$\mathcal{H}$-matrix accelerated second moment analysis for potentials with rough correlation

Jürgen Dölz[1], Helmut Harbrecht[1], Michael Peters[1] and Christoph Schwab[2]

[1]Department für Mathematik und Informatik, Universität Basel
[2]Seminar für Angewandte Mathematik, Eidgenössische Technische Hochschule Zürich

Pro*Doc Retreat Disentis, August 2014

Outline

Motivation

The Dirichlet problem in a domain D

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

can e.g. be solved with finite elements or boundary elements:

Motivation

The Dirichlet problem in a domain D

$$\begin{aligned} \Delta u &= 0 \quad \text{in } D, \\ u &= f \quad \text{on } \partial D, \end{aligned}$$

can e.g. be solved with finite elements or boundary elements:

Single layer potential ansatz in 3D for some $\rho \in H^{-1/2}(\partial D)$:

$$f(x) = (\mathcal{V}\rho)(x) = \int_{\partial D} \frac{\rho(y)}{4\pi\|x-y\|} \mathrm{d}\sigma_y, \qquad x \in \partial D,$$

$$u(x) = (\tilde{\mathcal{V}}\rho)(x) = \int_{\partial D} \frac{\rho(y)}{4\pi\|x-y\|} \mathrm{d}\sigma_y, \qquad x \in D.$$

Problem: Input data might not be known exactly.

Stochastic problem I

If input data are not exactly known:

$\Rightarrow$ Solution u depends of uncertainties of input data

$\Rightarrow$ Use of highly accurate solution u limited

Can we quantify the behaviour of u?
Especially the mean $\mathbb{E}_u$ and the variance $\mathbb{V}_u$?

Stochastic problem I

If input data are not exactly known:

- $\Rightarrow$ Solution u depends of uncertainties of input data
- $\Rightarrow$ Use of highly accurate solution u limited

Can we quantify the behaviour of u?
Especially the mean $\mathbb{E}_u$ and the variance $\mathbb{V}_u$?

Let $(\Omega, \Sigma, \mathbb{P})$ a probability space and $D \subset \mathbb{R}^3$ a domain

$$\left.\begin{aligned} \Delta_x u(x,\omega) &= 0, & x &\in D \\ u(x,\omega) &= f(x,\omega), & x &\in \partial D \end{aligned}\right\} \text{for } \mathbb{P}\text{-a.e. } \omega \in \Omega,$$

where

$$f(x,\cdot) : \Omega \to H^{1/2}(\partial D).$$

Stochastic problem II

$$\mathbb{E}_f(x) = \int_\Omega f(x,\omega)\mathrm{d}\mathbb{P}(\omega)$$

Linearity of the mean yields

$$\begin{aligned} \mathcal{V}\mathbb{E}_\rho(x) &= \mathbb{E}_f(x), \quad && x \in \partial D, \\ \mathbb{E}_u(x) &= \tilde{\mathcal{V}}\mathbb{E}_\rho(x), && x \in D. \end{aligned}$$

Stochastic problem II

$$\mathbb{E}_f(x) = \int_\Omega f(x,\omega)\mathrm{d}\mathbb{P}(\omega)$$

Linearity of the mean yields

$$\begin{aligned} \mathcal{V}\mathbb{E}_\rho(x) &= \mathbb{E}_f(x), \quad x \in \partial D, \\ \mathbb{E}_u(x) &= \tilde{\mathcal{V}}\mathbb{E}_\rho(x), \quad x \in D. \end{aligned}$$

$$\mathrm{Cor}_f(x,y) = \int_\Omega f(x,\omega)f(y,\omega)\mathrm{d}\mathbb{P}(\omega)$$

Tensorizing $\mathcal{V}\rho = f$ and integration over ω yields

$$\begin{aligned} (\mathcal{V}\otimes\mathcal{V})\mathrm{Cor}_\rho(x,y) &= \mathrm{Cor}_f(x,y), && x,y \in \partial D, \\ \mathrm{Cor}_u(x,y) &= (\tilde{\mathcal{V}}\otimes\tilde{\mathcal{V}})\mathrm{Cor}_\rho(x,y), && x,y \in D, \\ \mathbb{V}_u(x) &= \mathrm{Cor}_u(x,x) - \mathbb{E}_u^2(x). \end{aligned}$$

