Second moment analysis of elliptic problems with random input parameters

Helmut Harbrecht
Mathematisches Institut
Universität Basel
Switzerland

University of Basel

Overview

- Motivation
- PDEs with random input data
  - random loading
  - random coefficients
  - random domain
- Solution of tensor product type boundary value problems
  - pivoted Cholesky decomposition
  - sparse tensor product approximation
  - $\mathcal{H}$-matrices
- Numerical results and applications

Part 1. Motivation

Motivation and background

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

Examples: uncertain material parameters, uncertain loadings,
but also uncertain domains

Model problem:

$$\boxed{\begin{aligned} -\operatorname{div}\left[\mathbf{A}(\omega)\nabla u(\omega)\right] &= f(\omega) \quad \text{in } D(\omega) \\ u(\omega) &= g(\omega) \quad \text{on } \partial D(\omega) \end{aligned}}$$

Statistical quantities

- Expectation or mean:

$$\mathbb{E}[u](\mathbf{x}) = \int_\Omega u(\mathbf{x},\omega)\,\mathrm{d}\mathbb{P}(\omega)$$

- Correlation:

$$\mathrm{Cor}[u](\mathbf{x},\mathbf{y}) = \int_\Omega u(\mathbf{x},\omega)u(\mathbf{y},\omega)\,\mathrm{d}\mathbb{P}(\omega) = \mathbb{E}[u(\mathbf{x})u(\mathbf{y})]$$

- Covariance:

$$\mathrm{Covar}[u](\mathbf{x},\mathbf{y}) = \mathrm{Cor}[u](\mathbf{x},\mathbf{y}) - \mathbb{E}[u](\mathbf{x})\mathbb{E}[u](\mathbf{y})$$

- Variance:

$$\mathbb{V}[u](\mathbf{x}) = \mathrm{Covar}[u](\mathbf{x},\mathbf{y})\big|_{\mathbf{x}=\mathbf{y}}$$

Goal of computation: For given mean and two-point correlation of the random input parameter, compute, with leading order in the size of the random perturbation, the mean and the two-point correlation of the random solution of the boundary value problem.

Part 2. Modelling

Random loadings I

Random boundary value problem:

$$\boxed{-\operatorname{div}\left[\mathbf{A}\nabla u(\omega)\right] = f(\omega) \text{ in } D, \qquad u(\omega) = g(\omega) \text{ on } \partial D}$$

$\longrightarrow$ the random solution depends linearly on the random input data:

$$\underbrace{\mathbb{E}\Big[-\operatorname{div}\left[\mathbf{A}\nabla u(\omega)\right]\Big]}_{=-\operatorname{div}\left[\mathbf{A}\nabla\mathbb{E}[u(\omega)]\right]} = \mathbb{E}[f(\omega)] \text{ in } D, \qquad \mathbb{E}[u(\omega)] = \mathbb{E}[g(\omega)] \text{ on } \partial D$$

Consequently, the solution's expectation is given by:

$$\boxed{-\operatorname{div}[\mathbf{A}\nabla\mathbb{E}[u]] = \mathbb{E}[f] \text{ in } D, \qquad \mathbb{E}[u] = \mathbb{E}[g] \text{ on } \partial D}$$

Question: How to compute the solution's variance?

$\longrightarrow$ use $\mathbb{V}[u](\mathbf{x}) = \operatorname{Covar}[u](\mathbf{x},\mathbf{y})\big|_{\mathbf{x}=\mathbf{y}}$

i.e., compute it from the trace of the correlation $\operatorname{Cor}[u](\mathbf{x},\mathbf{y}) = \mathbb{E}[u(\mathbf{x},\omega)u(\mathbf{y},\omega)]$

Random loadings II

Boundary value problem for $u(\mathbf{x},\omega)u(\mathbf{y},\omega)$:

$$\begin{aligned}
\operatorname{div}_{\mathbf{x}}\left[\mathbf{A}(\mathbf{x})\nabla_{\mathbf{x}}u(\mathbf{x},\omega)\right]\operatorname{div}_{\mathbf{y}}\left[\mathbf{A}(\mathbf{y})\nabla_{\mathbf{y}}u(\mathbf{y},\omega)\right] &= f(\mathbf{x},\omega)f(\mathbf{y},\omega), && \mathbf{x},\mathbf{y}\in D\\
-\operatorname{div}_{\mathbf{x}}\left[\mathbf{A}(\mathbf{x})\nabla_{\mathbf{x}}u(\mathbf{x},\omega)\right]u(\mathbf{y},\omega) &= f(\mathbf{x},\omega)g(\mathbf{y},\omega), && \mathbf{x}\in D,\ \mathbf{y}\in\partial D\\
-\operatorname{div}_{\mathbf{y}}\left[\mathbf{A}(\mathbf{y})\nabla_{\mathbf{y}}u(\mathbf{y},\omega)\right]u(\mathbf{x},\omega) &= f(\mathbf{y},\omega)g(\mathbf{x},\omega), && \mathbf{y}\in D,\ \mathbf{x}\in\partial D\\
u(\mathbf{x},\omega)u(\mathbf{y},\omega) &= g(\mathbf{x},\omega)g(\mathbf{y},\omega), && \mathbf{x},\mathbf{y}\in\partial D.
\end{aligned}$$

Random loadings III

Take the expectations on the left and on the right hand sides:

$$\mathbb{E}\Big[\operatorname{div}_{\mathbf{x}}\big[\mathbf{A}(\mathbf{x})\nabla_{\mathbf{x}}u(\mathbf{x},\omega)\big]\operatorname{div}_{\mathbf{y}}\big[\mathbf{A}(\mathbf{y})\nabla_{\mathbf{y}}u(\mathbf{y},\omega)\big]\Big] = \mathbb{E}\big[f(\mathbf{x},\omega)f(\mathbf{y},\omega)\big], \qquad \mathbf{x},\mathbf{y}\in D$$

$$\mathbb{E}\Big[-\operatorname{div}_{\mathbf{x}}\big[\mathbf{A}(\mathbf{x})\nabla_{\mathbf{x}}u(\mathbf{x},\omega)\big]u(\mathbf{y},\omega)\Big] = \mathbb{E}\big[f(\mathbf{x},\omega)g(\mathbf{y},\omega)\big], \qquad \mathbf{x}\in D,\ \mathbf{y}\in\partial D$$

$$\mathbb{E}\Big[-\operatorname{div}_{\mathbf{y}}\big[\mathbf{A}(\mathbf{y})\nabla_{\mathbf{y}}u(\mathbf{y},\omega)\big]u(\mathbf{x},\omega)\Big] = \mathbb{E}\big[f(\mathbf{y},\omega)g(\mathbf{x},\omega)\big], \qquad \mathbf{y}\in D,\ \mathbf{x}\in\partial D$$

$$\mathbb{E}\big[u(\mathbf{x},\omega)u(\mathbf{y},\omega)\big] = \mathbb{E}\big[g(\mathbf{x},\omega)g(\mathbf{y},\omega)\big], \qquad \mathbf{x},\mathbf{y}\in\partial D.$$

Random loadings VI

Use the linearity of the expectation to arrive at:

$$\operatorname{div}_{\mathbf{x}} \operatorname{div}_{\mathbf{y}} \Big[\mathbf{A}(\mathbf{x})\mathbf{A}(\mathbf{y})\nabla_{\mathbf{x}}\nabla_{\mathbf{y}}\mathbb{E}\big[u(\mathbf{x},\omega)u(\mathbf{y},\omega)\big]\Big] = \mathbb{E}\big[f(\mathbf{x},\omega)f(\mathbf{y},\omega)\big], \qquad \mathbf{x},\mathbf{y} \in D$$

$$-\operatorname{div}_{\mathbf{x}} \Big[\mathbf{A}(\mathbf{x})\nabla_{\mathbf{x}}\mathbb{E}\big[u(\mathbf{x},\omega)u(\mathbf{y},\omega)\big]\Big] = \mathbb{E}\big[f(\mathbf{x},\omega)g(\mathbf{y},\omega)\big], \qquad \mathbf{x} \in D,\ \mathbf{y} \in \partial D$$

$$-\operatorname{div}_{\mathbf{y}} \Big[\mathbf{A}(\mathbf{y})\nabla_{\mathbf{y}}\mathbb{E}\big[u(\mathbf{y},\omega)u(\mathbf{x},\omega)\big]\Big] = \mathbb{E}\big[f(\mathbf{y},\omega)g(\mathbf{x},\omega)\big], \qquad \mathbf{y} \in D,\ \mathbf{x} \in \partial D$$

$$\mathbb{E}\big[u(\mathbf{x},\omega)u(\mathbf{y},\omega)\big] = \mathbb{E}\big[g(\mathbf{x},\omega)g(\mathbf{y},\omega)\big], \qquad \mathbf{x},\mathbf{y} \in \partial D.$$

Random loadings

Theorem (Schwab/Todor [2003]): For the boundary value problem with random loading

$$-\operatorname{div}[\mathbf{A}\nabla u(\omega)] = f(\omega) \text{ in } D, \qquad u(\omega) = g(\omega) \text{ on } \partial D$$

one has

$$-\operatorname{div}[\mathbf{A}\nabla \mathbb{E}[u]] = \mathbb{E}[f] \text{ in } D, \qquad \mathbb{E}[u] = \mathbb{E}[g] \text{ on } \partial D$$

and

$$\begin{aligned}
(\operatorname{div}_{\mathbf{x}} \otimes \operatorname{div}_{\mathbf{y}}) \left[\big(\mathbf{A}(\mathbf{x}) \otimes \mathbf{A}(\mathbf{y})\big) (\nabla_{\mathbf{x}} \otimes \nabla_{\mathbf{y}}) \operatorname{Cor}[u](\mathbf{x},\mathbf{y}) \right] &= \operatorname{Cor}[f](\mathbf{x},\mathbf{y}), && \mathbf{x},\mathbf{y} \in D \\
-\operatorname{div}_{\mathbf{x}} \left[\mathbf{A}(\mathbf{x}) \nabla_{\mathbf{x}} \operatorname{Cor}[u](\mathbf{x},\mathbf{y}) \right] &= \operatorname{Cor}[f,g](\mathbf{x},\mathbf{y}), && \mathbf{x} \in D,\ \mathbf{y} \in \partial D \\
-\operatorname{div}_{\mathbf{y}} \left[\mathbf{A}(\mathbf{y}) \nabla_{\mathbf{y}} \operatorname{Cor}[u](\mathbf{x},\mathbf{y}) \right] &= \operatorname{Cor}[g,f](\mathbf{x},\mathbf{y}), && \mathbf{x} \in \partial D,\ \mathbf{y} \in D \\
\operatorname{Cor}[u](\mathbf{x},\mathbf{y}) &= \operatorname{Cor}[g](\mathbf{x},\mathbf{y}), && \mathbf{x},\mathbf{y} \in \partial D.
\end{aligned}$$

Random diffusion matrix

Random boundary value problem:

$$-\operatorname{div}\left[\mathbf{A}(\omega)\nabla u(\omega)\right] = f \text{ in } D, \qquad u(\omega) = g \text{ on } \partial D$$

$\longrightarrow$ the random solution depends nonlinearly on the random input data

$\longrightarrow$ linearize the random solution: needs sensitivity analysis

Theorem: Let $\mathbf{A} \in L^\infty(D;\mathbb{R}^{d\times d})$ be uniformly elliptic, i.e.,

$$\underline{a}\|\xi\|_2^2 \le \xi^T\mathbf{A}(\mathbf{x})\xi \le \overline{a}\|\xi\|_2^2, \quad \mathbf{x} \in D$$

and $u \in H^1(D)$ given by

$$-\operatorname{div}[\mathbf{A}\nabla u] = f \text{ in } D, \qquad u = g \text{ on } \partial D.$$

Then the mapping

$$F : L^\infty(D;\mathbb{R}^{d\times d}) \to \left\{v \in H^1(D) : v\big|_{\partial D} = g\right\}, \quad \mathbf{A} \mapsto F(\mathbf{A}) = u$$

is Fréchet-differentiable, where the derivative $\delta u = \delta u[\mathbf{B}]$ in the direction $\mathbf{B} \in L^\infty(D;\mathbb{R}^{d\times d})$ is given by

$$-\operatorname{div}[\mathbf{A}\nabla\delta u] = \operatorname{div}[\mathbf{B}\nabla u] \text{ in } D, \qquad \delta u = 0 \text{ on } \partial D.$$

Random Taylor expansion

Random diffusion matrix:

Let $\overline{\mathbf{A}} \in L^\infty(D;\mathbb{R}^{n\times n})$ be uniformly elliptic and

$$\mathbf{A}(\mathbf{x},\omega) = \overline{\mathbf{A}}(\mathbf{x}) + \varepsilon\mathbf{B}(\mathbf{x},\omega) \in L^2_{\mathbb{P}}\big(\Omega; L^\infty(D;\mathbb{R}^{d\times d})\big)$$

with

$$\|\mathbf{B}(\omega)\|_{L^\infty(D;\mathbb{R}^{d\times d})} \leq 1 \ \mathbb{P}\text{-a.e. } \omega \in \Omega, \qquad \mathbb{E}[\mathbf{B}](\mathbf{x}) = \mathbf{0}.$$

Theorem: The first order random Taylor expansion

$$u(\omega) = \overline{u} + \varepsilon\delta u(\omega) + O(\varepsilon^2)$$

holds almost surely in $H^1(D)$ where

$$-\operatorname{div}[\overline{\mathbf{A}}\nabla\overline{u}] = f \text{ in } D, \qquad \overline{u} = g \text{ on } \partial D$$

and

$$\delta u(\omega) := \delta\overline{u}[\mathbf{B}(\omega)],$$

satisfying

$$-\operatorname{div}[\mathbf{A}\nabla\delta u(\omega)] = \operatorname{div}[\mathbf{B}(\omega)\nabla\overline{u}] \text{ in } D, \qquad \delta u(\omega) = 0 \text{ on } \partial D.$$

Bochner spaces

- For a given Banach space X, the Bochner space $L^p_{\mathbb{P}}(\Omega;X)$, $1 \le p \le \infty$, consists of all equivalence classes of strongly measurable functions $v : \Omega \to X$ whose norm

$$\|v\|_{L^p_{\mathbb{P}}(\Omega;X)} := \begin{cases} \left(\int_\Omega \|v(\cdot,\omega)\|_X^p \, \mathrm{d}\mathbb{P}(\omega) \right)^{1/p}, & p < \infty \\ \operatorname*{ess\,sup}_{\omega \in \Omega} \|v(\cdot,\omega)\|_X, & p = \infty \end{cases}$$

  is finite.
- If $p = 2$ and X is a separable Hilbert space, then the Bochner space is isomorphic to the tensor product space $L^2_{\mathbb{P}}(\Omega) \otimes X$.

