

Numerical solution of elliptic diffusion problems on random domains

Helmut Harbrecht, Michael Peters and Markus Siebenmorgen

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Problem Formulation

- ▶ As model problem, we consider the Laplace equation

$$-\Delta u(\mathbf{x}, \omega) = f(\mathbf{x}) \text{ in } D(\omega), \quad u(\mathbf{x}, \omega) = 0 \text{ on } \Gamma(\omega).$$

- ▶ We are interested in computing the *mean* $\mathbb{E}[u](\mathbf{x})$ and the *variance* $\mathbb{V}[u](\mathbf{x})$ with respect to a fixed reference domain D_{ref} .
- ▶ Here, $D_{\text{ref}} \subset \mathbb{R}^d$ for $d = 2$ or $d = 3$ denotes a domain with Lipschitz continuous boundary $\Gamma := \partial D_{\text{ref}}$.
- ▶ Moreover, we model the stochastic parameter with respect to the complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$ where Ω is a separable set, $\mathcal{F} \subset 2^\Omega$ a σ -field and \mathbb{P} a probability measure.

- ▶ Let $\mathbf{V}: \overline{D_{\text{ref}}} \times \Omega \rightarrow \mathbb{R}^d$ be an invertible vector field of class C^2 , i.e. \mathbf{V} is twice continuously differentiable with respect to \mathbf{x} .
- ▶ Thus, \mathbf{V} defines a family of domains

$$D(\omega) := \mathbf{V}(D_{\text{ref}}, \omega).$$

- ▶ Additionally, we shall assume that the singular-values of the vector field \mathbf{V} 's Jacobian $\mathbf{J}(\mathbf{x}, \omega)$ satisfy

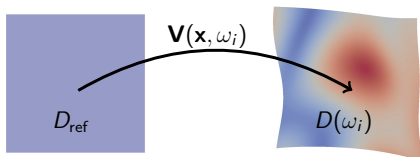
$$0 < \underline{\sigma} \leq \min \{ \sigma(\mathbf{J}(\mathbf{x}, \omega)) \} \leq \max \{ \sigma(\mathbf{J}(\mathbf{x}, \omega)) \} \leq \bar{\sigma} < \infty.$$

\rightsquigarrow uniform ellipticity

- ▶ 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

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

Reformulation for the reference domain



- ▶ The main tool in the regularity analysis will be the equivalence between the diffusion problem on $D(\omega)$ and the diffusion problem pulled back to the reference domain D_{ref} .
- ▶ This equivalence is described by the vector field $\mathbf{V}(\mathbf{x}, \omega)$. For a function v on $D(\omega)$, the transported function is given by

$$\hat{v}(\mathbf{x}, \omega) := (v \circ \mathbf{V})(\mathbf{x}, \omega).$$

Due to the chain rule, we have for $v \in C^1(D(\omega))$

$$(\nabla v)(\mathbf{V}(\mathbf{x}, \omega)) = \mathbf{J}(\mathbf{x}, \omega)^{-\top} \nabla \hat{v}(\mathbf{x}, \omega).$$

- For given $\omega \in \Omega$, the variational formulation for the model problem is given as follows: Find $u(\omega) \in H_0^1(D(\omega))$ such that

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

- Thus, with

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

and

$$f_{\text{ref}}(\mathbf{x}, \omega) := \hat{f}(\mathbf{x}, \omega) \det \mathbf{J}(\mathbf{x}, \omega),$$

we obtain the variational formulation with respect to the reference domain: Find $\hat{u}(\omega) \in H_0^1(D_{\text{ref}})$ such that for all $\hat{v}(\omega) \in H_0^1(D_{\text{ref}})$

$$\int_{D_{\text{ref}}} \langle \mathbf{A}(\omega) \nabla_{\mathbf{x}} \hat{u}(\omega), \nabla_{\mathbf{x}} \hat{v}(\omega) \rangle \, d\mathbf{x} = \int_{D_{\text{ref}}} f_{\text{ref}}(\omega) \hat{v}(\omega) \, d\mathbf{x}.$$

