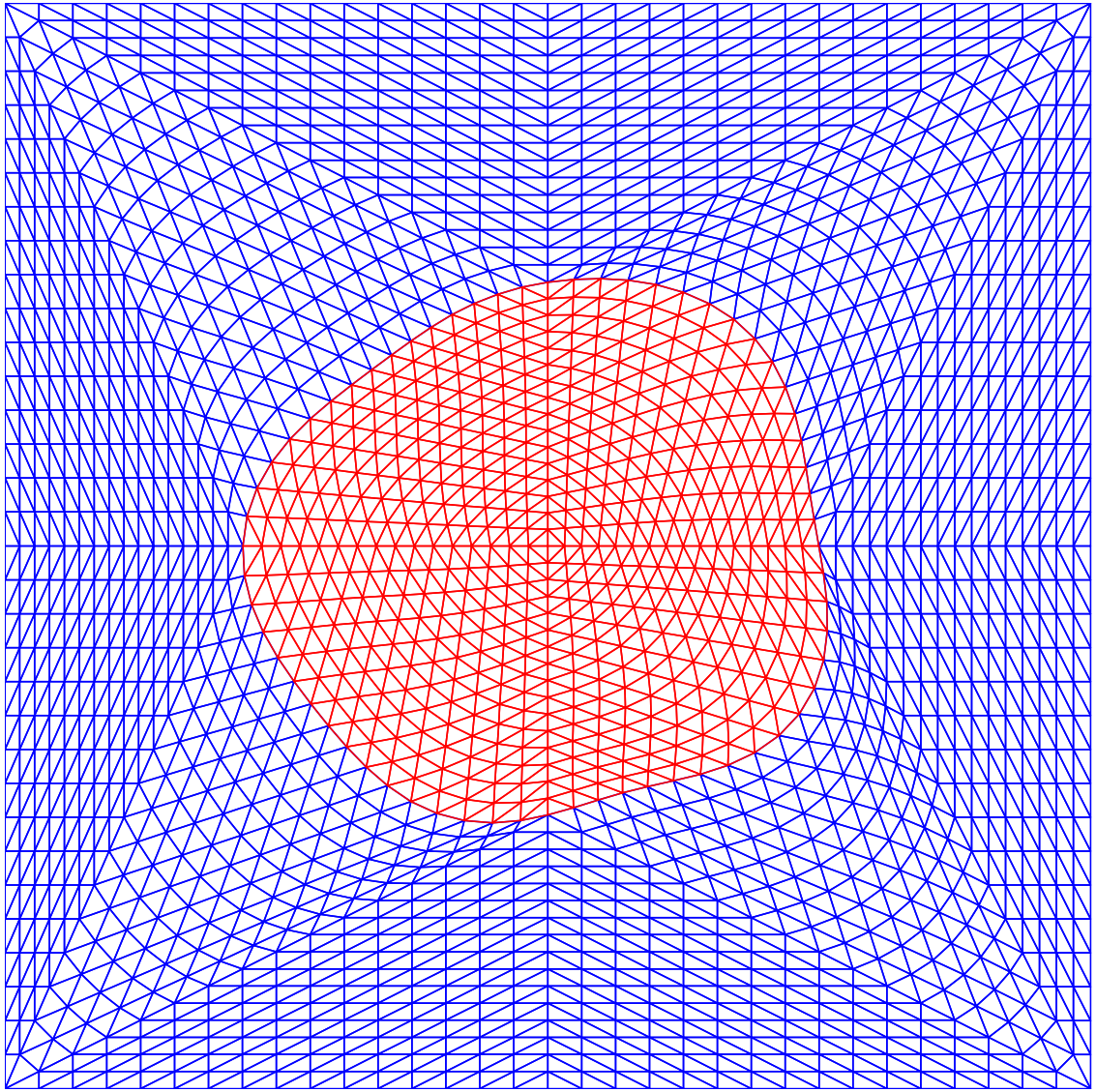
Sample ($\varepsilon = 0.02$)



Sample ($\varepsilon = 0.02$)



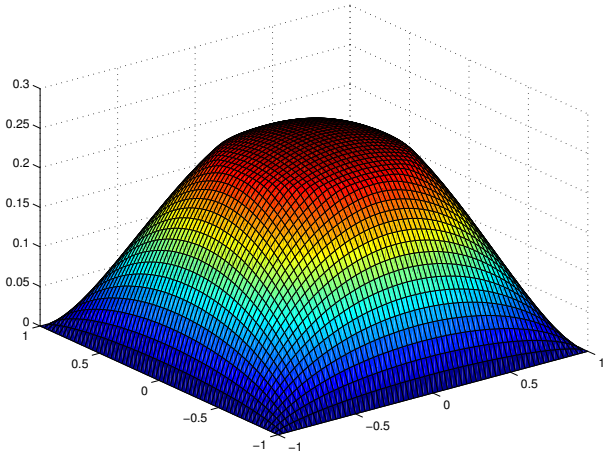
Sample ($\varepsilon = 0.02$)