Expectation of the random solution

Theorem: There holds

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

in $H^1(D)$, where

$$-\operatorname{div}[\overline{\mathbf{A}}\nabla\overline{u}] = f \text{ in } D, \qquad \overline{u} = g \text{ on } \partial D.$$

Proof: Use the random Taylor expansion:

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

Herein, there holds $\mathbb{E}\big[\delta u(\omega)\big) = 0$ due to

$$-\operatorname{div}\big[\overline{\mathbf{A}}\nabla\mathbb{E}[\delta u]\big] = \operatorname{div}\big[\underbrace{\mathbb{E}[\mathbf{B}]}_{=\mathbf{0}}\nabla\overline{u}\big] \text{ in } D, \qquad \mathbb{E}[\delta u] = 0 \text{ on } \partial D. \qquad \square$$

Variance of the random solution

Theorem: There holds

$$\mathbb{V}[u] = \varepsilon^2 \mathbb{E}\big[\delta u(\omega)^2\big] + O\big(\varepsilon^3\big)$$

in $W^{1,1}(D)$, where

$$\mathbb{E}\big[\delta u(\mathbf{x},\omega)^2\big] = \mathrm{Cor}[\delta u](\mathbf{x},\mathbf{y})\big|_{\mathbf{x}=\mathbf{y}}$$

and

$$\begin{aligned}
&(\mathrm{div}_{\mathbf{x}} \otimes \mathrm{div}_{\mathbf{y}})\big[\big(\overline{\mathbf{A}}(\mathbf{x}) \otimes \overline{\mathbf{A}}(\mathbf{y})\big)(\nabla_{\mathbf{x}} \otimes \nabla_{\mathbf{y}})\,\mathrm{Cor}[\delta u](\mathbf{x},\mathbf{y})\big] \\
&\qquad = (\mathrm{div}_{\mathbf{x}} \otimes \mathrm{div}_{\mathbf{y}})\big[\mathrm{Cor}[\mathbf{B}](\nabla_{\mathbf{x}} \otimes \nabla_{\mathbf{y}})\big(\overline{u}(\mathbf{x}) \otimes \overline{u}(\mathbf{y})\big)\big], && \mathbf{x},\mathbf{y} \in D \\
&\qquad \mathrm{div}_{\mathbf{x}}\big[\overline{\mathbf{A}}(\mathbf{x})\nabla_{\mathbf{x}}\mathrm{Cor}[\delta u](\mathbf{x},\mathbf{y})\big] = 0, && \mathbf{x} \in D,\ \mathbf{y} \in \partial D \\
&\qquad \mathrm{div}_{\mathbf{y}}\big[\overline{\mathbf{A}}(\mathbf{y})\nabla_{\mathbf{y}}\mathrm{Cor}[\delta u](\mathbf{x},\mathbf{y})\big] = 0, && \mathbf{x} \in \partial D,\ \mathbf{y} \in D \\
&\qquad \mathrm{Cor}[\delta u](\mathbf{x},\mathbf{y}) = 0, && \mathbf{x},\mathbf{y} \in \partial D.
\end{aligned}$$

Proof: Use the random Taylor expansion to derive

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

Taking the trace yields the assertion. □

PDEs on random domains

Applications:

- tolerances in the shape of products fabricated by line production
- domains arising from inverse problems, e.g. tomography
- biological problems

Random boundary value problem:

$$\boxed{-\operatorname{div}\left[\mathbf{A}\nabla u(\omega)\right] = f \text{ in } D(\omega), \qquad u(\omega) = g \text{ on } \partial D(\omega)}$$

$\longrightarrow$ the random solution depends nonlinearly on the random input data
$\longrightarrow$ linearize the random solution: needs sensitivity analysis

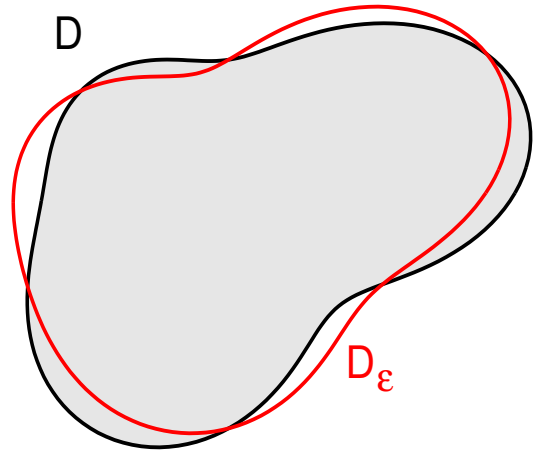
Assumption:

- security set $\mathbb{D} \supset D(\omega)$
- smooth data $\mathbf{A}, f, g \in C^\infty(\mathbb{D})$
- smooth random domains $D(\omega) \in C^{2,1}$

First order shape Taylor expansion

- **Boundary variation:** $\mathbf{V} := \kappa\mathbf{n}$ where $\kappa \in C^{2,1}(\partial D)$ satisfies $\|\kappa\|_{C^{2,1}(\partial D)} \leq 1$
- **Perturbed domain:** $\partial D_\varepsilon[\mathbf{V}] := \{\mathbf{x} + \varepsilon\mathbf{V}(\mathbf{x}) : \mathbf{x} \in \partial D\}$
- **Local shape derivative:**

  Consider the boundary value problems



$$-\operatorname{div}[\mathbf{A}\nabla u] = f \text{ in } D, \qquad u = g \text{ on } \partial D,$$
$$-\operatorname{div}\left[\mathbf{A}\nabla u_\varepsilon[\mathbf{V}]\right] = f \text{ in } D_\varepsilon[\mathbf{V}], \qquad u_\varepsilon[\mathbf{V}] = g \text{ on } \partial D_\varepsilon[\mathbf{V}].$$

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

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

  reads as

$$\boxed{\operatorname{div}\left[\mathbf{A}\nabla\delta u[\mathbf{V}]\right] = 0 \text{ in } D, \qquad \delta u[\mathbf{V}] = \langle \nabla(g-u), \mathbf{V}\rangle = \kappa\frac{\partial(g-u)}{\partial\mathbf{n}} \text{ on } \partial D}$$

$\rightsquigarrow$ **First order shape Taylor expansion:**

$$\boxed{u_\varepsilon(\mathbf{x}) = u(\mathbf{x}) + \varepsilon\delta u[\mathbf{V}](\mathbf{x}) + O(\varepsilon^2), \quad \mathbf{x} \in K \Subset D \cap D_\varepsilon[\mathbf{V}]}$$

Random domains

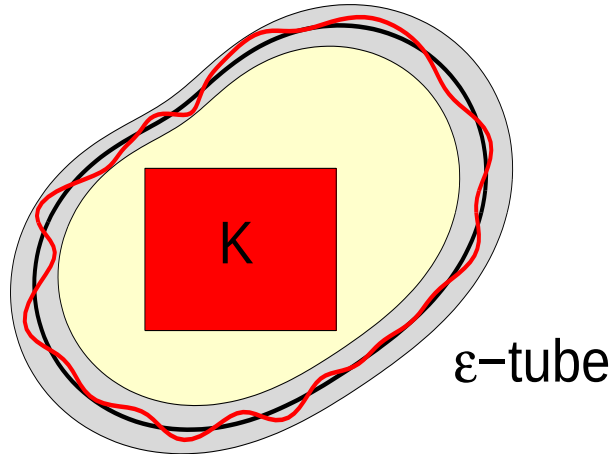
Consider a random boundary variation $\mathbf{V}(\mathbf{x},\omega) = \kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x})$ where

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

The random domain is described via its boundary

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

with $\varepsilon > 0$ being a sufficiently small parameter.



Random boundary value problem:

$$-\operatorname{div}[\mathbf{A}\nabla u(\omega)] = f \text{ in } D(\omega), \qquad u(\omega) = g \text{ on } \partial D(\omega)$$

Random shape Taylor expansion:

$$u(\mathbf{x},\omega) = \overline{u}(\mathbf{x}) + \varepsilon\delta u(\mathbf{x},\omega) + O(\varepsilon^2), \quad \mathbf{x} \in K, \quad \text{for } \mathbb{P}\text{-a.e. } \omega \in \Omega$$

where $\overline{u} \in H^1(\overline{D})$ denotes the solution of the deterministic Dirichlet problem

$$-\operatorname{div}[\mathbf{A}\nabla\overline{u}] = f \text{ in } \overline{D}, \qquad \overline{u} = g \text{ on } \partial\overline{D}$$

and

$$\delta u(\omega) := \delta\overline{u}[\kappa(\omega)\mathbf{n}].$$

Expectation and variance of the random solution

Theorem: There holds

$$\mathbb{E}[u](\mathbf{x}) = \overline{u}(\mathbf{x}) + O(\varepsilon^2), \qquad \mathbb{V}[u](\mathbf{x}) = \varepsilon^2 \mathbb{E}\big[\delta u(\mathbf{x},\omega)^2\big] + O(\varepsilon^3)$$

for all $\mathbf{x} \in K$.

$\longrightarrow$ Recall: $\mathbb{E}\big(\delta u(\mathbf{x},\omega)^2\big) = \mathrm{Cor}[\delta u](\mathbf{x},\mathbf{y})\big|_{\mathbf{x}=\mathbf{y}}$

Theorem: The two-point correlation $\mathrm{Cor}[\delta u]$ is given by boundary value problem

$$\begin{aligned}
(\mathrm{div}_{\mathbf{x}} \otimes \mathrm{div}_{\mathbf{y}})\big[\big(\mathbf{A}(\mathbf{x}) \otimes \mathbf{A}(\mathbf{y})\big)(\nabla_{\mathbf{x}} \otimes \nabla_{\mathbf{y}})\,\mathrm{Cor}[\delta u](\mathbf{x},\mathbf{y})\big] &= 0, && \mathbf{x},\mathbf{y} \in \overline{D} \\
\mathrm{div}_{\mathbf{x}}\big[\mathbf{A}(\mathbf{x})\nabla_{\mathbf{x}}\,\mathrm{Cor}[\delta u](\mathbf{x},\mathbf{y})\big] &= 0, && \mathbf{x} \in \overline{D},\ \mathbf{y} \in \partial\overline{D} \\
\mathrm{div}_{\mathbf{y}}\big[\mathbf{A}(\mathbf{y})\nabla_{\mathbf{y}}\,\mathrm{Cor}[\delta u](\mathbf{x},\mathbf{y})\big] &= 0, && \mathbf{x} \in \partial\overline{D},\ \mathbf{y} \in \overline{D} \\
\mathrm{Cor}[\delta u](\mathbf{x},\mathbf{y}) &= \mathrm{Cor}[\kappa](\mathbf{x},\mathbf{y})\left[\frac{\partial(g-\overline{u})}{\partial\mathbf{n}}(\mathbf{x}) \otimes \frac{\partial(g-\overline{u})}{\partial\mathbf{n}}(\mathbf{y})\right], && \mathbf{x},\mathbf{y} \in \partial\overline{D}.
\end{aligned}$$

Part 3. Numerics

Tensor product boundary value problems

Introduce Sobolev spaces of dominant mixed derivatives:

$$H^{s,t}_{\text{mix}}(D_1 \times D_2) := H^s(D_1) \otimes H^t(D_2).$$

Problem: Seek $u \in H^{1,1}_{\text{mix}}(D \times D)$ such that it holds

$$\begin{aligned}
(\operatorname{div}_{\mathbf{x}} \otimes \operatorname{div}_{\mathbf{y}}) \left[(\mathbf{A}(\mathbf{x}) \otimes \mathbf{A}(\mathbf{y}))(\nabla_{\mathbf{x}} \otimes \nabla_{\mathbf{y}}) u(\mathbf{x},\mathbf{y}) \right] &= f(\mathbf{x},\mathbf{y}), && \mathbf{x},\mathbf{y} \in D \\
-\operatorname{div}_{\mathbf{x}} \left[\mathbf{A}(\mathbf{x}) \nabla_{\mathbf{x}} u(\mathbf{x},\mathbf{y}) \right] &= h(\mathbf{x},\mathbf{y}), && \mathbf{x} \in D,\ \mathbf{y} \in \partial D \\
-\operatorname{div}_{\mathbf{y}} \left[\mathbf{A}(\mathbf{y}) \nabla_{\mathbf{y}} u(\mathbf{x},\mathbf{y}) \right] &= h(\mathbf{y},\mathbf{x}), && \mathbf{x} \in \partial D,\ \mathbf{y} \in D \\
u(\mathbf{x},\mathbf{y}) &= g(\mathbf{x},\mathbf{y}), && \mathbf{x},\mathbf{y} \in \partial D.
\end{aligned}$$

Shift property: If $f \in H^{s-2,s-2}_{\text{mix}}(D \times D)$,
$h \in H^{s-2,s-1/2}_{\text{mix}}(D \times \Gamma)$,
$g \in H^{s-1/2,s-1/2}_{\text{mix}}(\Gamma \times \Gamma)$, then it holds

$$u \in H^{s,s}_{\text{mix}}(D \times D)$$

provided that D is sufficiently smooth.