- ▶ The spaces $H_0^1(D_{\text{ref}})$ and $H_0^1(D(\omega))$ are isomorphic by the isomorphism

$$\mathcal{E}: H_0^1(D_{\text{ref}}) \rightarrow H_0^1(D(\omega)), \quad v \mapsto v \circ \mathbf{V}(\omega)^{-1}.$$

The inverse mapping is given by $v \mapsto v \circ \mathbf{V}(\omega)$.

- ▶ The space of test functions is not dependent on $\omega \in \Omega$: It holds $H_0^1(D(\omega)) = \{\mathcal{E}(v) : v \in H_0^1(D_{\text{ref}})\}$. Thus, for $\mathcal{E}(v) \in H_0^1(D(\omega))$, we have

$$\widehat{\mathcal{E}(v)} = \mathcal{E}(v) \circ \mathbf{V} = v \circ \mathbf{V}^{-1} \circ \mathbf{V} = v \in H_0^1(D_{\text{ref}})$$

independent of $\omega \in \Omega$.

- ▶ In particular, the solutions u on $D(\omega)$ and \hat{u} on D_{ref} satisfy

$$\hat{u}(\omega) = u \circ \mathbf{V}(\omega) \quad \text{and} \quad u(\omega) = \hat{u} \circ \mathbf{V}(\omega)^{-1}.$$

- ▶ Now, we can specify the mean and the variance of u with respect to D_{ref} according to

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

and

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

Karhunen-Loève expansion

- ▶ We assume that the domain perturbation field $\mathbf{V}(\mathbf{x}, \omega)$ is given by a truncated *Karhunen-Loève expansion*, i.e.

$$\mathbf{V}(\mathbf{x}, \omega) = \mathbb{E}[\mathbf{V}](\mathbf{x}) + \sum_{k=1}^M \sigma_k \varphi_k(\mathbf{x}) X_k(\omega).$$

- ▶ It can be computed up to a prescribed precision, e.g. by the *pivoted Cholesky decomposition*, cf. [Harbrecht,P.,Siebenmorgen14a] if the *mean*

$$\mathbb{E}[\mathbf{V}]: D_{\text{ref}} \rightarrow \mathbb{R}^d, \quad \mathbb{E}[\mathbf{V}](\mathbf{x}) = [\mathbb{E}[v_1](\mathbf{x}), \dots, \mathbb{E}[v_d](\mathbf{x})]^\top$$

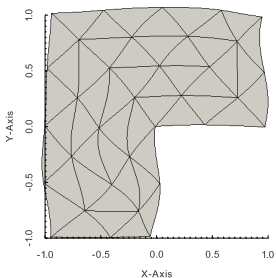
and the (matrix-valued) *covariance function*

$$\text{Cov}[\mathbf{V}]: D_{\text{ref}} \times D_{\text{ref}} \rightarrow \mathbb{R}^{d \times d}, \quad \text{Cov}[\mathbf{V}](\mathbf{x}, \mathbf{x}') = [\text{Cov}_{i,j}(\mathbf{x}, \mathbf{x}')]_{i,j=1}^d$$

are provided.

- ▶ In general, we cannot reconstruct the distribution of the random variables $\{X_k\}_k$ from the covariance function. Therefore, we have also to assume that the distribution is known or appropriately approximated.