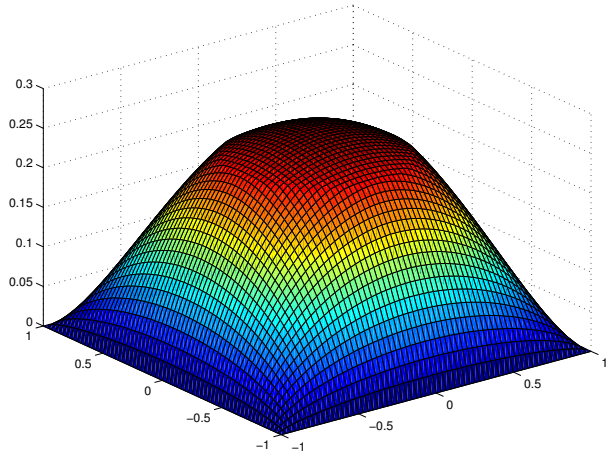
Interface problem II ($\alpha^- = 2$ and $\varepsilon = 0.02$)

expectation

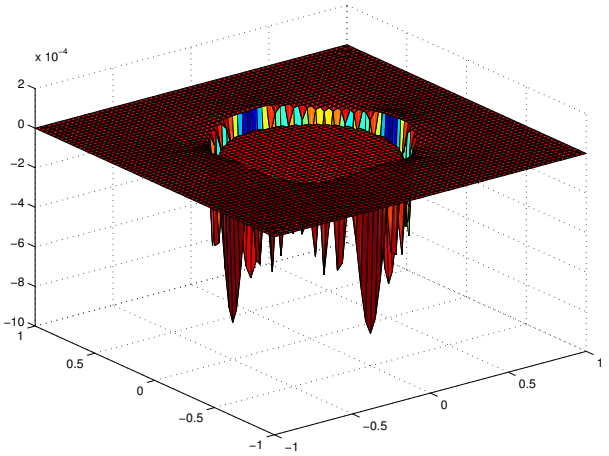
Monte Carlo approach



deterministic approach

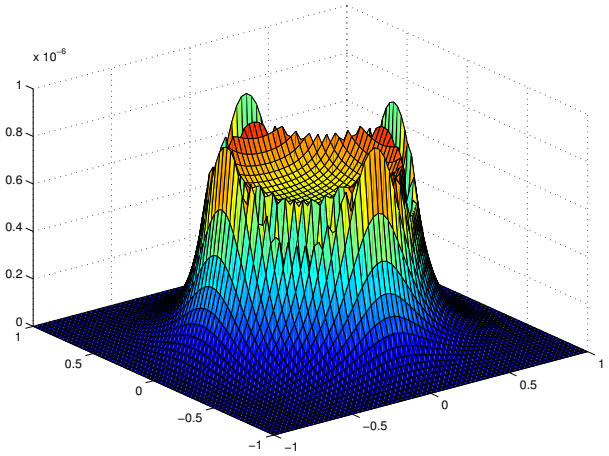


error

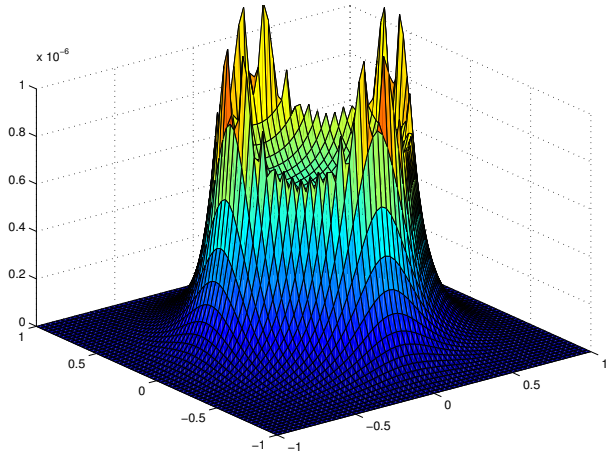


variance

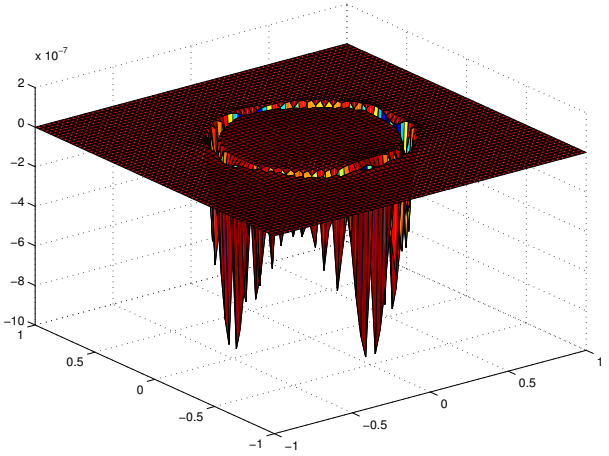
Monte Carlo approach



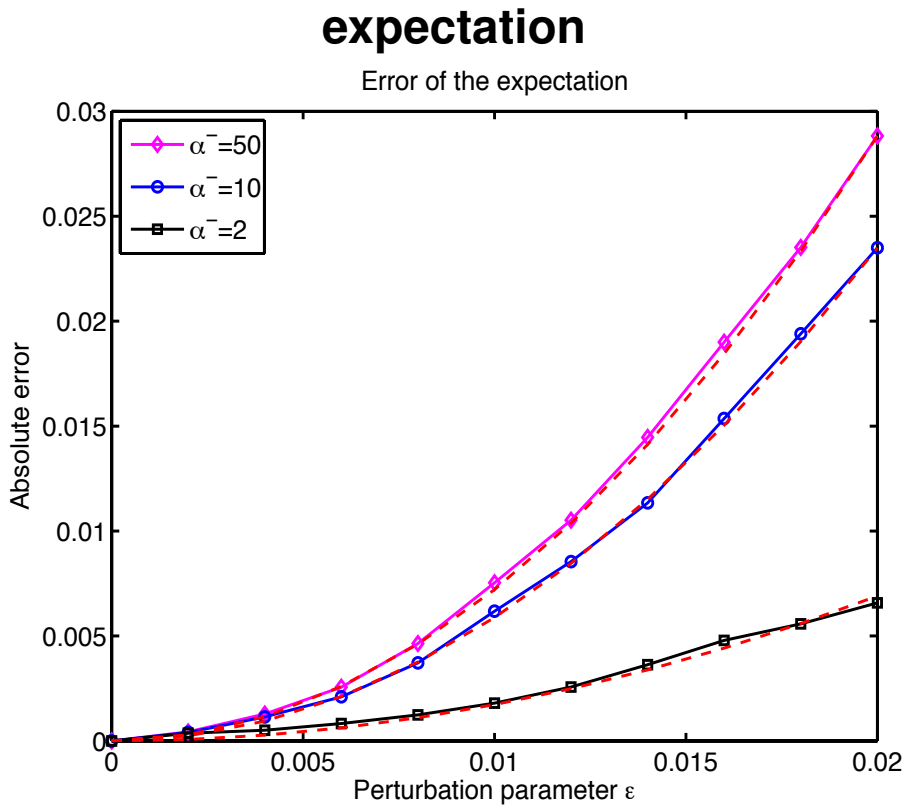
deterministic approach

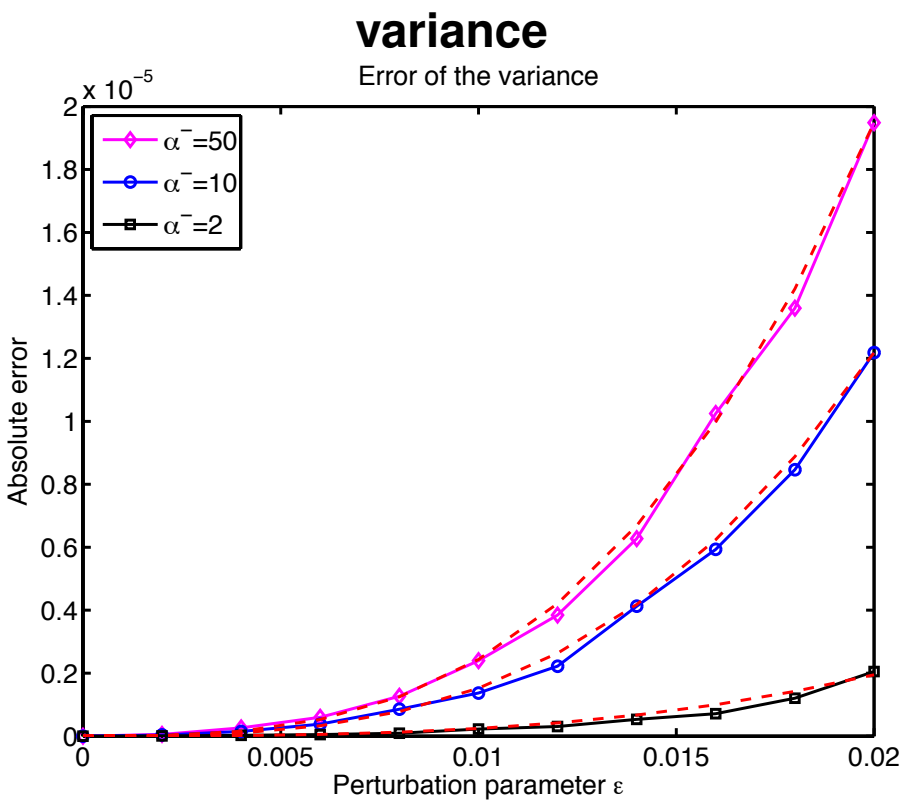


error



Interface problem III ($0 \leq \varepsilon \leq 0.02$)





Part 4. Eulerian specification: Thin layer approach

Random domain = domain with random layer

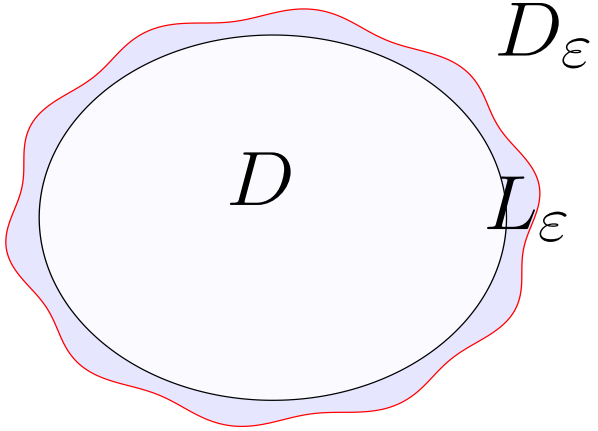
- **Idea.** The random domain can be seen as a fixed domain with thin random layer. We thus consider first the domain D with a deterministic layer

$$L_\varepsilon = \{\mathbf{x} + t\mathbf{n}(\mathbf{x}) : 0 \le t < \varepsilon h(\mathbf{x}),\ \mathbf{x} \in \partial D\}$$

  of thickness $0 < h_{\min} \le h(\mathbf{x}) \le h_{\max}$ for all $\mathbf{x} \in \partial D$.

- This leads to the transmission problem

$$\begin{cases} -\sigma_0 \Delta u_{\text{int}} = f & \text{in } D, \\ -\Delta u_{\text{ext}} = f & \text{in } L_\varepsilon, \\ u_{\text{int}} = u_{\text{ext}} & \text{on } \partial D, \\ \sigma_0 \frac{\partial u_{\text{int}}}{\partial \mathbf{n}} = \frac{\partial u_{\text{ext}}}{\partial \mathbf{n}} & \text{on } \partial D, \\ u_{\text{ext}} = 0 & \text{on } \partial D_\varepsilon. \end{cases}$$



- A heuristic way for replacing the boundary condition is given by Taylor's formula:

$$u_{\text{ext}}\big(\mathbf{x} + \varepsilon h(\mathbf{x})\mathbf{n}(\mathbf{x})\big) = u_{\text{ext}}(\mathbf{x}) + \varepsilon h(\mathbf{x}) \frac{\partial u_{\text{ext}}}{\partial \mathbf{n}}(\mathbf{x}) + O(\varepsilon^2), \quad \mathbf{x} \in \partial D.$$