Rough correlation

Let us assume, that Cor_f is isotropic, i.e.

$$\mathrm{Cor}_f(x,y) = \mathrm{Cor}_f(r), \qquad r = \|x-y\|,$$

and provides limited Sobolev smoothness, i.e.

$$\mathrm{Cor}_f \in H^s(\partial D \times \partial D) \text{ for } s > 0 \text{ small.}$$

Rough correlation

Let us assume, that Cor_f is isotropic, i.e.

$$\mathrm{Cor}_f(x, y) = \mathrm{Cor}_f(r), \qquad r = \|x - y\|,$$

and provides limited Sobolev smoothness, i.e.

$$\mathrm{Cor}_f \in H^s(\partial D \times \partial D) \text{ for } s > 0 \text{ small.}$$

- We cannot compute a reasonable low rank approximation.
- A sparse tensor product approach has only half of the rate of convergence of a full one.

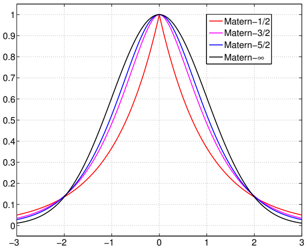
$\Rightarrow$ Find a way to approximate the full tensor product approach.

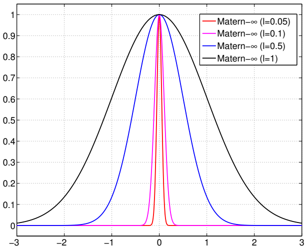
Matérn class of kernels

For $r = \|x - y\|$ let

$$\mathrm{Cor}_f(x,y) = k_\nu(r) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu} r}{\ell} \right)^\nu K_\nu \left(\frac{\sqrt{2\nu} r}{\ell} \right).$$

For $\nu \to \infty$ we receive the Gauss kernel, for $\nu = \frac{1}{2}$ we get the exponential kernel $\exp\left(\frac{r}{\ell}\right)$.





Galerkin discretization

For an ansatz space $V_h \subset H^{-1/2}(\partial D)$ the Galerkin scheme of $(\mathcal{V} \otimes \mathcal{V})\mathrm{Cor}_\rho = \mathrm{Cor}_f$ reads:

Find $\mathrm{Cor}_{\rho,h} \in V_h \otimes V_h$ such that

$$\big((\mathcal{V} \otimes \mathcal{V})\mathrm{Cor}_{\rho,h}, v_h\big)_{L^2(\partial D\times\partial D)} = (\mathrm{Cor}_f, v_h)_{L^2(\partial D\times\partial D)}$$

for all $v_h \in V_h \otimes V_h$.

We therefore get the following system of equations:

$$(\mathbf{V} \otimes \mathbf{V})\,\mathrm{vec}(\mathbf{C}_\rho) = \mathrm{vec}(\mathbf{C}_f) \Leftrightarrow \mathbf{V}\mathbf{C}_\rho\mathbf{V} = \mathbf{C}_f$$

Galerkin discretization

For an ansatz space $V_h \subset H^{-1/2}(\partial D)$ the Galerkin scheme of $(\mathcal{V} \otimes \mathcal{V})\mathrm{Cor}_\rho = \mathrm{Cor}_f$ reads:

Find $\mathrm{Cor}_{\rho,h} \in V_h \otimes V_h$ such that

$$\big((\mathcal{V} \otimes \mathcal{V})\mathrm{Cor}_{\rho,h}, v_h\big)_{L^2(\partial D \times \partial D)} = (\mathrm{Cor}_f, v_h)_{L^2(\partial D \times \partial D)}$$

for all $v_h \in V_h \otimes V_h$.