Multilevel finite elements

Assumption: Finite element spaces $V_j = \mathrm{span}\{\phi_{j,k} : k \in \Delta_j\}$ based on standard Lagrangian finite elements of order r, satisfying $h_j \sim 2^{-j}$

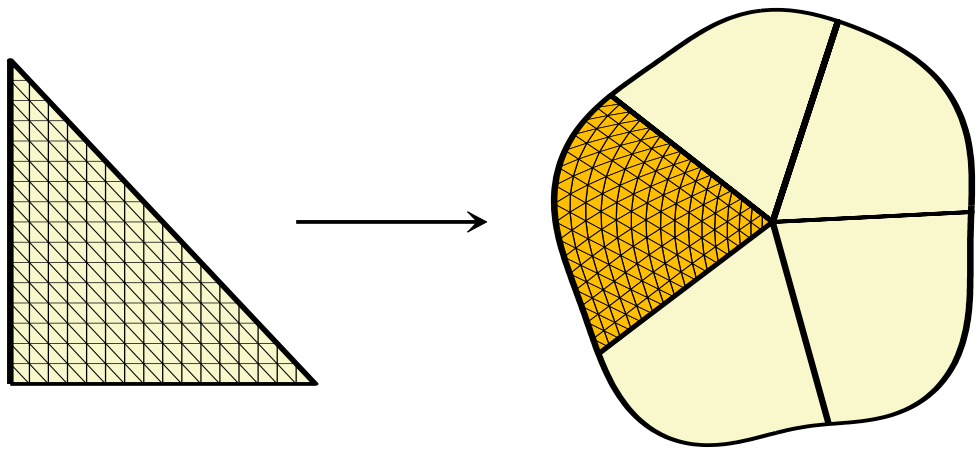
Multilevel hierarchy:

$$V_0 \subset V_1 \subset \cdots \subset V_j \subset V_{j+1} \subset \cdots \subset H^1(D)$$

Refinement $\longrightarrow$

Parametric finite elements:

- $\overline{D} = \bigcup_{i=1}^{M} \overline{D}_i, \quad D_i = \gamma_i(\triangle), \quad i = 1, \ldots, M$
- $\overline{D}_i \cap \overline{D}_j$, $i \neq j$, is either empty or a lower dimensional face
- parametric finite elements by lifting standard Lagrangian finite elements from $\triangle$ to D via the parametrization



Treatment of nontrivial boundary data

Ansatz:

$$u_J = \sum_{j+j'\le J} \sum_{k\in\triangle_j} \sum_{k'\in\triangle_{j'}} u_{(j,k),(j',k')}(\phi_{j,k}\otimes\phi_{j',k'}) = u_J^{D,D} + u_J^{D,\partial D} + u_J^{\partial D,D} + u_J^{\partial D,\partial D}$$

1. compute Dirichlet data on $\partial D\times\partial D$:

$$\big(\mathbf{G}_J^{\partial D}\otimes\mathbf{G}_J^{\partial D}\big)\mathbf{u}_J^{\partial D,\partial D} = \mathbf{g}_J^{\partial D,\partial D}$$

2. compute solution on $D\times\partial D$ and $\partial D\times D$:

$$\big(\mathbf{S}_J^{D}\otimes\mathbf{G}_J^{\partial D}\big)\mathbf{u}_J^{D,\partial D} = \mathbf{h}_J^{D,\partial D} - \big(\mathbf{S}_J^{\partial D}\otimes\mathbf{G}_J^{\partial D}\big)\mathbf{u}_J^{\partial D,\partial D}$$

$$\big(\mathbf{G}_J^{\partial D}\otimes\mathbf{S}_J^{D}\big)\mathbf{u}_J^{\partial D,D} = \mathbf{h}_J^{\partial D,D} - \big(\mathbf{G}_J^{\partial D}\otimes\mathbf{S}_J^{\partial D}\big)\mathbf{u}_J^{\partial D,\partial D}$$

3. compute the solution $D\times D$:

$$\big(\mathbf{S}_J^{D}\otimes\mathbf{S}_J^{D}\big)\mathbf{u}_J^{D,D} = \mathbf{f}_J^{D,D} - \big(\mathbf{S}_J^{\partial D}\otimes\mathbf{S}_J^{\partial D}\big)\mathbf{u}_J^{\partial D,\partial D} - \big(\mathbf{S}_J^{D}\otimes\mathbf{S}_J^{\partial D}\big)\mathbf{u}_J^{D,\partial D} - \big(\mathbf{S}_J^{\partial D}\otimes\mathbf{S}_J^{D}\big)\mathbf{u}_J^{\partial D,D}$$

Theorem: The approximate solution $\widehat{u}_J\in\widehat{V}_J$ satisfies the error estimate

$$\|u-u_J\|_{H^{1,1}_{\mathsf{mix}}(D\times D)} \lesssim 2^{-J(r-1)}\|u\|_{H^{r,r}_{\mathsf{mix}}(D\times D)}$$

provided that the given data are sufficiently smooth.

How to solve tensor product problems?

High-dimensional problem: $(\mathcal{A} \otimes \mathcal{A})u = f$ on $D \times D$

► **Low rank approximation (e.g. by truncated Karhunen-Loève expansion):**

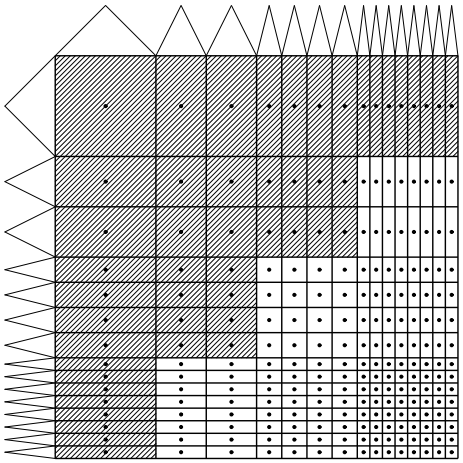
Replace $f \in L^2(D \times D)$ by a low rank approximation

$$f(\mathbf{x}, \mathbf{y}) \approx \sum_{m=1}^{M} \alpha_m \varphi_m(\mathbf{x}) \psi_m(\mathbf{y})$$

and compute

$$u(\mathbf{x}, \mathbf{y}) \approx \sum_{m=1}^{M} \alpha_m \left(\mathcal{A}^{-1} \varphi_m\right)(\mathbf{x}) \left(\mathcal{A}^{-1} \psi_m\right)(\mathbf{y})$$

► **Sparse grids or sparse tensor product spaces:**



Pivoted Cholesky decomposition I

Lemma. Let the matrix

$$\mathbf{A} = \left[\begin{array}{c|c} a & \mathbf{b}^T \\ \hline \mathbf{b} & \mathbf{C} \end{array}\right] \in \mathbb{R}^{n \times n}$$

be symmetric and positive semi-definite with $a > 0$. Then, the Schur complement

$$\mathbf{S} := \mathbf{C} - \frac{1}{a}\mathbf{b}\mathbf{b}^T \in \mathbb{R}^{(n-1)\times(n-1)}$$

is well-defined and also symmetric and positive semi-definite.

► **Observation.** Pivoting enables to apply the Cholesky decomposition to positive semi-definite matrices. Hence, if $\mathbf{A}$ has finite rank m, the pivoted Cholesky decomposition terminates with a rank m decomposition

$$\mathbf{A} = \mathbf{L}_m \mathbf{L}_m^T.$$

► **Question.** What happens if $\mathbf{A}$ is nearly positive semi-definite, i.e.,

$$\|\mathbf{A} - \mathbf{A}_m\|_2 \leq \varepsilon$$

with $\mathbf{A}_m$ being a positive definite rank m matrix?

Pivoted Cholesky decomposition II

► **Trace norm.** The best possible reduction of the trace error in one Cholesky step is achieved if the trace of the Schur complement becomes as small as possible. This amounts to the problem

$$\operatorname{trace}(\mathbf{A}-\mathbf{A}_m) = \operatorname{trace}\mathbf{S} = \operatorname{trace}(\mathbf{A}-\mathbf{A}_{m-1}) - \frac{1}{a_{i,i}^{(m-1)}}\left\|\mathbf{a}_i^{(m-1)}\right\|_2^2 \to \min_{i=1}^{n}.$$

$\rightsquigarrow$ too expensive!

► **Strategy.** Remove the largest diagonal coefficient of the remainder matrix:

$$\operatorname{trace}(\mathbf{A}-\mathbf{A}_m) = \operatorname{trace}\mathbf{S} = \operatorname{trace}(\mathbf{A}-\mathbf{A}_{m-1}) - \max_i a_{i,i}^{(m-1)}.$$

$\rightsquigarrow$ total pivoting!

Algorithm (total pivoting): Permute the matrix such that the largest diagonal element is at the $(1,1)$-position and compute then the Cholesky step:

$$\mathbf{A} = \mathbf{A}_m + \mathbf{E}_m = \mathbf{L}_m\mathbf{L}_m^T + \mathbf{E}_m \quad \text{with} \quad \mathbf{E}_m := \mathbf{P}_1\mathbf{P}_2\cdots\mathbf{P}_m \left[\begin{array}{c|c} \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{S}_m \end{array}\right] \mathbf{P}_m\cdots\mathbf{P}_2\mathbf{P}_1.$$

Algorithm: cost $O(nm^2)$

Data: matrix $\mathbf{A} = [a_{i,j}] \in \mathbb{R}^{n\times n}$ and error tolerance $\varepsilon > 0$
Result: low-rank approximation $\mathbf{A}_m = \sum_{i=1}^{m} \boldsymbol{\ell}_i \boldsymbol{\ell}_i^T$ such that
$\operatorname{trace}(\mathbf{A} - \mathbf{A}_m) \leq \varepsilon$

begin
- set $m := 1$;
- set $\mathbf{d} := \operatorname{diag}(\mathbf{A})$ and $error := \|\mathbf{d}\|_1$;
- initialize $\boldsymbol{\pi} := (1, 2, \ldots, n)$;
- **while** $error > \varepsilon$ **do**
  - set $i := \arg\max\{d_{\pi_j} : j = m, m+1, \ldots, n\}$;
  - swap π_m and π_i;
  - set $\ell_{m,\pi_m} := \sqrt{d_{\pi_m}}$;
  - **for** $m + 1 \leq i \leq n$ **do**
    - compute $\ell_{m,\pi_i} := \left(a_{\pi_m,\pi_i} - \sum_{j=1}^{m-1} \ell_{j,\pi_m}\ell_{j,\pi_i}\right) \Big/ \ell_{m,\pi_m}$;
    - update $d_{\pi_i} := d_{\pi_i} - \ell_{m,\pi_m}\ell_{m,\pi_i}$;
  - compute $error := \sum_{i=m+1}^{n} d_{\pi_i}$;
  - increase $m := m + 1$;

end

Features

- the method was introduced by Beebe & Linderberg (1977)
- symmetric low-rank approximation: $\mathbf{A} \approx \mathbf{A}_m = \mathbf{L}_m \mathbf{L}_m^T$
- approximation error is rigorously controlled in terms of the trace norm
- stable variant of the Cholesky decomposition, especially if the eigenvalues decay rapidly
- only the diagonal coefficients and the m columns of $\mathbf{A}$, associated with the pivot elements, need to be computed
- extremely simple to implement
- coincides with the adaptive cross approximation for symmetric matrices
- a purely algebraic convergence proof is available

Convergence

Theorem: Assume that the eigenvalues of $\mathbf{A} \in \mathbb{R}^{n\times n}$ satisfy

$$4^m \lambda_m \lesssim \exp(-bm)$$

for some $b > 0$ uniformly in n. Then, the pivoted Cholesky approximation $\mathbf{A}_m$ with rank $m \sim |\log(\varepsilon/n)|$ satisfies $\operatorname{trace}(\mathbf{A}_m - \mathbf{A}) \lesssim \varepsilon$ uniformly as ε tends to zero.

Proof. Assume that $\mathbf{A}$ is permuted such that the k-th pivot is found at the (k,k)-position for all $k = 1, 2, \ldots, n$. Then, $\mathbf{L}_m \in \mathbb{R}^{n\times m}$ is always a lower triangular matrix. It follows from

$$\mathbf{A}_m = \mathbf{L}_m \mathbf{L}_m^T = \begin{bmatrix} \mathbf{L}_{1,1} & \mathbf{0} \\ \mathbf{L}_{2,1} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{L}_{1,1}^T & \mathbf{L}_{2,1}^T \\ \mathbf{0} & \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{L}_{1,1}\mathbf{L}_{1,1}^T & \mathbf{L}_{1,1}\mathbf{L}_{2,1}^T \\ \mathbf{L}_{2,1}\mathbf{L}_{1,1}^T & \mathbf{L}_{2,1}\mathbf{L}_{2,1}^T \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{1,1} & \mathbf{A}_{1,2} \\ \mathbf{A}_{2,1} & \mathbf{L}_{2,1}\mathbf{L}_{2,1}^T \end{bmatrix}$$

that $\mathbf{L}_{1,1}\mathbf{L}_{1,1}^T$ is the (pivoted) Cholesky decomposition of $\mathbf{A}_{1,1}$. Consequently, we have

$$\frac{1}{\lambda_m(\mathbf{A}_{1,1})} = \|\mathbf{A}_{1,1}^{-1}\|_2 = \|\mathbf{L}_{1,1}^{-1}\|_2^2 \overset{\text{sharp!}}{\leq} \frac{4^m + 6m - 1}{9\ell_{m,m}^2} \leq \frac{4^m}{\ell_{m,m}^2}.$$

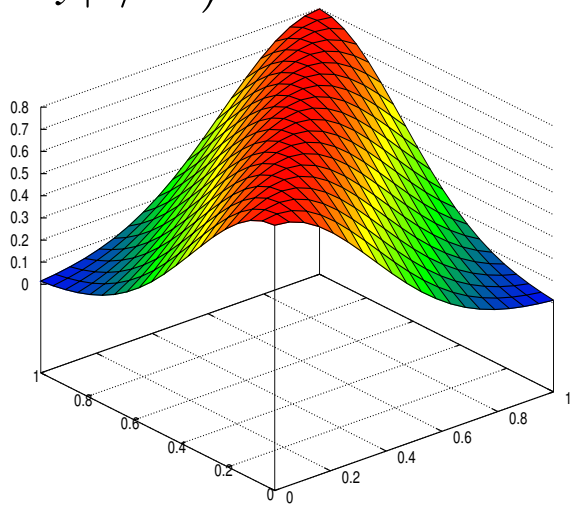
The trace norm of $\mathbf{A} - \mathbf{A}_m$ is bounded by $(n-m)$-times the pivot element $\ell_{m,m}^2$:

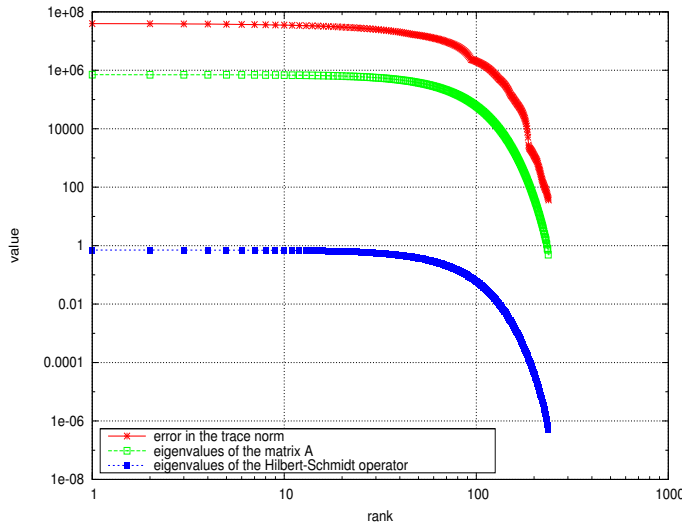
$$\operatorname{trace}(\mathbf{A} - \mathbf{A}_m) \leq (n-m)\ell_{m,m}^2 \leq 4^m n \lambda_m(\mathbf{A}_{1,1}) \underset{\text{Fischer}}{\overset{\text{Courant}}{\leq}} 4^m n \lambda_m(\mathbf{A}). \qquad \square$$