  Hence, the Dirichlet boundary condition on ∂D_ε implies approximately

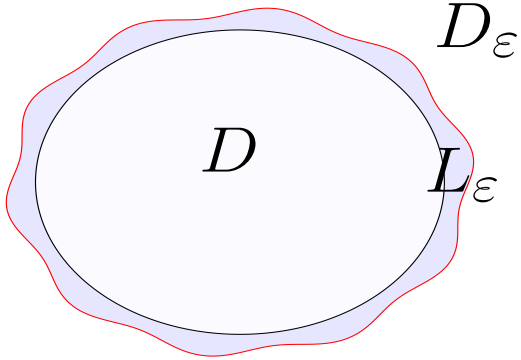
$$-\sigma_0 \Delta u_{\text{int}} = f \text{ in } D, \quad u_{\text{int}} + \varepsilon h \sigma_0 \frac{\partial u_{\text{int}}}{\partial \mathbf{n}} \approx 0 \text{ on } \partial D.$$

Random domain = domain with random layer

Idea. The random domain can be seen as a fixed domain with thin random layer. So, we first consider the deterministic layer

$$L_\varepsilon = \{\mathbf{x} + t\mathbf{n}(\mathbf{x}) : 0 \le t < \varepsilon h(\mathbf{x}),\ \mathbf{x} \in \partial D\}$$

of thickness $0 < h_{\min} \le h(\mathbf{x}) \le h_{\max}$ for all $\mathbf{x} \in \partial D$.



Theorem: Consider

$$-\operatorname{div}(\sigma \nabla u_\varepsilon) = f \text{ in } D_\varepsilon, \quad u = 0 \text{ on } \partial D_\varepsilon,$$

with $\sigma = \sigma_0$ in D and $\sigma = 1$ in L_ε. Then, it holds for the approximations

$$-\sigma_0 \Delta u^{[1]} = f \text{ in } D, \qquad u^{[1]} + \varepsilon h \sigma_0 \frac{\partial u^{[1]}}{\partial \mathbf{n}} = 0 \text{ on } \partial D,$$

$$-\sigma_0 \Delta u^{[2]} = f \text{ in } D, \quad \left(1 + \frac{\kappa h \varepsilon}{2}\right) u^{[2]} + \varepsilon \sigma_0 h \frac{\partial u^{[2]}}{\partial \mathbf{n}} = \frac{\varepsilon^2 h^2}{2} f \text{ on } \partial D,$$

the error estimates

$$\left\| u_\varepsilon - u^{[1]} \right\|_{H^1(D)} \lesssim \varepsilon^2, \quad \left\| u_\varepsilon - u^{[2]} \right\|_{H^1(D)} \lesssim \varepsilon^3.$$

Randomly varying layer

- **Random layer.** Let the layer be random according to

$$L_\varepsilon(\omega) = \{\mathbf{x} + t\mathbf{n}(\mathbf{x}) : 0 \le t < \varepsilon h(\mathbf{x},\omega),\ \mathbf{x} \in \partial D\},$$

  where

$$h(\mathbf{x},\omega) = \overline{h}(\mathbf{x}) + \widetilde{h}(\mathbf{x},\omega) \quad \text{with} \quad \overline{h}(\mathbf{x}) = \mathbb{E}\big(h(\mathbf{x},\omega)\big).$$

- **Uniform boundedness.** The random layer

$$h(\mathbf{x},\omega) = \overline{h}(\mathbf{x}) + \widetilde{h}(\mathbf{x},\omega) \quad \text{with} \quad \overline{h}(\mathbf{x}) = \mathbb{E}\big(h(\mathbf{x},\omega)\big)$$

  satisfies

$$0 < h_{\min} \le \overline{h}(\mathbf{x}) \le h_{\max} \quad \text{and} \quad |\widetilde{h}(\mathbf{x},\omega)| \le q|\overline{h}(\mathbf{x})| \text{ for some } 0 \le q < 1$$

  for all $\mathbf{x} \in \partial D$ and for $\mathbb{P}$-almost all $\omega \in \Omega$.

- **Uniform regularity.** The function $\mathbf{x} \mapsto h(\mathbf{x},\omega)$ is uniformly bounded in $C^1(\partial D)$ for all ω in Ω, that is, the random field h belongs to the Bochner space $L^\infty_{\mathbb{P}}\big(\Omega, C^1(\partial D)\big)$.

- **Variational formulation.** Seek $u^{[2]} \in L^2_{\mathbb{P}}\big(\Omega, H^1(D)\big)$ such that

$$\int_\Omega \left\{ \sigma_0 \int_D \nabla u^{[2]}(\omega) \nabla v(\omega)\, \mathrm{d}\mathbf{x} + \frac{1}{\varepsilon\sigma_0} \int_{\partial D} \left[\frac{1}{h(\omega)} + \frac{\varepsilon}{2}\kappa \right] u^{[2]}(\omega) v(\omega)\, \mathrm{d}o \right\} \mathrm{d}\mathbb{P}(\omega)$$
$$= \int_\Omega \left\{ \int_D f v(\omega)\, \mathrm{d}\mathbf{x} + \int_{\partial D} \frac{\varepsilon h(\omega)}{2\sigma_0} f v(\omega)\, \mathrm{d}o \right\} \mathrm{d}\mathbb{P}(\omega).$$

Randomly varying layer

Theorem: Under the condition

$$0 < h_{\min} \leq \overline{h}(\mathbf{x}) \leq h_{\max} \quad \text{and} \quad |\widetilde{h}(\mathbf{x},\omega)| \leq q|\overline{h}(\mathbf{x})|,$$

there exists a unique solution $u^{[2]}$ in $L^2_{\mathbb{P}}\big(\Omega, H^1(D)\big)$ provided that ε is so small that

$$|\varepsilon\kappa(\mathbf{x})| \leq \frac{1}{(1+q)h_{\max}} \text{ for all } \mathbf{x} \in \partial D.$$