We therefore get the following system of equations:

$$(\mathbf{V} \otimes \mathbf{V})\,\mathrm{vec}(\mathbf{C}_\rho) = \mathrm{vec}(\mathbf{C}_f) \Leftrightarrow \mathbf{V}\mathbf{C}_\rho\mathbf{V} = \mathbf{C}_f$$

Using the standard boundary element method, the matrices $\mathbf{V}$, $\mathbf{C}_\rho$ and $\mathbf{C}_f$ are in general **densely populated**.

Compressability I

$$(\cdot)_{ij} = \int_{\partial D} \int_{\partial D} k(x,y)\varphi_i(x)\varphi_j(y)\mathrm{d}\sigma_x \mathrm{d}\sigma_y, \qquad \text{for } \mathbf{V} \text{ and } \mathbf{C}_f$$

Compressability I

$$(\cdot)_{ij} = \int_{\partial D} \int_{\partial D} k(x,y)\varphi_i(x)\varphi_j(y)\mathrm{d}\sigma_x \mathrm{d}\sigma_y, \qquad \text{for } \mathbf{V} \text{ and } \mathbf{C}_f$$

Definition

The kernel $k(x,y) \in C^\infty$, $x \neq y$, is **asymptotically smooth** if

$$\left|\partial_x^\alpha \partial_y^\beta k(x,y)\right| \leq C \frac{(|\alpha| + |\beta|)!}{r_k^{|\alpha|+|\beta|}} \|x-y\|^{-2-2q-|\alpha|-|\beta|}.$$

Under certain conditions for x and y, we can find a local factorization to every asymptotically smooth kernel $k(x,y)$:

$$k(x,y) \approx \sum_{i=0}^{k'} g_i(x) h_i(y).$$

Compressability II

Theorem

Let Cor_f *be a sufficiently smooth Schwartz kernel on the smooth boundary* ∂D*. Then the Schwartz kernel* Cor_ρ *of the solution of*

$$\mathcal{V} \circ \mathrm{OPS}(\mathrm{Cor}_\rho) \circ \mathcal{V}^\star = \mathrm{OPS}(\mathrm{Cor}_f)$$

is asymptotically smooth. Hereby, $\mathrm{OPS}(k)$ *denotes the pseudo differential operator induced by the Schwartz kernel* k*.*

All matrices in

$$\mathbf{V}\mathbf{C}_\rho\mathbf{V} = \mathbf{C}_f$$

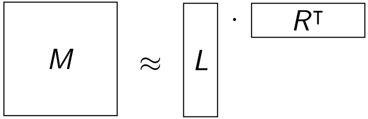
correspond to asymptotically smooth kernels.

Low rank matrices

If k' is small, we can use

$$k(x,y) \approx \sum_{i=0}^{k'} g_i(x) h_i(y)$$

to represent a corresponding matrix $M \in \mathbb{R}^{n' \times n'}$ in a data sparse way:



$$, \qquad L, R \in \mathbb{R}^{n' \times k'}.$$

Definition

We define the set of **rk-matrices** as

$$\mathcal{R}(k') = \left\{ M \in \mathbb{R}^{n' \times n'} : \text{ rank } M \leq k' \right\}.$$

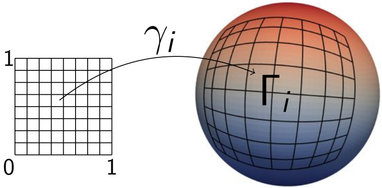
Surface representation

Assume that ∂D is a piecewise smooth Lipschitz boundary, i.e.

$$\partial D = \bigcup_{i=1}^{M} \Gamma_i,$$

where

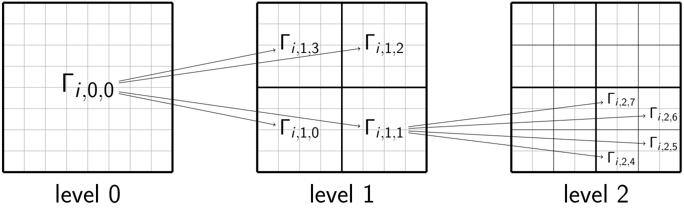
- $\Gamma_i \cap \Gamma_j$, $i \neq j$, is a vertex or an edge or empty,
- $\Gamma_i = \gamma_i(\square)$ with $\gamma_i : \square \to \Gamma_i$ a smooth diffeomorphism.