Example: Transformed domain



$$\mathbb{E}[\mathbf{V}](\mathbf{x}) = \mathbf{x}$$

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

Length of the Karhunen-Loève expansion:
 $M = 343$ (precision $\varepsilon = 10^{-6}$)

Figure: Transformed L-shape

Assumption

- (1) *The random variables $\{X_k\}_k$ are centered and take values in $[-1, 1]$, i.e. $X_k(\omega) \in [-1, 1]$ for all k and almost every $\omega \in \Omega$.*
- (2) *The random variables $\{X_k\}_k$ are independent and identically distributed.*
- (3) *The sequence $\{\gamma_k\}_k := \{\|\sigma_k \varphi_k\|_{W^{1,\infty}(D;\mathbb{R}^d)}\}_k$ is at least in $\ell^1(\mathbb{R})$. We denote its norm by $c_\gamma := \sum_{k=1}^{\infty} \gamma_k$.*

- Here, the space $W^{1,\infty}(D; \mathbb{R}^d)$ is equipped with the norm

$$\|\mathbf{v}\|_{W^{1,\infty}(D;\mathbb{R}^d)} = \max \left\{ \|\mathbf{v}\|_{L^\infty(D;\mathbb{R}^d)}, \|\mathbf{v}'\|_{L^\infty(D;\mathbb{R}^d \times d)} \right\},$$

where \mathbf{v}' denotes the Jacobian of \mathbf{v} .

- ▶ For the rest of this talk, we will refer to the randomness only via the coordinates

$$\mathbf{y} \in \square := [-1, 1]^M, \quad \text{where } \mathbf{y} = [y_1, \dots, y_M].$$

The related spaces $L^p(\square)$ for are equipped with the push-forward measure $\mathbb{P}_{\mathbf{X}}$.

- ▶ Wlog., we may assume that $\mathbb{E}[\mathbf{V}](\mathbf{x}) = \mathbf{x}$ is the identity mapping. Otherwise, we replace D_{ref} by

$$\tilde{D}_{\text{ref}} := \mathbb{E}[\mathbf{V}](D_{\text{ref}}) \quad \text{and} \quad \tilde{\varphi}_k := \sqrt{\det(\mathbb{E}[\mathbf{V}]^{-1})}' \varphi_k \circ \mathbb{E}[\mathbf{V}]^{-1}.$$

Therefore, we obtain

$$\mathbf{V}(\mathbf{x}, \mathbf{y}) = \mathbf{x} + \sum_{k=1}^M \sigma_k \varphi_k(\mathbf{x}) y_k \quad \text{and} \quad \mathbf{J}(\mathbf{x}, \mathbf{y}) = \mathbf{I} + \sum_{k=1}^M \sigma_k \varphi_k'(\mathbf{x}) y_k,$$

where $\mathbf{I} \in \mathbb{R}^{d \times d}$ denotes the identity matrix.

- ▶ By this construction, we recognize, that D_{ref} is in fact the mean of the domains $D(\omega)$. It holds

$$\int_{\Omega} D(\omega) d\mathbb{P}(\omega) = \int_{\Omega} V(D_{\text{ref}}, \omega) d\mathbb{P}(\omega) = D_{\text{ref}},$$

since the random variable $\{X_k\}_k$ are centered.

- ▶ For the subsequent regularity results, we introduce the space $L^\infty(\square; L^\infty(D_{\text{ref}}; \mathbb{R}^d))$ consisting of all maps $\mathbf{V}: \square \rightarrow L^\infty(D_{\text{ref}}; \mathbb{R}^d)$ with

$$\|\mathbf{V}\|_d := \text{ess sup}_{\mathbf{y} \in \square} \|\mathbf{V}(\mathbf{y})\|_{L^\infty(D_{\text{ref}}; \mathbb{R}^d)} < \infty.$$

- ▶ Furthermore, the space $L^\infty(\square; L^\infty(D_{\text{ref}}; \mathbb{R}^{d \times d}))$ consists of all matrix-valued functions $\mathbf{M}: \square \rightarrow L^\infty(D_{\text{ref}}; \mathbb{R}^{d \times d})$ with

$$\|\mathbf{M}\|_{d \times d} := \text{ess sup}_{\mathbf{y} \in \square} \|\mathbf{M}(\mathbf{y})\|_{L^\infty(D_{\text{ref}}; \mathbb{R}^{d \times d})} < \infty.$$