Numerical results I

Gauss kernel: $(2\pi\sigma^2)^{-1/2}\exp\left(|x-y|^2/\sigma^2\right)$

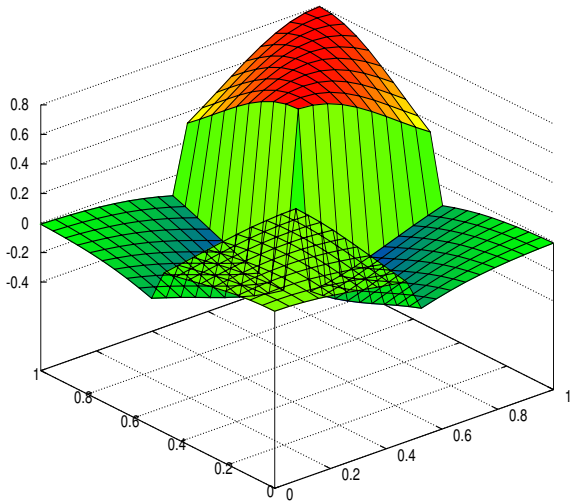
ε	value of σ				
	1	0.5	0.1	0.05	0.01
10^{-1}	2	3	10	19	89
10^{-2}	3	5	15	28	137
10^{-3}	4	5	19	36	173
10^{-4}	5	6	21	39	187
10^{-5}	5	7	24	46	214
10^{-6}	5	8	27	50	238

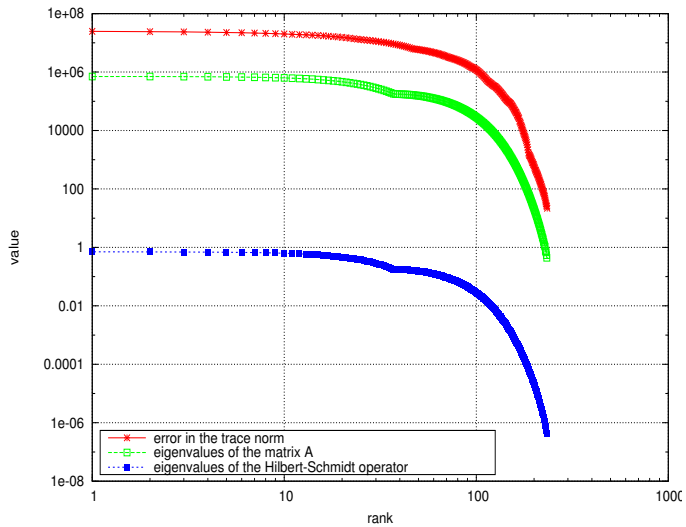




Jumping Gauss kernel:

ε	value of σ				
	1	0.5	0.1	0.05	0.01
10^{-1}	2	3	10	17	81
10^{-2}	3	4	15	28	131
10^{-3}	4	5	18	34	168
10^{-4}	4	6	21	39	186
10^{-5}	5	7	24	45	211
10^{-6}	5	8	26	50	234

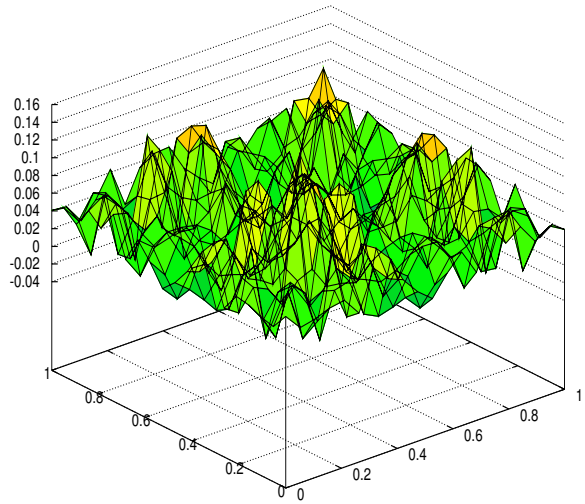


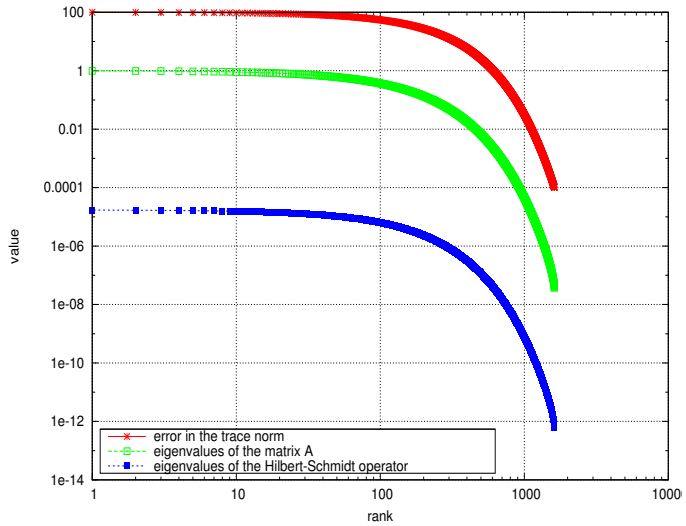


Numerical results II

Random kernel: $\mathbf{A} = \sum_{k=1}^{m} \lambda_k \mathbf{v}_k \mathbf{v}_k^T,\ \lambda_k = \exp(-\sigma k),\ \mathbf{v}_k^T \mathbf{v}_\ell = \delta_{k,\ell}$

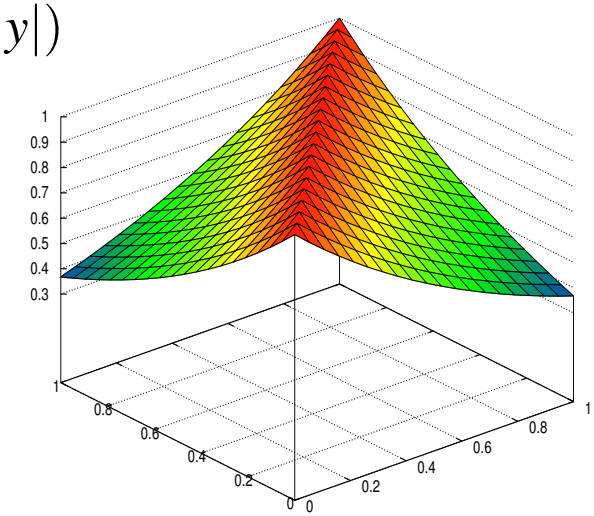
ε	value of σ				
	1	0.5	0.1	0.05	0.01
10^{-1}	3	6	29	61	333
10^{-2}	6	11	56	115	610
10^{-3}	8	15	81	167	873
10^{-4}	10	21	106	216	1126
10^{-5}	13	25	130	266	1375
10^{-6}	15	30	154	315	1618

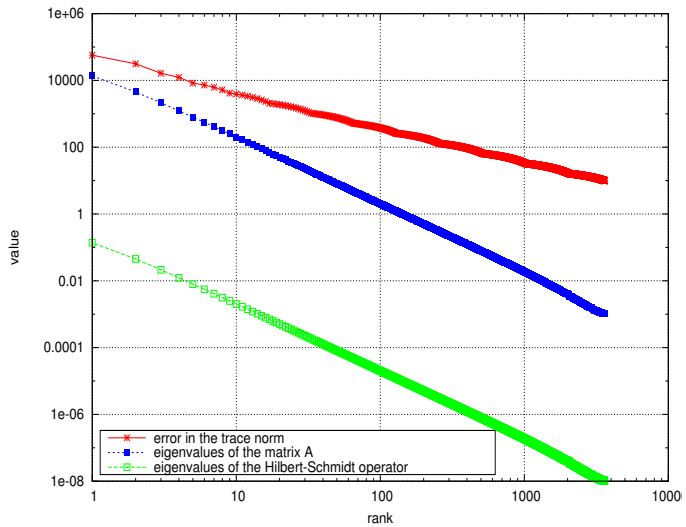




Exponential kernel: $\exp(-\sigma|x-y|)$

ε	value of σ				
	1	10^{-1}	10^{-2}	10^{-3}	10^{-4}
10^{-1}	5	1	1	1	1
10^{-2}	36	5	1	1	1
10^{-3}	376	36	5	1	1
10^{-4}	3616	376	36	5	1





Numerical results III

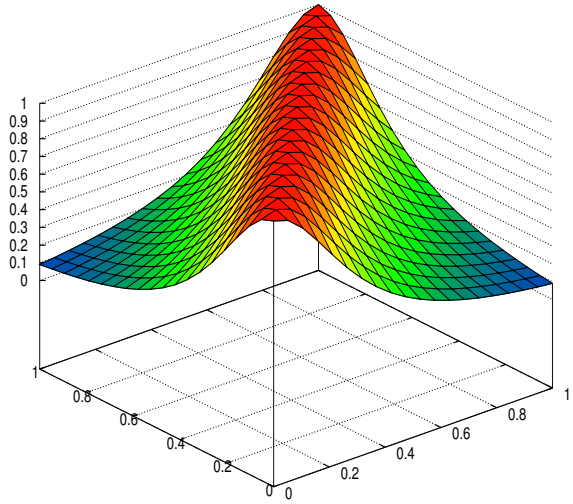
Problem: $(\Delta \otimes \Delta)\,\mathrm{Cor}[u] = \mathrm{Cor}[f]$ on $D \times D$, $\quad \mathrm{Cor}[u] = 0$ on $\partial(D \times D)$

Approximate

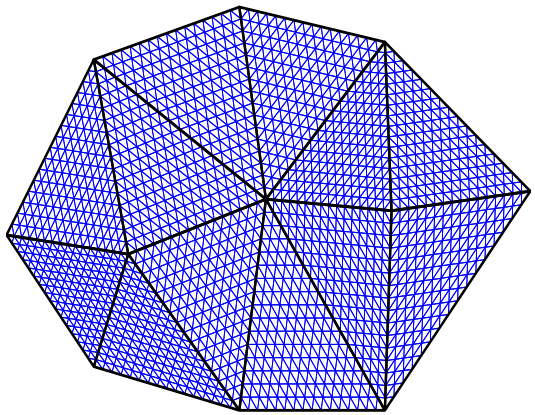
$$\mathrm{Cor}[f](\mathbf{x},\mathbf{y}) = \frac{1}{\sigma + \|\mathbf{x}-\mathbf{y}\|^2} \approx \sum_{i=1}^{m} \psi_i(\mathbf{x})\psi_i(\mathbf{y})$$

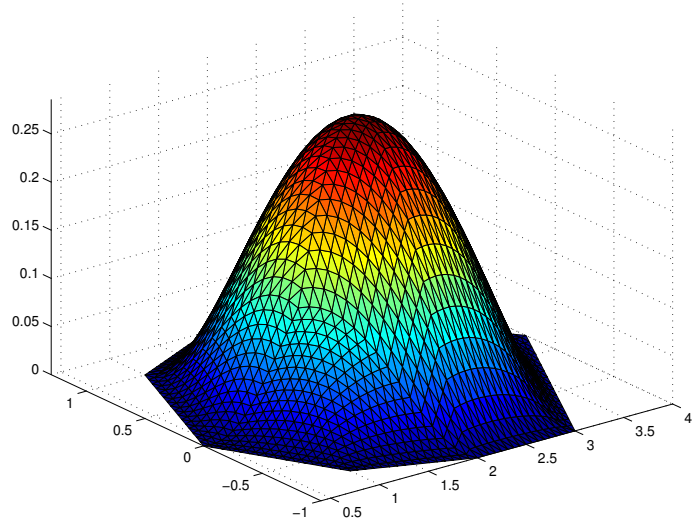
by the pivoted Cholesky decomposition, solve $-\Delta\varphi_i = \psi_i$ for all i, and compute

$$\mathrm{Cor}[u](\mathbf{x},\mathbf{y}) \approx \sum_{i=1}^{m} \varphi_i(\mathbf{x})\varphi_i(\mathbf{y}),\ \mathbb{V}[u](\mathbf{x}) \approx \sum_{i=1}^{m} \varphi_i^2(\mathbf{x}) - \mathbb{E}[u]^2(\mathbf{x}).$$

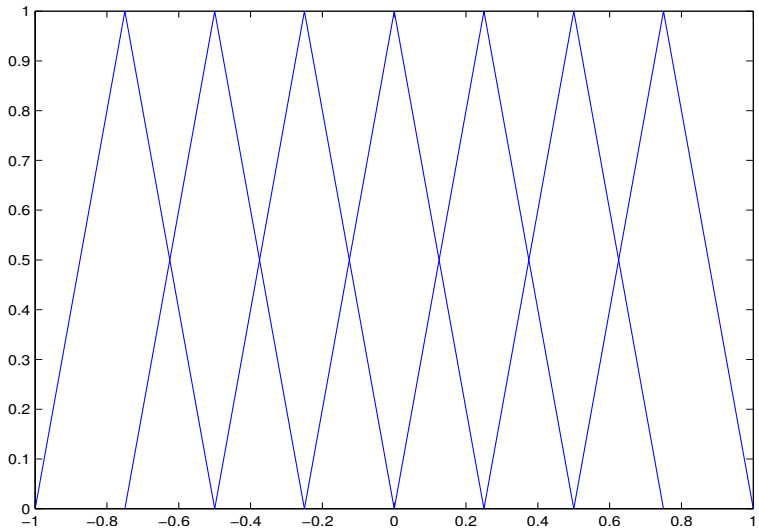


ε	value of σ				
	0.1	0.2	0.4	0.8	1.6
10^{-1}	85	46	27	14	9
10^{-2}	234	122	66	37	21
10^{-3}	442	236	123	68	38
10^{-4}	710	371	198	108	61
10^{-5}	1038	539	290	157	87
10^{-6}	1426	748	395	214	118