No loss of accuracy due to surface approximation.

Cluster tree

A mesh on the square gives us a mesh on the surface. Thus, a hierarchical mesh on the square gives us a hierarchical mesh on the surface.
We call it the **cluster tree** $\mathcal{T}$.



For each Γ_i we get a quad tree with 4^J elements on level J.
$\Rightarrow$ For J levels we have $4^J M$ elements in total.

Block cluster tree

Using piecewise constant ansatz functions, $\mathcal{T} \times \mathcal{T}$ corresponds to a full matrix with a hierarchical structure.

Use the admissibility condition

$$\max\big(\operatorname{diam}(\Gamma_\lambda), \operatorname{diam}(\Gamma_{\lambda'})\big) \leq \eta \operatorname{dist}(\Gamma_\lambda, \Gamma_{\lambda'}), \qquad 0 < \eta \text{ fixed}$$

to extract two subtrees of $\mathcal{T} \times \mathcal{T}$:

- **Farfield $\mathcal{F}$:** Admissible blocks, low rank approximable
- **Nearfield $\mathcal{N}$:** Inadmissible blocks, not compressible

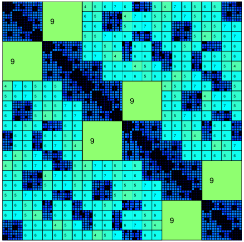
Block cluster tree $\mathcal{B} = \mathcal{F} \cup \mathcal{N}$ corresponds again to a matrix with hierarchical structure.

$\Rightarrow$ We know which parts of the matrix are compressible, use adaptive cross approximation.

$\mathcal{H}$-matrices

Definition

An $\mathcal{H}$-**matrix** is a matrix with block wise low rank in $\mathcal{F}$. We denote the set of $\mathcal{H}$-matrices with maximal rank k by $\mathcal{H}(\mathcal{B}, k)$.

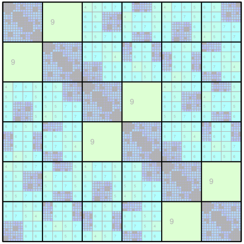


Problem: In order to solve $\mathbf{V}\mathbf{C}_\rho\mathbf{V} = \mathbf{C}_f$ we have to explain addition and multiplication in $\mathcal{H}(\mathcal{B}, k)$.

$\mathcal{H}$-matrices

Definition

An $\mathcal{H}$-**matrix** is a matrix with block wise low rank in $\mathcal{F}$. We denote the set of $\mathcal{H}$-matrices with maximal rank k by $\mathcal{H}(\mathcal{B}, k)$.



$$= \begin{bmatrix} \mathbf{H}_{1,1} & \dots & \mathbf{H}_{1,M} \\ \vdots & & \vdots \\ \mathbf{H}_{M,1} & \dots & \mathbf{H}_{M,M} \end{bmatrix}$$

Problem: In order to solve $\mathbf{VC}_\rho\mathbf{V} = \mathbf{C}_f$ we have to explain addition and multiplication in $\mathcal{H}(\mathcal{B}, k)$.

$\mathcal{H}$-matrix addition

We have

$$\begin{bmatrix} \mathbf{H}_{1,1} & \dots & \mathbf{H}_{1,M} \\ \vdots & & \vdots \\ \mathbf{H}_{M,1} & \dots & \mathbf{H}_{M,M} \end{bmatrix} \quad \text{where} \quad \mathbf{H}_{i,j} \in \begin{cases} \mathcal{H}(\mathcal{B}', k) & \text{or} \\ \mathcal{R}(k) & \text{or} \\ \mathbb{R}^{n' \times n'}. \end{cases}$$

The special structure of $\mathcal{B}$ yields that all blocks on the same level are quadratic and of the same size.