In particular, introducing the spatial energy norm

$$|||v||| := \sqrt{\sigma_0 |v|^2_{H^1(D)} + \frac{1}{\varepsilon\sigma_0}\|T(v)\|^2_{L^2(\partial D)}},$$

where $T : H^1(D) \to L^2(\partial D)$ is the trace operator, we have the stability estimate

$$\sqrt{\int_\Omega |||u^{[2]}(\omega)|||^2 \, \mathrm{d}\mathbb{P}(\omega)} \leq C\big\{\|f\|_{\widetilde{H}^{-1}(D)} + \|T(f)\|_{L^2(\partial D)}\big\}$$

uniformly as ε tends to 0, where $\|\cdot\|_{\widetilde{H}^{-1}(D)}$ denotes as usual the dual norm to $\|\cdot\|_{H^1(D)}$.

Error estimates

- **Expectation.**

$$\mathbb{E}\big(u^{[2]}\big)(\mathbf{x}) = \int_\Omega u^{[2]}(\mathbf{x},\omega)\,\mathrm{d}\mathbb{P}(\omega), \quad \mathbf{x} \in D.$$

- **Variance.**

$$\mathbb{V}\big(u^{[2]}\big)(\mathbf{x}) = \int_\Omega \big[u^{[2]}(\mathbf{x},\omega) - \mathbb{E}\big(u^{[2]}\big)(\mathbf{x})\big]^2\,\mathrm{d}\mathbb{P}(\omega), \quad \mathbf{x} \in D.$$

Theorem: The random solution $u^{[2]} \in L^2_{\mathbb{P}}\big(\Omega, H^1(D)\big)$ satisfies the error estimates

$$\big\|\mathbb{E}(u_\varepsilon) - \mathbb{E}\big(u^{[2]}\big)\big\|_{H^1(D)} \lesssim \varepsilon^3, \quad \big\|\mathbb{V}(u_\varepsilon) - \mathbb{V}\big(u^{[2]}\big)\big\|_{W^{1,1}(D)} \lesssim \varepsilon^4.$$

Regularity of the solution I

- **Karhunen-Loève expansion.** Assume that the layer is given by

$$h(\mathbf{x},\omega) = \overline{h}(\mathbf{x}) + \sum_{k=1}^{m} \sigma_k \varphi_k(\mathbf{x}) Y_k(\omega) \quad \longrightarrow \quad h(\mathbf{x},\mathbf{y}) = \overline{h}(\mathbf{x}) + \sum_{k=1}^{m} \sigma_k \varphi_k(\mathbf{x}) y_k$$

  where the random variables $\{Y_k(\omega)\}$ are independent and uniformly distributed in $[-1/2, 1/2]$ and the sequence $\{\gamma_k\}_k := \left\{ \|\sigma_k \varphi_k\|_{L^\infty(\partial D)} \right\}_k$ fulfills $\sum_{k=1}^{m} \gamma_k < \infty$.

- **Uniform boundedness.** The random layer $h(\mathbf{x},\mathbf{y}) = \overline{h}(\mathbf{x}) + \widetilde{h}(\mathbf{x},\mathbf{y})$ satisfies

$$0 < h_{\min} \le \overline{h}(\mathbf{x}) \le h_{\max} \quad \text{and} \quad |\widetilde{h}(\mathbf{x},\mathbf{y})| \le q\overline{h}(\mathbf{x}) \text{ for some } 0 \le q < 1.$$

Theorem: The derivatives of the solution $u \in L^2\big(\square, H^1(D)\big)$ satisfy the pointwise estimate

$$\left\| \left| \partial_{\mathbf{y}}^{\alpha} u^{[2]}(\mathbf{y}) \right| \right\| \le c_f |\alpha|! \left(\frac{c_u}{(1-q)h_{\min}} \right)^{|\alpha|} \gamma^{\alpha},$$

for all $\mathbf{y} \in \square := [-1/2, 1/2]^m$ and $\alpha \in \mathbb{N}^m$. The constant c_f depends only on $\|f\|_{\widetilde{H}^{-1}(D)}$, $\|T(f)\|_{L^2(\partial D)}$ and σ_0, but not on the layer thickness ε, while the constant c_u is given by

$$c_u = 2 \max \left\{ \frac{1}{(1-q)h_{\min}}, \frac{2(1+q)h_{\max}}{(1-q)h_{\min}} \right\} \ge 2.$$

Regularity of the solution II

Remarks.

- The solution $u(\mathbf{y})$ depends analytically on the parameter $\mathbf{y}$.
- Dimension independent sampling methods do work if the sequence $\{\gamma_k\}$ decays sufficiently fast.
- The quadrature error of QMC based on N Halton points satisfies the estimate

$$\left\| \mathbb{E}\left[u^{[2]}\right] - \frac{1}{N}\sum_{i=1}^{N} u^{[2]}(\cdot,\mathbf{y}_i) \right\| \lesssim N^{-1+\delta}$$

  for all $\delta > 0$ with a constant which depends on δ provided that $\gamma_k \lesssim k^{-2-\varepsilon}$.

Numerical results I

- Consider the Poisson equation

$$-\Delta u(\omega) = 4 \text{ in } D_\varepsilon(\omega), \quad u(\omega) = 0 \text{ on } \partial D_\varepsilon(\omega),$$

on the random domain $D_\varepsilon(\omega) = D \cup L_\varepsilon(\omega)$ where D is a disk of radius $1-\varepsilon$ and $L_\varepsilon(\omega) = \{\mathbf{x} + t\mathbf{n}(\mathbf{x}) : 0 \le t < \varepsilon h(\mathbf{x},\omega),\ \mathbf{x} \in \partial D\}$ is a random layer.