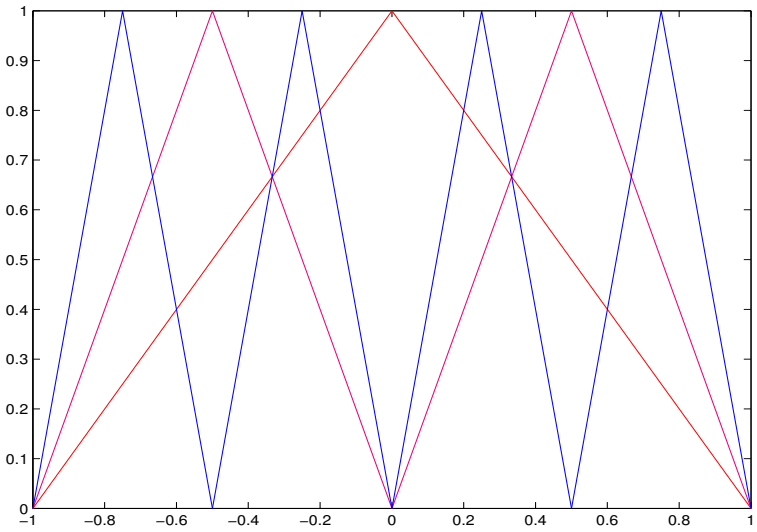




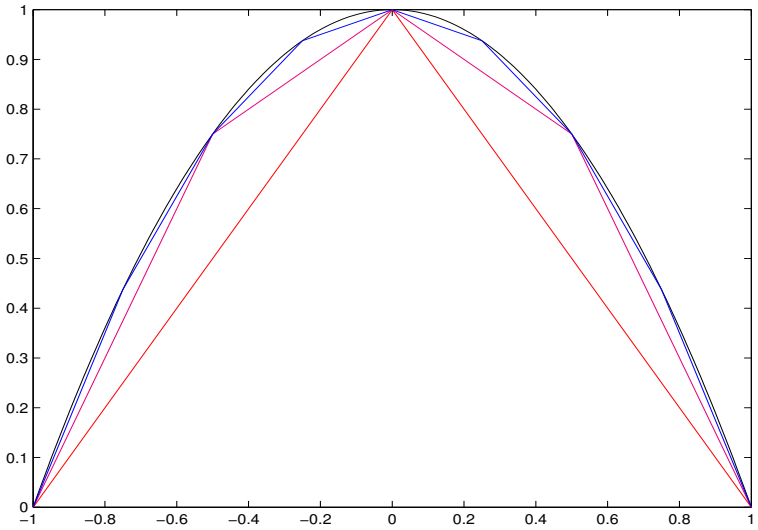
Sparse tensor product spaces I



piecewise linear basis $\{\phi_{J,k}\}_k$



hierarchical basis $\{\psi_{j,k}\}_{j,k}$



$$a_{0,0} = 1$$

$$a_{1,0} = a_{1,1} = 1/4$$

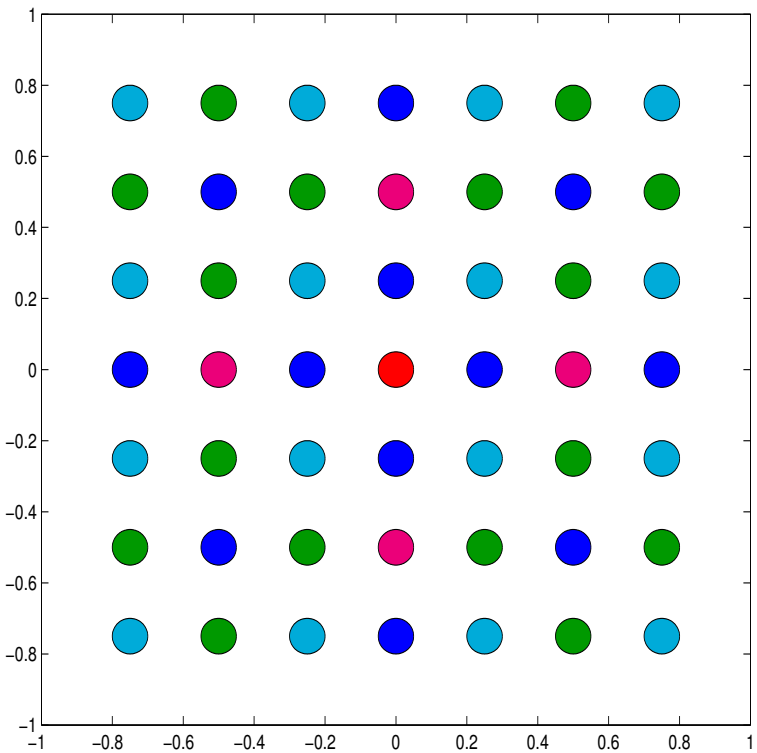
$$a_{2,0} = a_{2,1} = a_{2,2} = a_{2,3} = 1/16$$

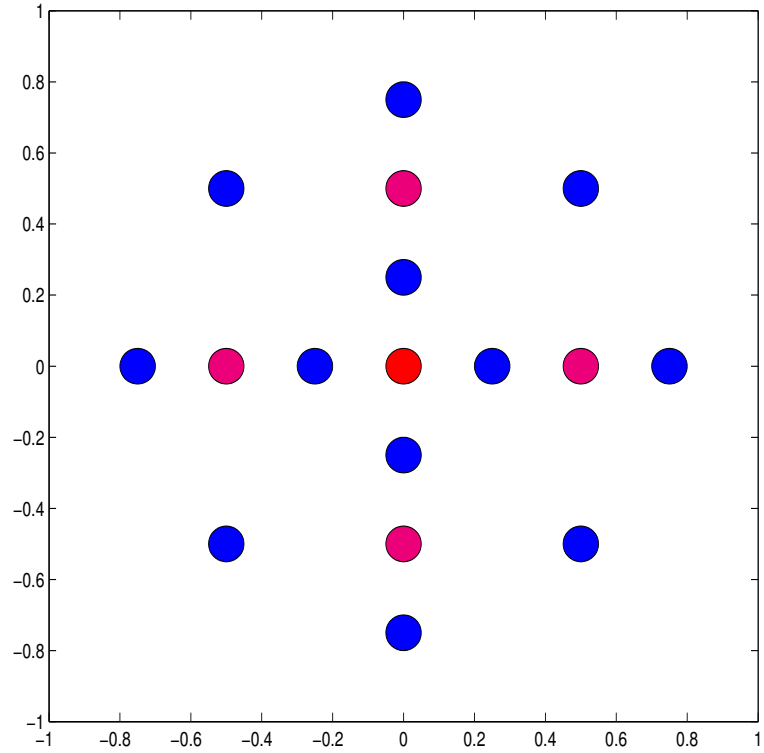
$$a_{3,0} = a_{3,1} = \ldots = a_{3,7} = 1/64$$

$$\vdots$$

Sparse tensor product spaces II

● = 1 ● = 1/4 ● = 1/16 ● = 1/64 ● = 1/256





full tensor product space:

$$V_J \otimes V_J := \sum_{j,j' \le J} W_j \otimes W_{j'}$$

$$\dim(V_J \otimes V_J) = N_J^2$$

$$\inf \|f - f_J\|_{L^2(\square)} \lesssim h_J^r \|f\|_{H^r(\square)}$$

sparse grid approach:

$$\widehat{V}_J := \sum_{j+j' \le J} W_j \otimes W_{j'}$$

$$\dim \widehat{V}_J = N_J \log N_J$$

$$\inf \|f - f_J\|_{L^2(\square)} \lesssim h_J^r \sqrt{|\log h_J|} \|f\|_{H^{r,r}_{\text{mix}}(\square)}$$

Sparse tensor discretization of the second moment

Problem:

$$\boxed{\begin{gathered}(\mathrm{div}\otimes\mathrm{div})\big[(\mathbf{A}\otimes\mathbf{A})(\nabla\otimes\nabla)\,\mathrm{Cor}[u]\big] = \mathrm{Cor}[f] \text{ on } D\times D \\ \mathrm{Cor}[u] = 0 \text{ on } \partial(D\times D)\end{gathered}}$$

Introduce the Galerkin projection

$$P_j : H_0^1(D) \to V_j, \quad w \mapsto P_j w =: w_j$$

$$\text{where } \langle \mathbf{A}(\nabla w - \nabla w_j), \nabla v_j\rangle_{L^2(D)} = 0 \text{ for all } v_j \in V_j$$

and define the complement spaces

$$\boxed{W_j := (P_j - P_{j-1})H_0^1(D) \subset V_j \text{ for } j \geq 1, \quad W_0 := V_0.}$$

This yields the multilevel decomposition

$$V_J = W_0 \oplus W_1 \oplus \cdots \oplus W_J.$$

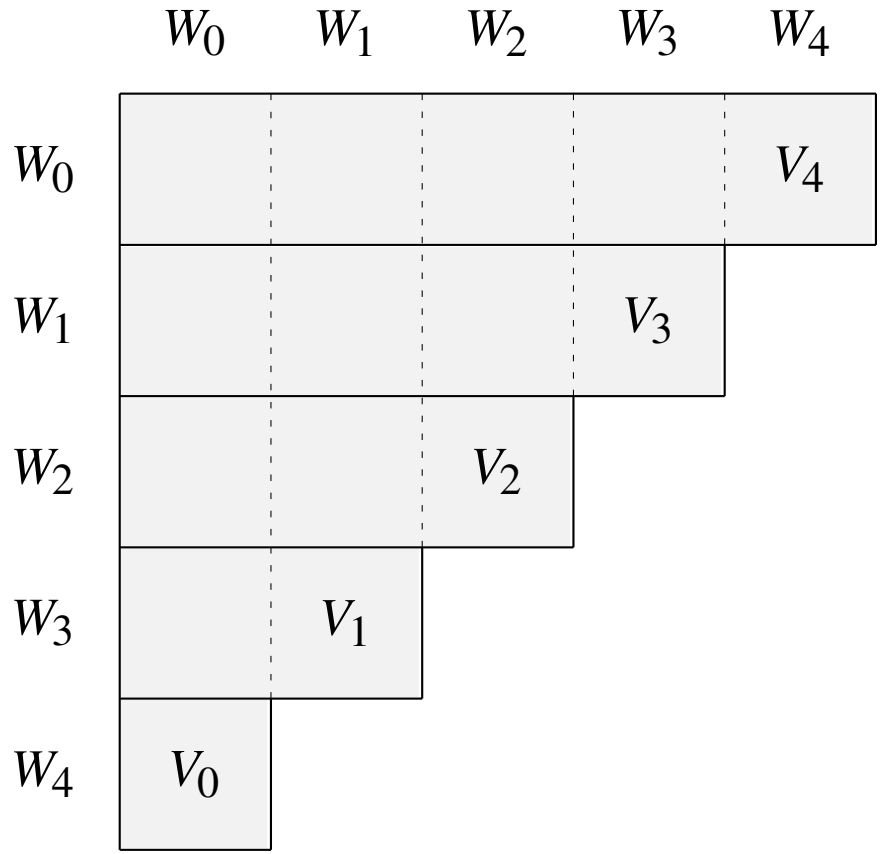
Sparse tensor product spaces

- The starting point is multilevel decomposition

$$V_J = W_0 \oplus W_1 \oplus \cdots \oplus W_J$$

- The sparse tensor product space is given by

$$\begin{aligned}\widehat{V}_J &= \bigoplus_{j+j' \le J} W_j \otimes W_{j'} \\ &= \bigoplus_{j=0}^{J} W_j \left(\bigoplus_{\ell'=0}^{j-\ell} W_{\ell'} \right) \\ &= \bigoplus_{j=0}^{J} W_j \otimes V_{J-j}\end{aligned}$$



- The dimension of $\widehat{V}_J$ is $\widehat{N}_J := \dim \widehat{V}_J \sim N_J \log N_J \ll N_J^2 = \dim(V_J \otimes V_J)$ while the approximation power of $\widehat{V}_J$ is nearly as good as in the full tensor product space $V_J \otimes V_J$.

Combination technique I

Lemma: The related Galerkin system decouples since for arbitrary functions $\widehat{\varphi}_j \in W_j \otimes V_{J-j}$ and $\widehat{\psi}_{j'} \in W_{j'} \otimes V_{J-j'}$ there holds

$$\langle (\mathbf{A} \otimes \mathbf{A})(\nabla \otimes \nabla)\widehat{\varphi}_j, (\nabla \otimes \nabla)\widehat{\psi}_{j'} \rangle_{L^2(D \times D)} = 0 \text{ if } j \neq j'.$$

Proof.

$$\langle (\mathbf{A} \otimes \mathbf{A})(\nabla \otimes \nabla) \overbrace{\sum_k \alpha_{j,k} \otimes \beta_{J-j,k}}^{=\widehat{\varphi}_j}, (\nabla \otimes \nabla) \overbrace{\sum_{k'} \gamma_{j',k'} \otimes \delta_{J-j',k'}}^{=\widehat{\psi}_{j'}} \rangle_{L^2(D \times D)}$$

$$= \sum_{k,k'} \underbrace{\langle \mathbf{A}\nabla\alpha_{j,k}, \nabla\gamma_{j',k'} \rangle_{L^2(D)}}_{=0 \text{ if } j \neq j'} \langle \mathbf{A}\nabla\beta_{J-j,k}, \nabla\delta_{J-j',k'} \rangle_{L^2(D)}.$$

□

Theorem: The discretization of $\mathrm{Cor}[u]$ in $\widehat{V}_j$ leads to the decomposition

$$\widehat{\mathrm{Cor}}_J[u] = \sum_{j=0}^{J} v_j \quad \text{with} \quad \underbrace{v_j}_{\in W_j \otimes V_{J-j}} = \underbrace{p_{j,J-j}}_{\in V_j \otimes V_{J-j}} - \underbrace{p_{j-1,J-j}}_{\in V_{j-1} \otimes V_{J-j}}$$

where the $p_{j,j'} \in V_j \otimes V_{j'}$ satisfy the sub-problems

$$\langle (\mathbf{A} \otimes \mathbf{A})(\nabla \otimes \nabla) p_{j,j'}, (\nabla \otimes \nabla) q_{j,j'} \rangle_{L^2(D \times D)} = \langle f, q_{j,j'} \rangle_{L^2(D \times D)}$$

for all $q_{j,j'} \in V_j \otimes V_j'$.

Combination technique II

With the ansatz $p_{j,j'} = \sum_{k\in\Delta_j}\sum_{k'\in\Delta_{j'}} p_{(j,k),(j',k')}(\phi_{j,k}\otimes\phi_{j',k'})$, the solution of the j-th sub-problem is given by

$$(\mathbf{S}_j \otimes \mathbf{S}_{j'})\mathbf{p}_{j,j'} = \mathbf{f}_{j,j'} \quad \text{with} \quad \mathbf{S}_j = \Big[\langle \mathbf{A}\nabla\phi_{j,k'}, \phi_{j',k'}\rangle_{L^2(D)}\Big]_{k,k'\in\Delta_j},$$

$$\mathbf{f}_{j,j'} = -\Big[\langle f, \varphi_{j,k}\otimes\phi_{j',k'}\rangle_{L^2(D\times D)}\Big]_{k\in\Delta_j, k'\in\Delta_{j'}}.$$

Theorem: The cost of computing the Galerkin solution $\widehat{\mathrm{Cor}}_J[u]$ via the combination technique is of optimal order $O(N_J \log N_J)$. The approximation error is bounded by

$$\|\mathrm{Cor}[u] - \widehat{\mathrm{Cor}}_J[u]\|_{H^{1,1}_{\mathrm{mix}}(D\times D)} \lesssim 2^{-J(r-1)} J \|\mathrm{Cor}[u]\|_{H^{r,r}_{\mathrm{mix}}(D\times D)}$$

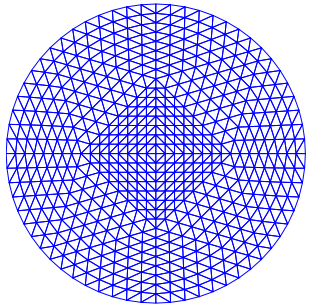
provided that the given data are sufficiently smooth.