$\mathcal{H}$-matrix addition

We have

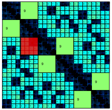
$$\begin{bmatrix} \mathbf{H}_{1,1} & \dots & \mathbf{H}_{1,M} \\ \vdots & & \vdots \\ \mathbf{H}_{M,1} & \dots & \mathbf{H}_{M,M} \end{bmatrix} \quad \text{where} \quad \mathbf{H}_{i,j} \in \begin{cases} \mathcal{H}(\mathcal{B}', k) & \text{or} \\ \mathcal{R}(k) & \text{or} \\ \mathbb{R}^{n' \times n'}. \end{cases}$$

The special structure of $\mathcal{B}$ yields that all blocks on the same level are quadratic and of the same size.

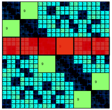
Addition of $\mathcal{H}$-matrices:

$+_{\mathcal{H}}$	$\mathcal{H}$-matrix	rk-matrix	full-matrix
$\mathcal{H}$-matrix	recursively		
rk-matrix		approximately	
full-matrix			exactly

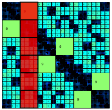
$\mathcal{H}$-matrix multiplication I



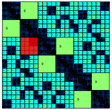
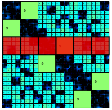
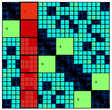
$+=$



$*_{\mathcal{H}}$



$\mathcal{H}$-matrix multiplication I

 $+=$  $*_{\mathcal{H}}$  $= \sum_{k=0}^{M} \left(\mathbf{H}^{(1)}_{3,k} *_{\mathcal{H}} \mathbf{H}^{(2)}_{k,2} \right)$

$*_{\mathcal{H}}$	$\mathcal{H}$-matrix	*rk*-matrix	full-matrix
$\mathcal{H}$-matrix	recursively	exactly	
rk-matrix	exactly	exactly	exactly
full-matrix		exactly	exactly

$+=_{\mathcal{H}}$	$\mathcal{H}$-matrix	*rk*-matrix	full-matrix
$\mathcal{H}$-matrix	recursively	recursively	
rk-matrix	approximately	approximately	approximately
full-matrix		exactly	exactly

Use a sparse eigensolver (e.g. ARPACK) to compute □ .

$\mathcal{H}$-matrix multiplication II

- Due to the special structure of $\mathcal{B}$: Interactions between $\mathcal{H}$-matrices and full matrices are completely omitted.

$\mathcal{H}$-matrix multiplication II

- Due to the special structure of $\mathcal{B}$: Interactions between $\mathcal{H}$-matrices and full matrices are completely omitted.
- Using the sparse eigensolver is superior to hierarchical approximation in literature.

$\mathcal{H}$-matrix multiplication II

- Due to the special structure of $\mathcal{B}$: Interactions between $\mathcal{H}$-matrices and full matrices are completely omitted.
- Using the sparse eigensolver is superior to hierarchical approximation in literature.
- It is possible to apply the eigensolver recursively to

$$\sum_{\alpha} \left(\mathbf{H}_{\alpha}^{(1)} \mathbf{H}_{\alpha}^{(2)} \right)$$

to compute a best approximation of the product (slow).

$\mathcal{H}$-matrix multiplication II

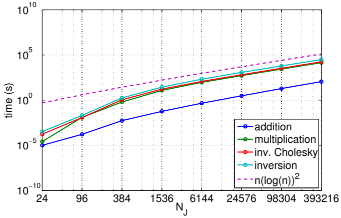
- Due to the special structure of $\mathcal{B}$: Interactions between $\mathcal{H}$-matrices and full matrices are completely omitted.
- Using the sparse eigensolver is superior to hierarchical approximation in literature.
- It is possible to apply the eigensolver recursively to

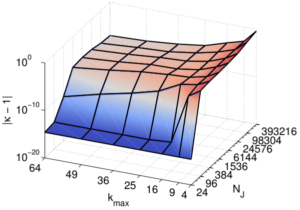
$$\sum_{\alpha} \left(\mathbf{H}_{\alpha}^{(1)} \mathbf{H}_{\alpha}^{(2)} \right)$$

  to compute a best approximation of the product (slow).
- An approximative inverse of an $\mathcal{H}$-matrix can be computed using recursive block Gaussian elimination.