- The random fluctuations are defined by the finite Karhunen-Loève expansion

$$h(\varphi,\omega) = 1 + \frac{1}{8}\sum_{k=0}^{5} \{a_k(\omega)\cos(k\varphi) + b_k(\omega)\sin(k\varphi)\},$$

where $0 \le \varphi < 2\pi$ is the polar angle of a given point $\mathbf{x} \in \partial D$ and $a_k, b_k \in [-1/2, 1/2]$ are independent and uniformly distributed random variables.

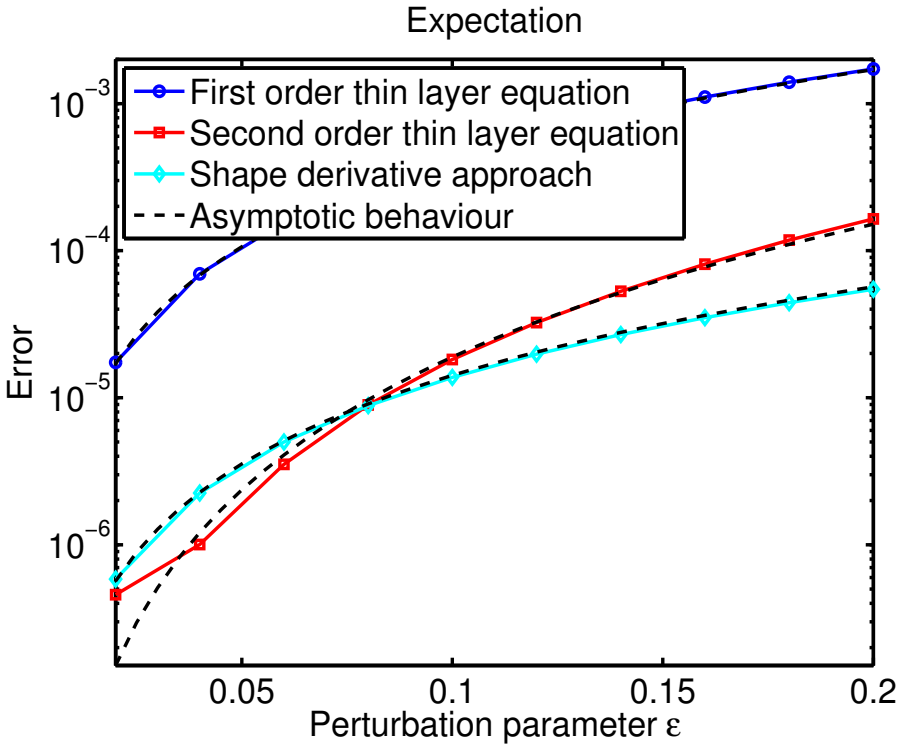
- The evaluation on the fixed set $K = \{\|\mathbf{x}\| \le 0.8\}$ yields:

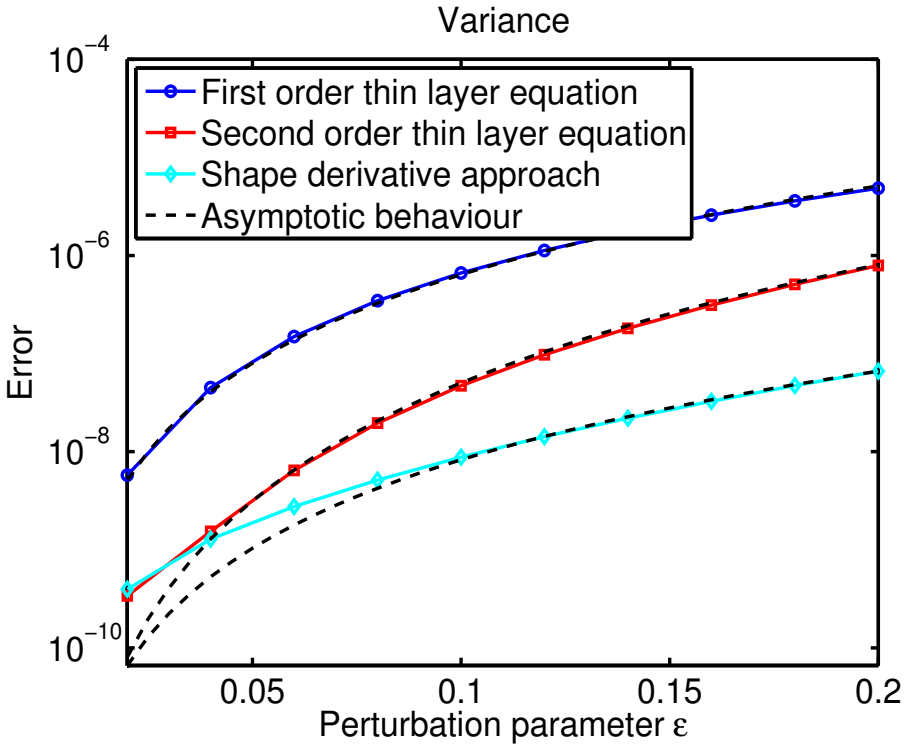
$$\left\|\mathbb{E}(u_\varepsilon) - \mathbb{E}\left(u^{[1]}\right)\right\|_{H^1(K)} \lesssim \varepsilon^2, \quad \left\|\mathbb{V}(u_\varepsilon) - \mathbb{V}\left(u^{[1]}\right)\right\|_{W^{1,1}(K)} \lesssim \varepsilon^3,$$
$$\left\|\mathbb{E}(u_\varepsilon) - \mathbb{E}\left(u^{[2]}\right)\right\|_{H^1(K)} \lesssim \varepsilon^3, \quad \left\|\mathbb{V}(u_\varepsilon) - \mathbb{V}\left(u^{[2]}\right)\right\|_{W^{1,1}(K)} \lesssim \varepsilon^4.$$