Numerical results I

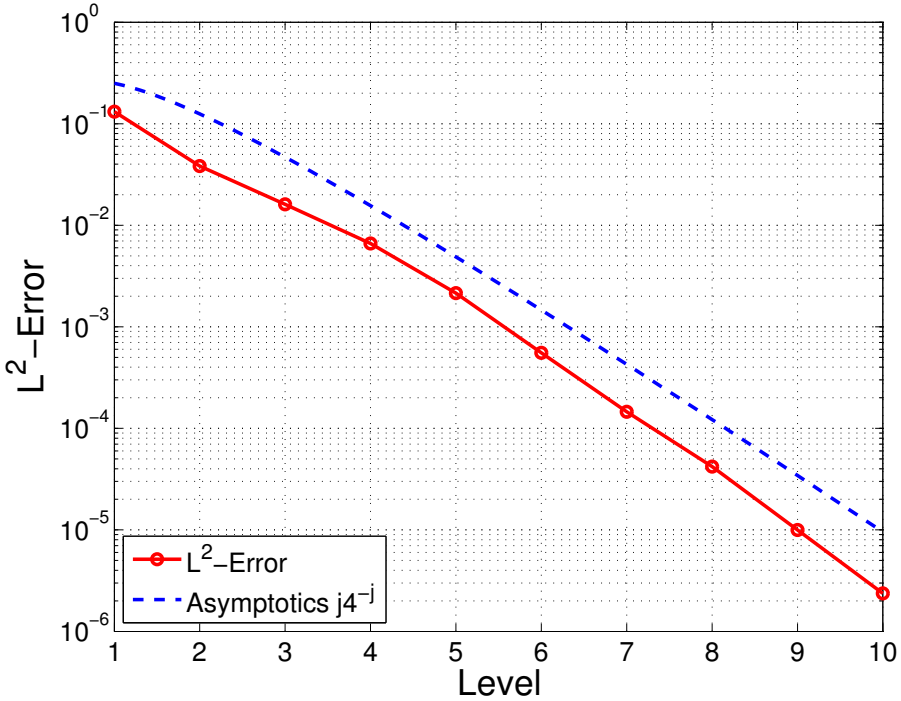
Deterministic boundary value problem on the tensorized unit disc:

$$(\Delta \otimes \Delta)u = f_1 \otimes f_2 \text{ on } D \times D, \quad u = 0 \text{ on } \partial(D \times D)$$

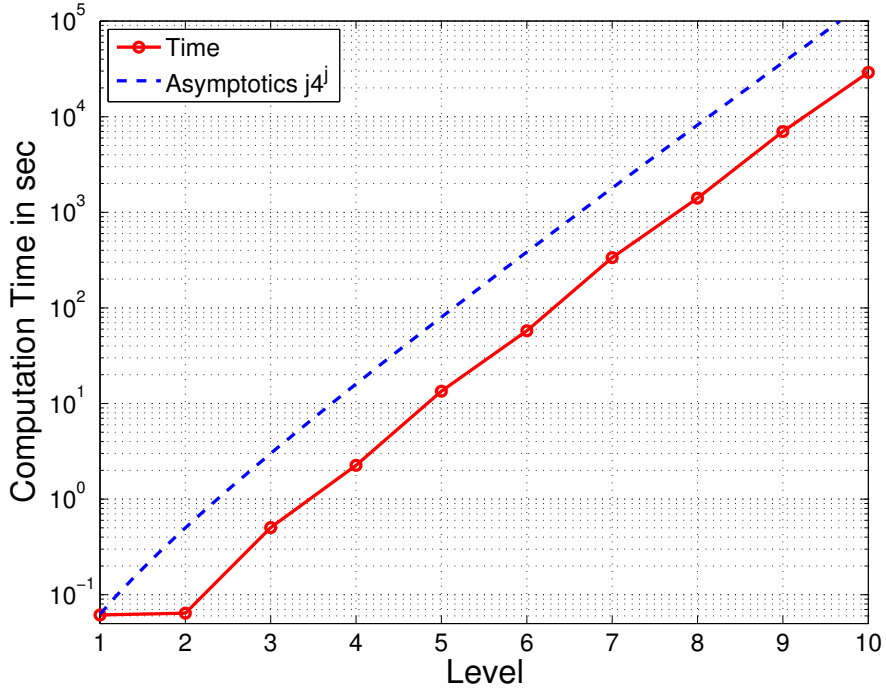
with $\quad f_1(x_1, x_2) = 1, \quad f_2(y_1, y_2) = y_1^2 + y_2^2 - \frac{1}{2}.$



relative L^2-error



computation time



Numerical results II

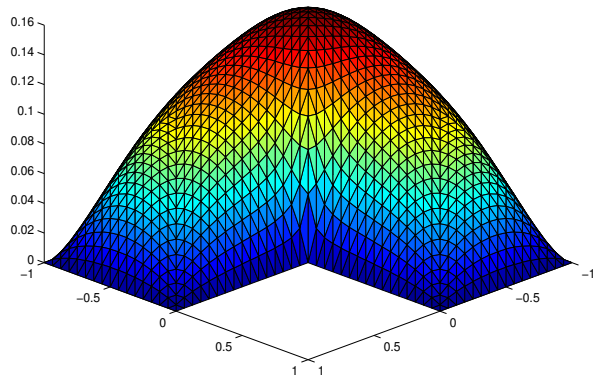
Random diffusion equation on an L-shaped domain

$$-\operatorname{div}\left[\alpha_\varepsilon(\omega)\nabla u_\varepsilon(\omega)\right] = 1 \text{ in } D, \quad u_\varepsilon(\omega) = 0 \text{ on } \partial\Omega,$$

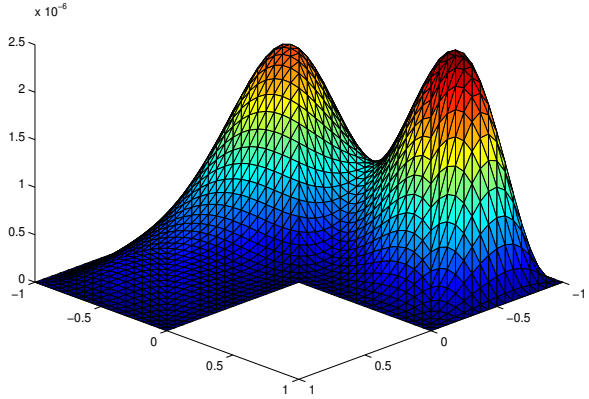
$$\alpha_\varepsilon(\mathbf{x},\omega) = 1 + \frac{\varepsilon}{4}\left[c_1(\mathbf{x})Y_1(\omega) + c_2(\mathbf{x})Y_2(\omega) + c_3(\mathbf{x})Y_3(\omega)\right].$$

The random variables $\{Y_i(\omega)\}$ are centered, independent and uniformly distributed, and

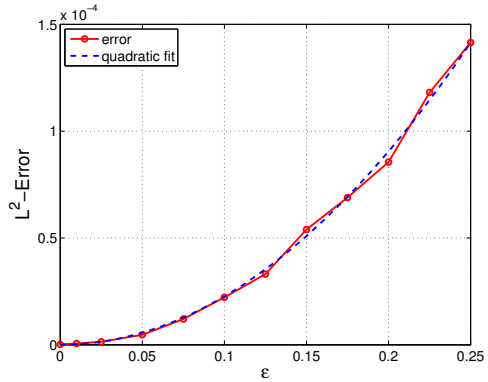
$$c_1(\mathbf{x}) = y(1-x), \quad c_2(\mathbf{x}) = x(1+y), \quad c_3(\mathbf{x}) = xy.$$

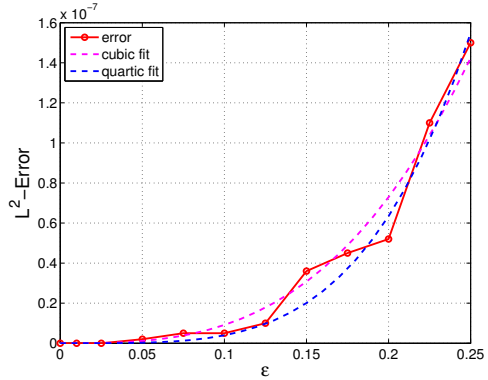


expectation



variance





Low-rank approximation vs. sparse grids

Karhunen-Loève expansion is based on the eigenpairs of the integral operator

$$(\mathcal{C}\varphi_k)(\mathbf{x}) = \int_D f(\mathbf{x},\mathbf{y})\varphi_k(\mathbf{y})\,\mathrm{d}\mathbf{y} = \lambda_k\varphi_k(\mathbf{x}), \quad \mathbf{x} \in D.$$

Remarks:

- the truncated Karhunen-Loève expansion defines the best low-rank decomposition
- truncation length heavily depends on the smoothness of the correlation function

Theorem: If $f \in H^{p,p}_{\text{mix}}(D \times D)$, then the eigenvalues $\{\lambda_m\}_{m\in\mathbb{N}}$ of $\mathcal{C}$ decay like

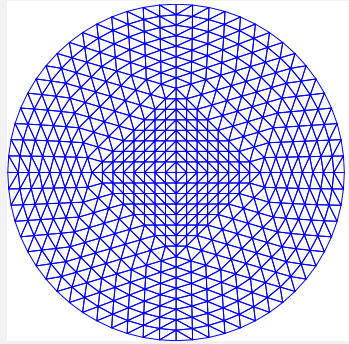
$$\lambda_m \lesssim \ell^{-(2p+d)/d} \quad \text{as } m \to \infty.$$

Consequence: If we consider an h-discretization, then the complexity of computing the Karhunen-Loève expansion is essentially larger than $N \log^{\alpha} N$ if f not analytic. Whereas, for fixed algebraic smoothness, the sparse grid approach has complexity $N \log N$.

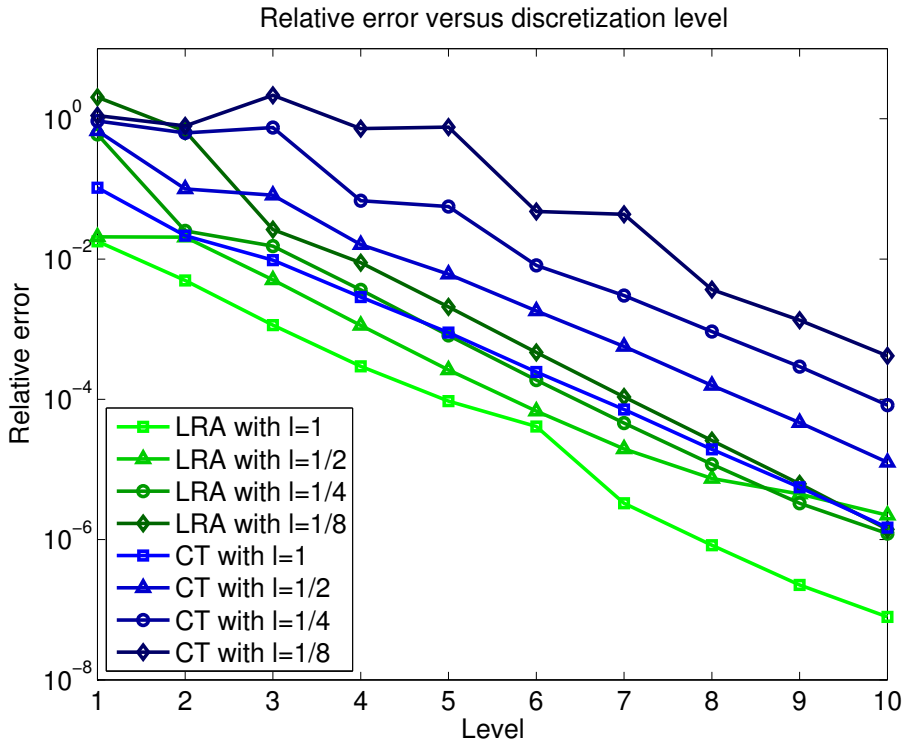
Robin boundary value problem I

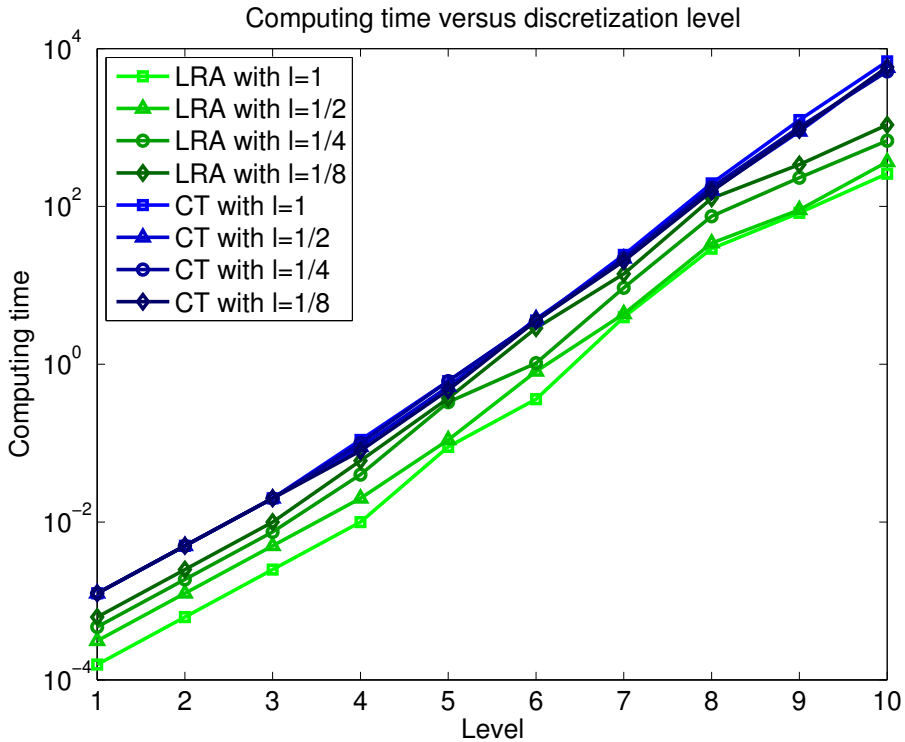
Problem: Robin boundary value problem on a random domain

$$\left.\begin{aligned} -\Delta u(\omega) &= 1 \quad \text{in } D(\omega) \\ u(\omega) + \frac{\partial u}{\partial \mathbf{n}}(\omega) &= 0 \quad \text{on } \partial D(\omega) \end{aligned}\right\} \quad \omega \in \Omega.$$