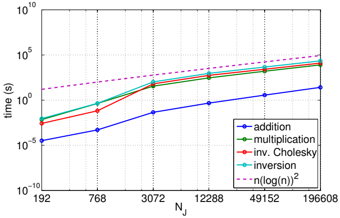
$\mathcal{H}$-matrix arithmetics

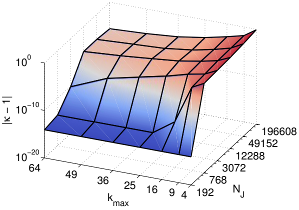
Sphere





Drilled cube





Lower pictures: cond $\left(\mathbf{V}\hat{\mathbf{V}}^{-1}\right) - 1$

Numerical solution I

To solve $\mathbf{V}\mathbf{C}_\rho\mathbf{V} = \mathbf{C}_f$, use the **iterative improvement**:

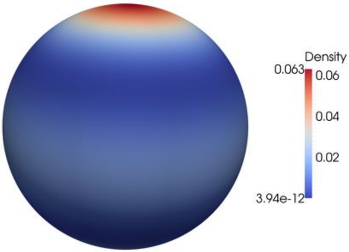
Compute an approximative inverse $\hat{\mathbf{V}}^{-1}$ of $\mathbf{V}$ and set

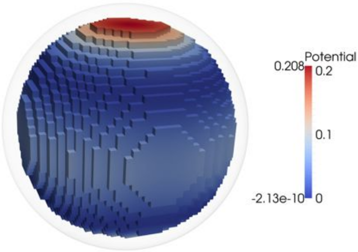
$$\mathbf{C}_\rho^{(0)} = \hat{\mathbf{V}}^{-1}\mathbf{C}_f\hat{\mathbf{V}}^{-1}.$$

Then compute

$$\begin{aligned} \mathbf{R}^{(k)} &= \mathbf{C}_f - \mathbf{V}\mathbf{C}_\rho^{(k)}\mathbf{V}, \\ \mathbf{C}_\rho^{(k+1)} &= \mathbf{C}_\rho^{(k)} + \hat{\mathbf{V}}^{-1}\mathbf{R}^{(k)}\hat{\mathbf{V}}^{-1}, \end{aligned} \qquad k = 0, 1, \ldots$$

Numerical solution II



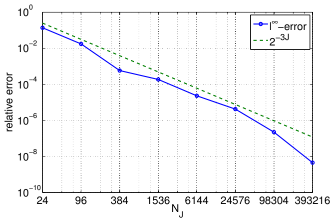


$$(\mathcal{V}\otimes\mathcal{V})(\rho\otimes\rho) = Y_2^0\otimes Y_2^0$$
$$(u\otimes u) = (\tilde{\mathcal{V}}\otimes\tilde{\mathcal{V}})(\rho\otimes\rho)$$

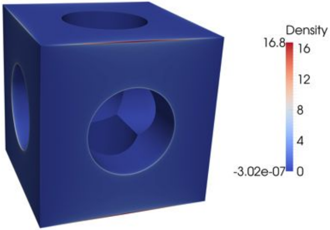
equivalent to

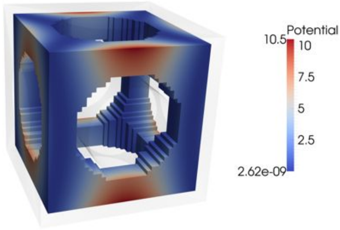
$$\mathcal{V}\rho = Y_2^0$$
$$u = \tilde{\mathcal{V}}\rho$$