- We compare this with a shape derivative approach which satisfies

$$\left\|\mathbb{E}(u_\varepsilon) - \mathbb{E}\left(u^{[\mathrm{sd}]}\right)\right\|_{H^1(K)} \lesssim \varepsilon^2, \quad \left\|\mathbb{V}(u_\varepsilon) - \mathbb{V}\left(u^{[\mathrm{sd}]}\right)\right\|_{W^{1,1}(K)} \lesssim \varepsilon^3.$$

Numerical results II





Part 5. Output functionals

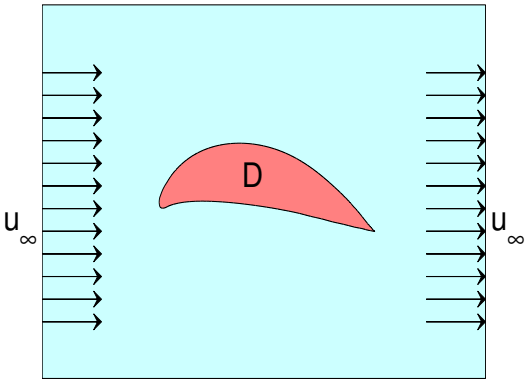
Random shape functionals I

Problem: Given a PDE on a random domain

$$-\Delta u(\omega) = f \text{ in } D(\omega), \quad u(\omega) = g \text{ on } \partial D(\omega).$$

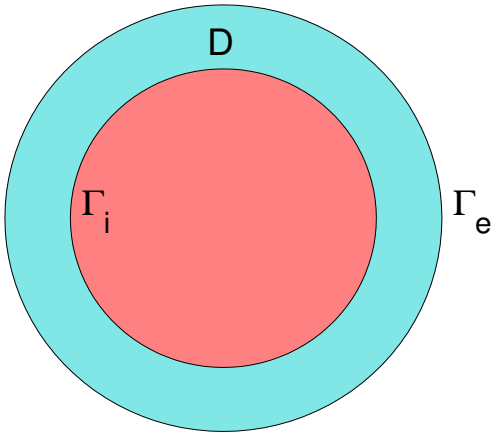
Often not the solution of the PDE is of interest, but the output functional

$$J\big(D(\omega); u(\omega)\big) = \int_{D(\omega)} j\big(u(\mathbf{x},\omega),\mathbf{x}\big)\,\mathrm{d}\mathbf{x}.$$



Random boundary variation $\mathbf{V}(\mathbf{x},\omega) = \mathbf{x} + \varepsilon\kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x})$ with

$$\mathbb{E}[\kappa] = 0 \text{ and } \|\kappa(\omega)\|_{C^{2,1}(\partial\overline{D})} \leq 1 \text{ for } \mathbb{P}\text{-a.e. } \omega \in \Omega.$$



The random domain is described via its boundary

$$\partial D(\omega) := \{\mathbf{x} + \varepsilon\kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x}) : \mathbf{x} \in \partial\overline{D}\}$$

where $\varepsilon > 0$ is a sufficiently small parameter.

Random shape functionals II

Theorem: There holds

$$\mathbb{E}[J] = J\big(\overline{D};\overline{u}\big) + O(\varepsilon^2),$$

$$\mathbb{V}[J] = \varepsilon^2 \int_{\partial\overline{D}\times\partial\overline{D}} \operatorname{Cor}[\kappa](\mathbf{x},\mathbf{y})\big(h(\mathbf{x})\otimes h(\mathbf{y})\big)\,\mathrm{d}\sigma_{(\mathbf{x},\mathbf{y})} + O(\varepsilon^3),$$

where

$$h(\mathbf{x}) = j(\overline{u},\mathbf{x}) + \frac{\partial p}{\partial \mathbf{n}}(\mathbf{x})\frac{\partial(g-\overline{u})}{\partial \mathbf{n}}(\mathbf{x})$$

and

$$-\Delta\overline{u} = f \text{ in } \overline{D}, \qquad \overline{u} = g \text{ on } \partial\overline{D},$$

$$-\Delta p = \frac{\partial j}{\partial \overline{u}}(\overline{u},\mathbf{x}) \text{ in } \overline{D}, \qquad p = 0 \text{ on } \partial\overline{D}.$$

Numerical results ($N = 5$)

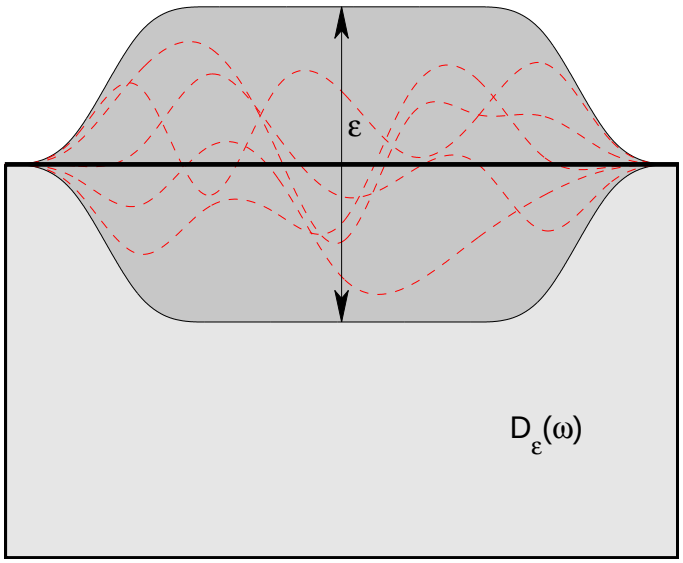
Problem:

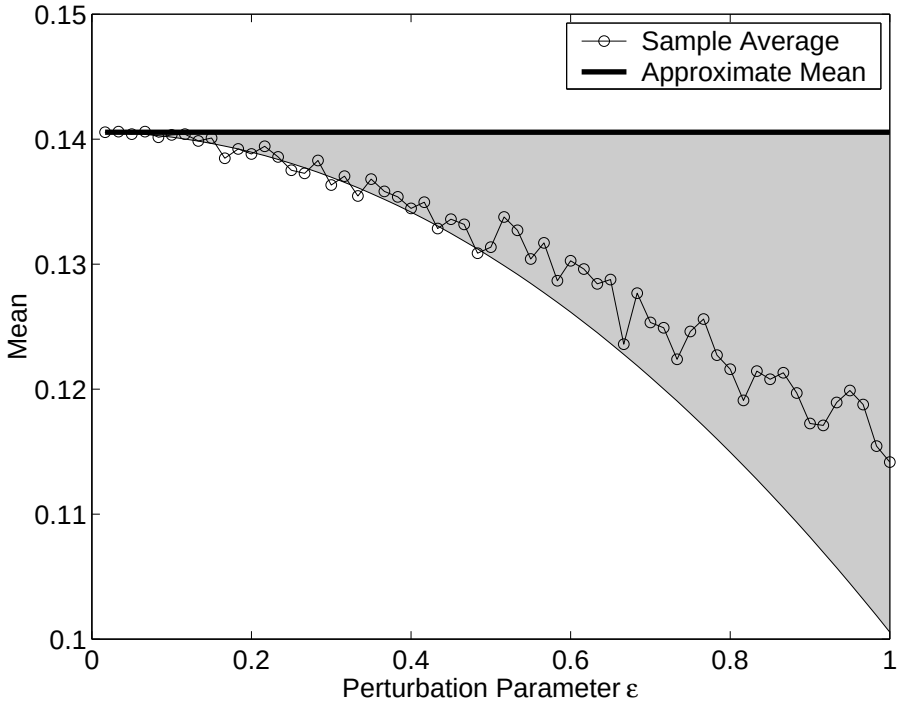
$$-\Delta u(\omega) = 1 \text{ in } D_\varepsilon(\omega), \quad u(\omega) = 0 \text{ on } \partial D_\varepsilon(\omega),$$

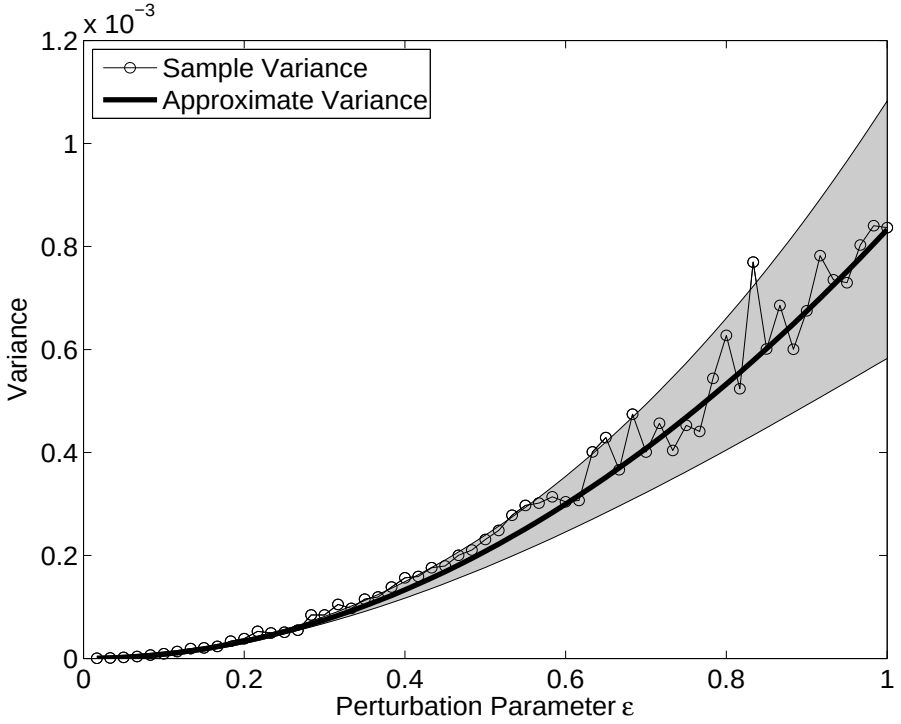
$$T\left(D_\varepsilon(\omega)\right) = \int_{D_\varepsilon(\omega)} u(\omega)\,\mathrm{d}\mathbf{x}$$

$\overline{D} = (0,1)^2$ and uncertain boundary at the top

$$f_\varepsilon(x,\omega) = \varepsilon \sum_{i=1}^{N} \alpha_i(\omega) B_4\left((N+3)x - i - 1\right).$$







Part 6. Summary

Summary

- We considered both, Eulerian coordinates and Lagrangian coordinates:

$$\dot{u}[\mathbf{V}] = \delta u[\mathbf{V}] + \langle \nabla u, \mathbf{V} \rangle.$$

- We developed and analyzed fast deterministic methods for the second moment analysis of random solutions to the elliptic boundary value problems on random domains.
- The domain mapping approach works for large deformations but needs complete knowledge on the domain perturbation field.
- The perturbation approach works for small deformations and needs only the knowledge on the boundary perturbation field.
- Use the local shape derivative to linearize the solution's dependence on the input data in case of the (first order) perturbation approach.
- The thin layer equation provides an alternative perturbation approach.
- Output functionals for PDEs on random domains can efficiently be solved by using the shape gradient or, for higher order approximations, by using the shape Hessian.