Gaussian covariance: $\mathrm{Covar}[\kappa](r) = \exp\left(-\frac{r^2}{\ell^2}\right), \quad r = \|\mathbf{x} - \mathbf{y}\|$

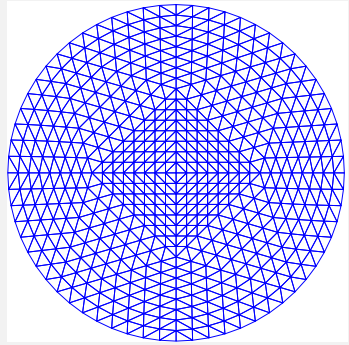




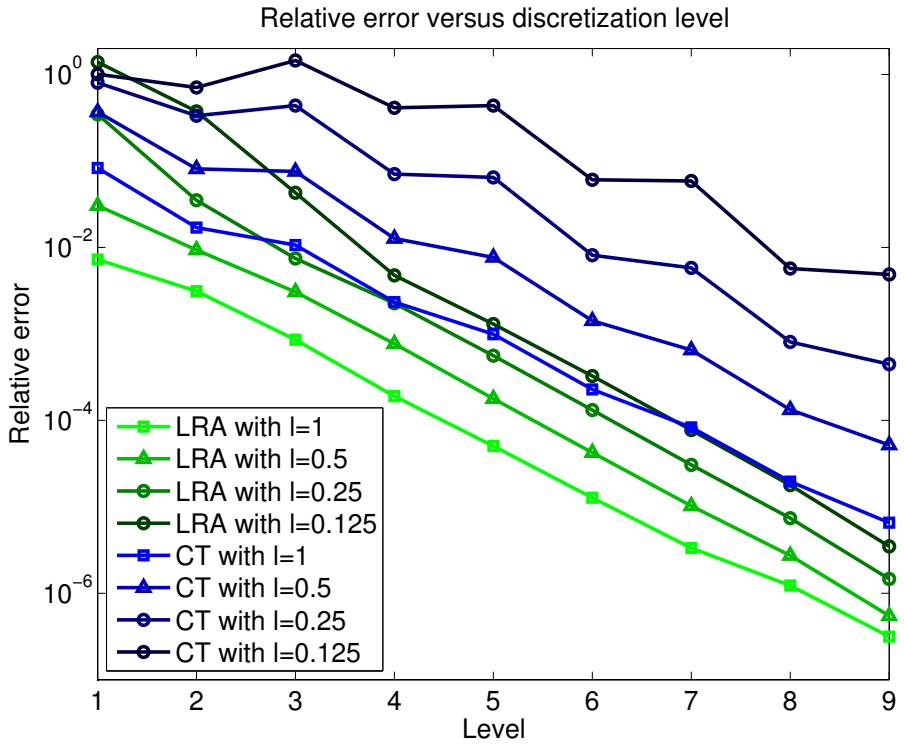
Robin boundary value problem II

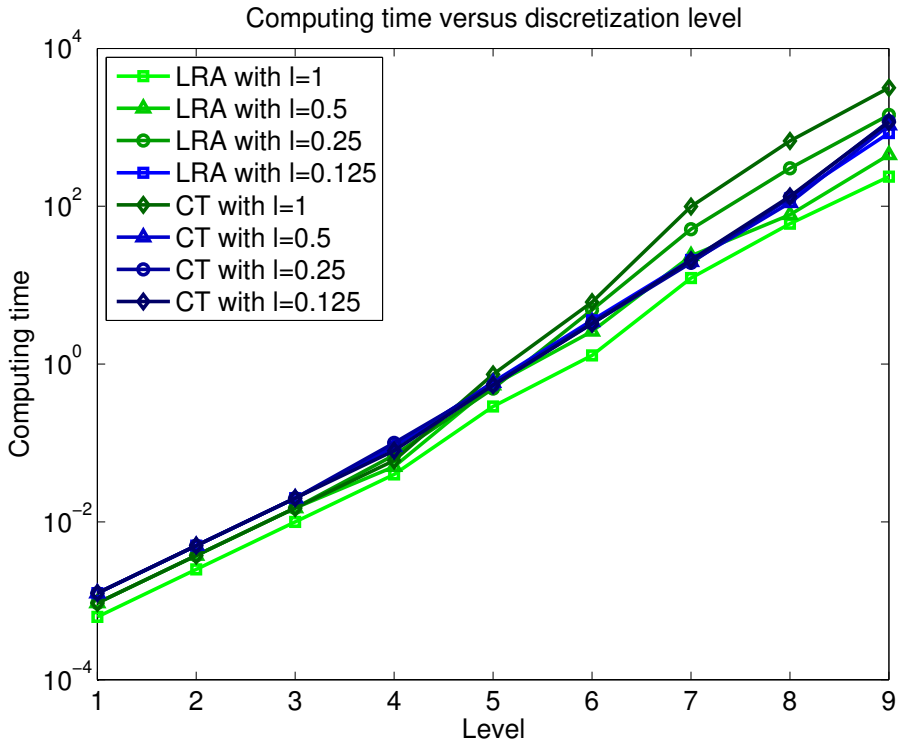
Problem: Robin boundary value problem on a random domain

$$\left.\begin{aligned} -\Delta u(\omega) &= 1 \quad \text{in } D(\omega) \\ u(\omega) + \frac{\partial u}{\partial \mathbf{n}}(\omega) &= 0 \quad \text{on } \partial D(\omega) \end{aligned}\right\} \quad \omega \in \Omega.$$



Matérn covariance: $\mathrm{Covar}[\kappa](r) = \left(1 + \frac{\sqrt{3}r}{\ell}\right) \exp\left(-\frac{\sqrt{3}r}{\ell}\right), \quad r = \|\mathbf{x} - \mathbf{y}\|$



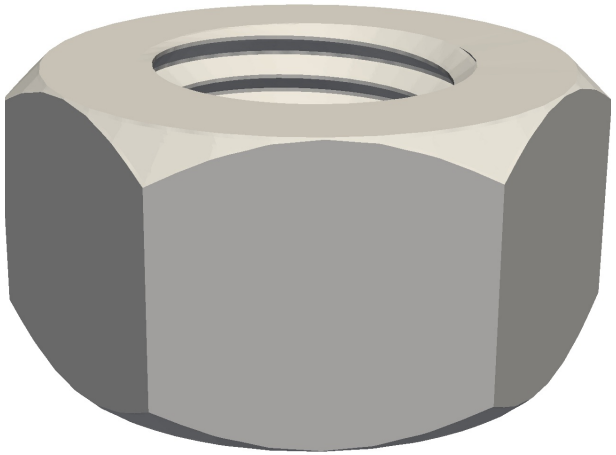


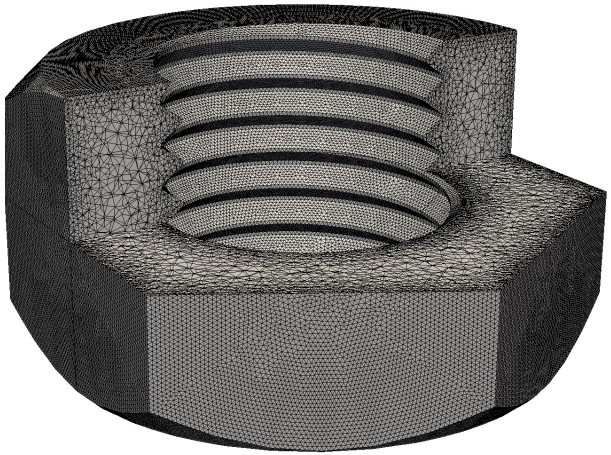
$\mathcal{H}$-matrix based second moment analysis

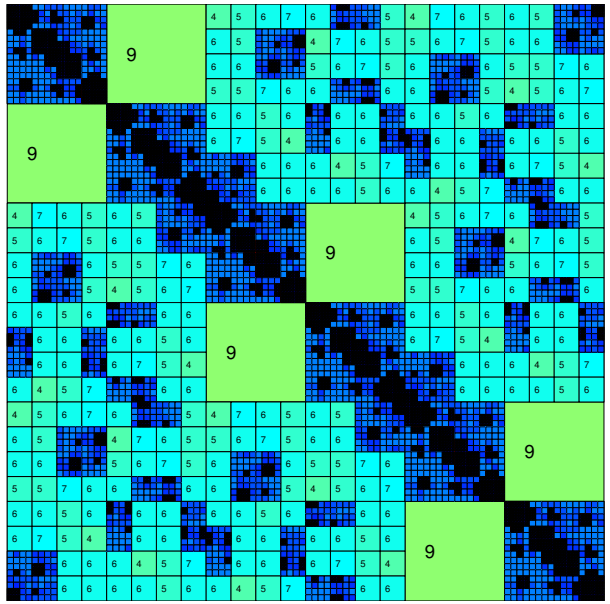
Problem: Solve the tensor product problem

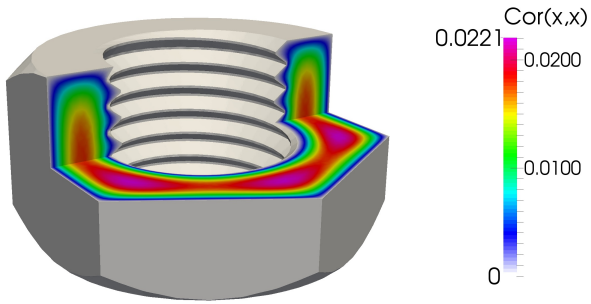
$$\mathbf{S}\mathbf{C}_u\mathbf{S}^\mathsf{T} = \mathbf{C}_f,$$

where $\mathbf{S}$ corresponds to a finite or boundary element matrix and $\mathbf{C}_f$ is the discretized correlation of the right-hand side.

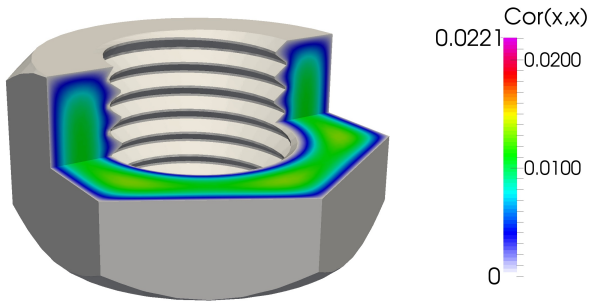




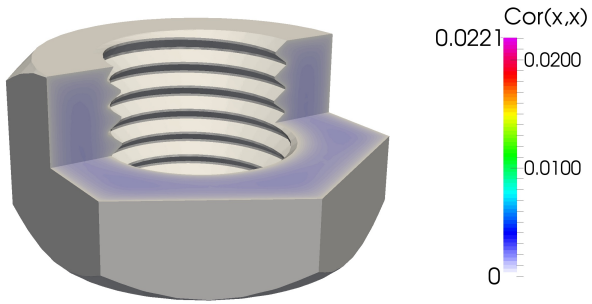




$$\ell = \frac{\mathrm{diam}(D)}{1}$$



$$\ell = \frac{\mathrm{diam}(D)}{10}$$



$$\ell = \frac{\mathrm{diam}(D)}{100}$$

Part 4. Application

On quadratic shape functionals with random load

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

$$\boxed{\begin{aligned} -\operatorname{div}\big[\mathbf{A}e\big(\mathbf{u}(\omega)\big)\big] &= \mathbf{f}(\omega) && \text{in } D,\\ \mathbf{A}e\big(\mathbf{u}(\omega)\big)\mathbf{n} &= \mathbf{0} && \text{on } \Gamma_N^{\text{free}},\\ \mathbf{A}e\big(\mathbf{u}(\omega)\big)\mathbf{n} &= \mathbf{g}(\omega) && \text{on } \Gamma_N^{\text{fix}},\\ \mathbf{u} &= \mathbf{0} && \text{on } \Gamma_D. \end{aligned}}$$

where $e(\mathbf{u}) = (\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathsf{T}})/2$ stands for the linearized strain tensor and $\mathbf{A}$ is given by

$$\mathbf{A}\mathbf{B} = 2\mu\mathbf{B} + \lambda\operatorname{tr}(\mathbf{B})\mathbf{I} \text{ for all } \mathbf{B} \in \mathbb{R}^{d\times d}$$

with the Lamé coefficients λ and μ satisfying $\mu > 0$ and $\lambda + 2\mu/d > 0$.

- Consider a quadratic shape functional, for example, the compliance of shapes:

$$\boxed{\begin{aligned} \mathcal{C}(D,\omega) &= \int_D \mathbf{A}e\big(\mathbf{u}(\mathbf{x},\omega)\big) : e\big(\mathbf{u}(\mathbf{x},\omega)\big)\,\mathrm{d}\mathbf{x}\\ &= \int_D \langle \mathbf{f}(\omega), \mathbf{u}(\omega)\rangle\,\mathrm{d}\mathbf{x} + \int_{\Gamma_N^{\text{fix}}} \langle \mathbf{g}(\mathbf{x},\omega), \mathbf{u}(\mathbf{x},\omega)\rangle\,\mathrm{d}\sigma_{\mathbf{x}}, \end{aligned}}$$

- We aim at minimizing the expectation $\mathbb{E}[\mathcal{C}(D,\omega)]$ of the quadratic shape functional.

Deterministic reformulation of the shape functional

Theorem. The expectation of the quadratic shape functional can be rewritten by

$$\mathbb{E}[\mathcal{C}(D,\omega)] = \int_D \big((\mathbf{A}e_{\mathbf{x}} : e_{\mathbf{y}})\,\mathrm{Cor}[\mathbf{u}]\big)(\mathbf{x},\mathbf{y})\big|_{\mathbf{x}=\mathbf{y}}\,\mathrm{d}\mathbf{x},$$

where

$$(\mathbf{A}e_{\mathbf{x}} : e_{\mathbf{y}}) : \big[H^1_{\Gamma_D}(D)\big]^d \otimes \big[H^1_{\Gamma_D}(D)\big]^d \to L^2(D) \otimes L^2(D)$$

is the linear operator induced from the bilinear mapping

$$\mathbf{u}\mathbf{v}^\mathsf{T} \mapsto \mathbf{A}e(\mathbf{u}) : e(\mathbf{v}).$$

Proof. The assertion follows from

$$\begin{aligned}
\mathbb{E}[\mathcal{C}(D,\omega)] &= \int_\Omega \int_D \mathbf{A}e\big(\mathbf{u}(\mathbf{x},\omega)\big) : e\big(\mathbf{u}(\mathbf{x},\omega)\big)\,\mathrm{d}\mathbf{x} \\
&= \int_D \left[(\mathbf{A}e_{\mathbf{x}} : e_{\mathbf{y}}) \int_\Omega \mathbf{u}(\mathbf{x},\omega)\mathbf{u}(\mathbf{y},\omega)^\mathsf{T}\,\mathrm{d}\mathbb{P}(\omega)\right]\Bigg|_{\mathbf{x}=\mathbf{y}}\,\mathrm{d}\mathbf{x} \\
&= \int_D \big((\mathbf{A}e_{\mathbf{x}} : e_{\mathbf{y}})\,\mathrm{Cor}[\mathbf{u}]\big)(\mathbf{x},\mathbf{y})\big|_{\mathbf{x}=\mathbf{y}}\,\mathrm{d}\mathbf{x}. \qquad \square
\end{aligned}$$

How to compute the correlation?