Y_2^0 spherical harmonic



Numerical solution III



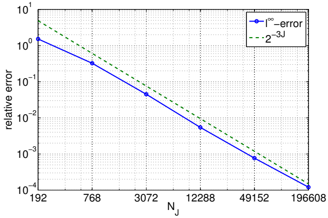


$$(\mathcal{V} \otimes \mathcal{V})(\rho \otimes \rho) = f \otimes f$$
$$(u \otimes u) = (\tilde{\mathcal{V}} \otimes \tilde{\mathcal{V}})(\rho \otimes \rho)$$

equivalent to

$$\mathcal{V}\rho = f$$
$$u = \tilde{\mathcal{V}}\rho$$

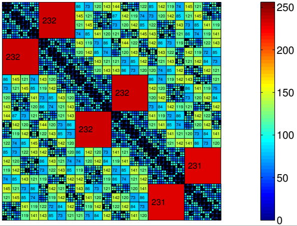
f harmonic polynomial

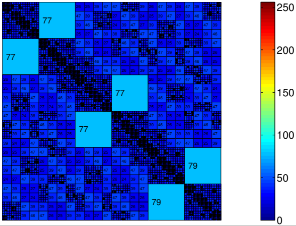


Compressibility of the solution

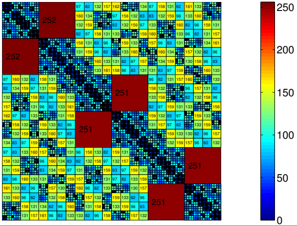
Compressability of Cor_u for $\mathrm{Cor}_f(r) = \exp(-r)$

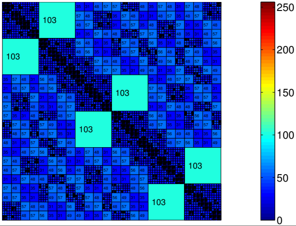
Sphere





Cube

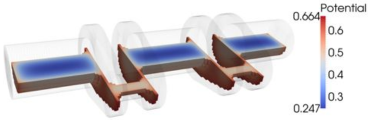


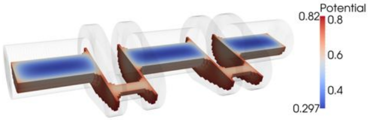


Rel. err. 10^{-8} 10^{-4}

Stochastic example

Matérn class as kernel for Cor_f, $k_{\max} = 81$ and $N_J = 145408$ boundary elements.
8.8 hours wall clock time on up to 32 cores.



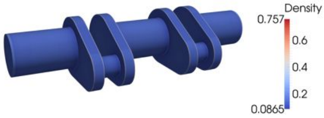


t.l.: $\mathrm{Cor}_u\big|_{x=y}$ for

$$\mathrm{Cor}_f(r) = \exp(-r)$$

t.r. $\mathrm{Cor}_u\big|_{x=y}$, l.r. $\mathrm{Cor}_\rho\big|_{x=y}$ for

$$\mathrm{Cor}_f(r) = (1 + \sqrt{3}r)\exp(-\sqrt{3}r)$$



Conclusions

- A new method to compute the solutions two-point correlation for strongly elliptic PDE with stochastic Dirichlet data with rough correlation.
- On smooth surfaces, $\mathcal{H}$-matrix compressibility of the solution is provable.
- The method scales log-linear in the number of boundary elements on the surface.

References:

Jürgen Dölz, Helmut Harbrecht, Michael Peters
$\mathcal{H}$-matrix accelerated second moment analysis for potentials with rough correlation.
Preprint 2014-03, Mathematisches Institut, Universität Basel, Switzerland, 2014.

Jürgen Dölz, Helmut Harbrecht, Christoph Schwab
Covariance regularity and $\mathcal{H}$-matrix approximation for rough random fields.
In preparation.

Conclusions

- A new method to compute the solutions two-point correlation for strongly elliptic PDE with stochastic Dirichlet data with rough correlation.
- On smooth surfaces, $\mathcal{H}$-matrix compressibility of the solution is provable.
- The method scales log-linear in the number of boundary elements on the surface.

Thank you!

References:

Jürgen Dölz, Helmut Harbrecht, Michael Peters
$\mathcal{H}$-matrix accelerated second moment analysis for potentials with rough correlation.
Preprint 2014-03, Mathematisches Institut, Universität Basel, Switzerland, 2014.

Jürgen Dölz, Helmut Harbrecht, Christoph Schwab
Covariance regularity and $\mathcal{H}$-matrix approximation for rough random fields.
In preparation.