Theorem. The two-point correlation function $\mathrm{Cor}[\mathbf{u}] \in [H^1_{\Gamma_D}(D)]^d \otimes [H^1_{\Gamma_D}(D)]^d$ is the unique solution to the following tensor-product boundary value problem:

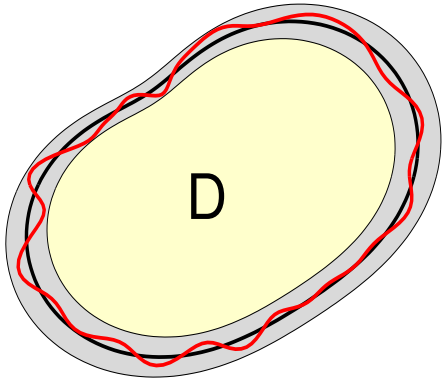
$$
\begin{aligned}
(\mathrm{div}_{\mathbf{x}} \otimes \mathrm{div}_{\mathbf{y}}) \big[(\mathbf{A}e_{\mathbf{x}} \otimes \mathbf{A}e_{\mathbf{y}}) \mathrm{Cor}[\mathbf{u}] \big] &= \mathrm{Cor}[\mathbf{f}] && \text{in } D \times D, \\
(\mathrm{div}_{\mathbf{x}} \otimes \mathbf{I}_{\mathbf{y}})(\mathbf{A}e_{\mathbf{x}} \otimes \mathbf{A}e_{\mathbf{y}}) \mathrm{Cor}[\mathbf{u}] (\mathbf{I}_{\mathbf{x}} \otimes \mathbf{n}_{\mathbf{y}}) &= \mathbf{0} && \text{on } D \times \Gamma_N^{\text{fix}\cup\text{free}}, \\
(\mathbf{I}_{\mathbf{x}} \otimes \mathrm{div}_{\mathbf{y}})(\mathbf{A}e_{\mathbf{x}} \otimes \mathbf{A}e_{\mathbf{y}}) \mathrm{Cor}[\mathbf{u}] (\mathbf{n}_{\mathbf{x}} \otimes \mathbf{I}_{\mathbf{y}}) &= \mathbf{0} && \text{on } \Gamma_N^{\text{fix}\cup\text{free}} \times D, \\
(\mathrm{div}_{\mathbf{x}} \otimes \mathbf{I}_{\mathbf{y}})(\mathbf{A}e_{\mathbf{x}} \otimes \mathbf{I}_{\mathbf{y}}) \mathrm{Cor}[\mathbf{u}] &= \mathbf{0} && \text{on } D \times \Gamma_D, \\
(\mathbf{I}_{\mathbf{x}} \otimes \mathrm{div}_{\mathbf{y}})(\mathbf{I}_{\mathbf{x}} \otimes \mathbf{A}e_{\mathbf{y}}) \mathrm{Cor}[\mathbf{u}] &= \mathbf{0} && \text{on } \Gamma_D \times D, \\
(\mathbf{A}e_{\mathbf{x}} \otimes \mathbf{A}e_{\mathbf{y}}) \mathrm{Cor}[\mathbf{u}] (\mathbf{n}_{\mathbf{x}} \otimes \mathbf{n}_{\mathbf{y}}) &= \mathbf{0} && \text{on } \big(\Gamma_N^{\text{fix}\cup\text{free}} \times \Gamma_N^{\text{fix}\cup\text{free}}\big) \\
& && \qquad \setminus (\Gamma_N^{\text{fix}} \times \Gamma_N^{\text{fix}}), \\
(\mathbf{A}e_{\mathbf{x}} \otimes \mathbf{A}e_{\mathbf{y}}) \mathrm{Cor}[\mathbf{u}] (\mathbf{n}_{\mathbf{x}} \otimes \mathbf{n}_{\mathbf{y}}) &= \mathrm{Cor}[\mathbf{g}] && \text{on } \Gamma_N^{\text{fix}} \times \Gamma_N^{\text{fix}}, \\
(\mathbf{A}e_{\mathbf{x}} \otimes \mathbf{I}_{\mathbf{y}}) \mathrm{Cor}[\mathbf{u}] (\mathbf{n}_{\mathbf{x}} \otimes \mathbf{I}_{\mathbf{y}}) &= \mathbf{0} && \text{on } \Gamma_N^{\text{fix}\cup\text{free}} \times \Gamma_D, \\
(\mathbf{I}_{\mathbf{x}} \otimes \mathbf{A}e_{\mathbf{y}}) \mathrm{Cor}[\mathbf{u}] (\mathbf{I}_{\mathbf{x}} \otimes \mathbf{n}_{\mathbf{y}}) &= \mathbf{0} && \text{on } \Gamma_D \times \Gamma_N^{\text{fix}\cup\text{free}}, \\
\mathrm{Cor}[\mathbf{u}] &= \mathbf{0} && \text{on } \Gamma_D \times \Gamma_D.
\end{aligned}
$$

Proof. The assertion follows by tensorizing the state equation and the exploiting the linearity when taking the expectation. □

Computing the shape gradient

Domain perturbation.

$$D_{\mathbf{V}} = (I+\mathbf{V})(D), \quad \mathbf{V} \in W^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d), \quad \|\mathbf{V}\|_{W^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)} \leq \frac{1}{2}.$$



Definition (Shape derivative). A functional $J(D)$ of the domain is shape differentiable at D if the underlying mapping $\mathbf{V} \mapsto J(D_{\mathbf{V}})$ which maps $W^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ into $\mathbb{R}$ is Fréchet-differentiable at $\mathbf{V} = \mathbf{0}$. The related Fréchet derivative $\mathbf{V} \mapsto \delta J(D)[\mathbf{V}]$ at D satisfies the following asymptotic expansion in the vicinity of $\mathbf{V} = \mathbf{0}$:

$$J(D_{\mathbf{V}}) = J(D) + \delta J(D)[\mathbf{V}] + o(\mathbf{V}), \text{ where } \frac{\|o(\mathbf{V})\|}{\|\mathbf{V}\|_{W^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)}} \xrightarrow{\mathbf{V}\to\mathbf{0}} 0.$$

Theorem. The functional $\mathbb{E}[J(D,\omega)]$ is shape differentiable at any shape $D \in \mathcal{U}_{ad}$ and its derivative reads

$$\frac{\mathrm{d}}{\mathrm{d}\mathbf{V}}\mathbb{E}[\mathcal{C}(D,\omega)] = \int_{\Gamma_N^{\text{free}}} \langle \mathbf{V}, \mathbf{n}\rangle \big((\mathbf{A}e_{\mathbf{x}} : e_{\mathbf{y}})\,\mathrm{Cor}[\mathbf{u}]\big)(\mathbf{x},\mathbf{y})\big|_{\mathbf{x}=\mathbf{y}}\,\mathrm{d}\sigma_{\mathbf{x}}.$$

Low-rank approximation

- **Approximation of the input correlation.** Assume low-rank approximations

$$\mathrm{Cor}[\mathbf{f}] \approx \sum_i \mathbf{f}_i \mathbf{f}_i^\mathsf{T}, \quad \mathrm{Cor}[\mathbf{g}] \approx \sum_j \mathbf{g}_j \mathbf{g}_j^\mathsf{T}.$$

  Such expansions can efficiently be computed by e.g. a pivoted Cholesky decomposition.

- **Approximation of the shape functional.** The shape functional is simply given by

$$\mathbb{E}[\mathcal{C}(D,\omega)] = \int_D \sum_{i,j} \mathbf{A} e(\mathbf{u}_{i,j}) : e(\mathbf{u}_{i,j}) \, \mathrm{d}\mathbf{x},$$

  where

$$\begin{aligned} -\operatorname{div}\left[\mathbf{A} e(\mathbf{u}_{i,j})\right] &= \mathbf{f}_i && \text{in } D, \\ \mathbf{A} e(\mathbf{u}_{i,j})\mathbf{n} &= \mathbf{0} && \text{on } \Gamma_N^{\text{free}}, \\ \mathbf{A} e(\mathbf{u}_{i,j})\mathbf{n} &= \mathbf{g}_j && \text{on } \Gamma_N^{\text{fix}}, \\ \mathbf{u}_{i,j} &= \mathbf{0} && \text{on } \Gamma_D. \end{aligned}$$

- **Approximation of the shape gradient.** The shape gradient is given by

$$\frac{\mathrm{d}}{\mathrm{d}\mathbf{V}} \mathbb{E}[J(D,\omega)] = \int_{\Gamma_N^{\text{free}}} \langle \mathbf{V}, \mathbf{n} \rangle \sum_{i,j} \mathbf{A} e(\mathbf{u}_{i,j}) : e(\mathbf{u}_{i,j}) \, \mathrm{d}\sigma_{\mathbf{x}}.$$

- **Alternative approach.** A direct discretization of $\mathrm{Cor}[\mathbf{u}]$ in a sparse grid space is possible as well.

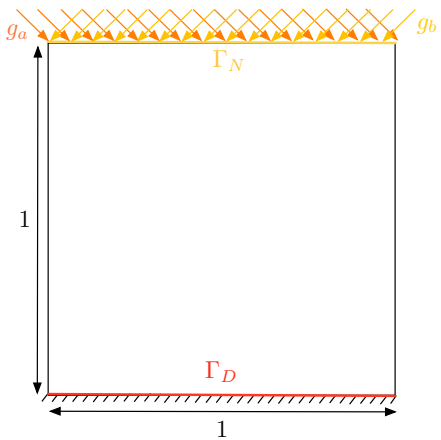
Compliance minimization

Problem: A bridge is clamped on its lower part and two sets of loads are applied on its top:

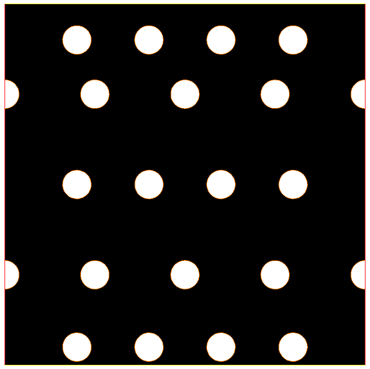
$$\mathbf{g}(\mathbf{x},\omega) = \xi_1(\omega)\begin{bmatrix}+1\\-1\end{bmatrix} + \xi_2(\omega)\begin{bmatrix}-1\\+1\end{bmatrix}.$$

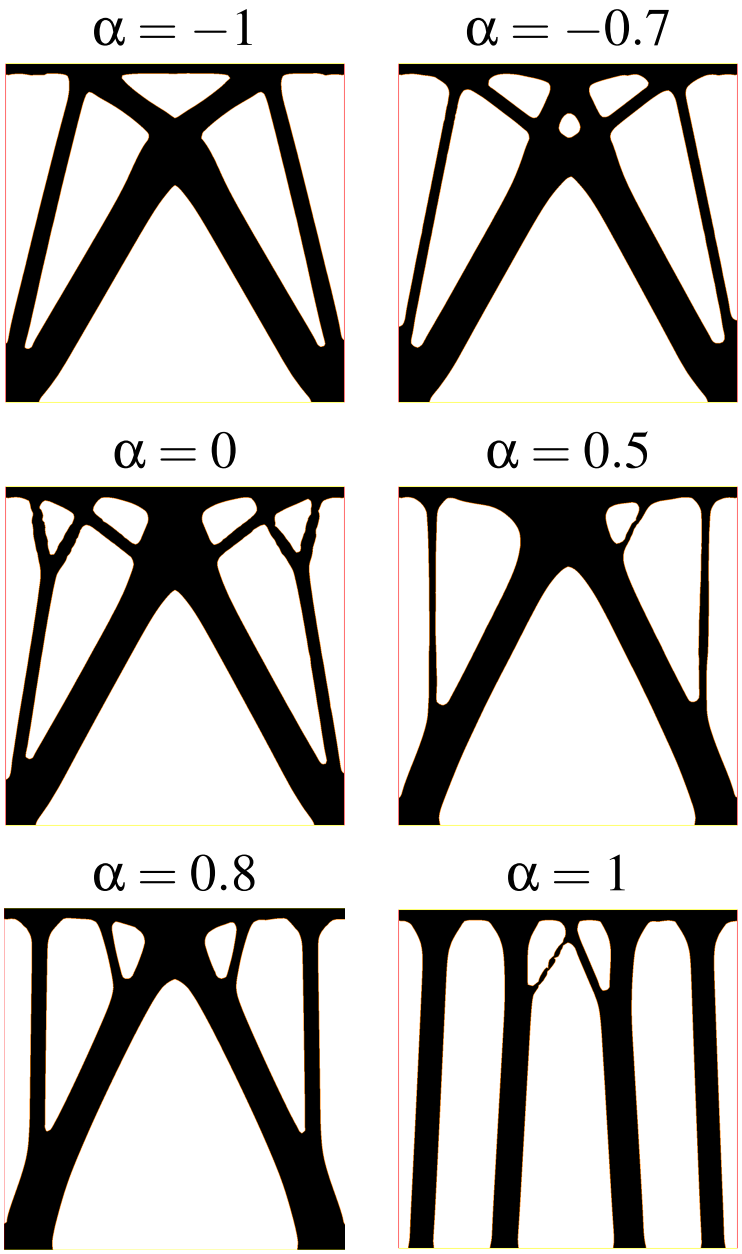
We choose $\mathbb{E}[\xi_i] = 0$, $\mathbb{V}[\xi_i] = 1$, and $\mathrm{Cor}[\xi_1, \xi_2] = \alpha$ with $-1 \leq \alpha \leq 1$.

Sketch



Initial guess





Part 5. Summary

Summary

- We developed and analyzed a fast deterministic method for the second moment analysis of random solutions to elliptic equation with random input data.
- The statistics of random loadings is computed exactly.
- The statistics of random coefficients or random domains is computed with leading order by means of sensitivity analysis.
- Only first order Fréchet derivatives are explicitly required to express the solution's non-linear dependence on the input data.
- The pivoted Cholesky decomposition gives a simple algorithm to solve second moment equations.
- Finite element methods arising from multilevel hierarchies are applied by means of the sparse grid combination technique to realize log-linear complexity in the number of degrees of freedom on D.
- $\mathcal{H}$-matrix techniques can be used in case of rough correlations.