Regularity results

- ▶ For the numerical approximation of $\mathbb{E}[u]$ and $\mathbb{V}[u]$ by e.g. the quasi-Monte Carlo quadrature or stochastic collocation, we have to provide regularity results for the solution \hat{u} .
- ▶ To that end, we have to analyze the derivatives of the diffusion matrix

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

and the right hand side

$$f_{\text{ref}}(\mathbf{x}, \mathbf{y}) = \hat{f}(\mathbf{x}, \mathbf{y}) \det \mathbf{J}(\mathbf{x}, \mathbf{y}),$$

on D_{ref} .

Lemma

It holds for the derivatives of $(\mathbf{J}(\mathbf{x}, \mathbf{y})^\top \mathbf{J}(\mathbf{x}, \mathbf{y}))^{-1}$ under the conditions of the assumption that

$$\|\partial_{\mathbf{y}}^{\alpha} (\mathbf{J}^\top \mathbf{J})^{-1}\|_{d \times d} \leq |\alpha|! \frac{\gamma^{\alpha}}{\underline{\sigma}^2} \left(\frac{2(1 + c_{\gamma})}{\underline{\sigma}^2 \log 2} \right)^{|\alpha|}.$$

Lemma

It holds for the derivatives of $\det \mathbf{J}(\mathbf{x}, \mathbf{y})$ under the condition of the assumption that

$$\|\partial_{\mathbf{y}}^{\alpha} \det \mathbf{J}\|_{L^{\infty}(\square; L^{\infty}(D_{\text{ref}}))} \leq (|\alpha|!)^2 \bar{\sigma}^d \left(\frac{d}{\underline{\sigma} \log 2} \right)^{|\alpha|} \gamma^{\alpha}.$$

Lemma

For the univariate derivatives of $\det \mathbf{J}(\mathbf{x}, \mathbf{y})$ it holds under the condition of the assumption that

$$\left\| \partial_{y_i}^\alpha \det \mathbf{J} \right\|_{L^\infty(\square; L^\infty(D_{\text{ref}}))} \leq \alpha! \bar{\sigma}^d \left(\frac{2d}{\underline{\sigma}} \right)^\alpha \gamma_i^\alpha.$$

- ▶ The proofs of these Lemmata are obtained by an application of the multivariate *Faà di Bruno formula* (generalized chain rule). For the determinant, we apply the identity $\det \mathbf{M} = \exp(\text{tr} \log \mathbf{M})$.
- ▶ In the multivariate case, the successive application of Faà di Bruno's formula yields an additional factor $|\alpha|!$ in our estimates. For univariate derivatives, this factor can be avoided, but up to now, we were not able to avoid it in the multivariate case.

Theorem

The derivatives of the diffusion matrix $\mathbf{A}(\mathbf{x}, \mathbf{y})$ satisfy

$$\|\|\partial_{\mathbf{y}}^{\alpha} \mathbf{A}\|\|_{d \times d} \leq 2(|\alpha|!)^2 \frac{\bar{\sigma}^d}{\underline{\sigma}^2} \left(\frac{2d(1+c_{\gamma})}{\underline{\sigma}^2 \log 2} \right)^{|\alpha|} \gamma^{\alpha}.$$

Theorem

It holds for the univariate derivatives of the diffusion matrix $\mathbf{A}(\mathbf{x}, \mathbf{y})$ that

$$\|\|\partial_{y_i}^{\alpha} \mathbf{A}\|\|_{d \times d} \leq (\alpha + 1)! \frac{\bar{\sigma}^d}{\underline{\sigma}^2} \left(\frac{2d(1+c_{\gamma})}{\underline{\sigma}^2 \log 2} \right)^{\alpha} \gamma_i^{\alpha}.$$

Theorem

Given that $f(\mathbf{x})$ is analytic, the derivatives of the right hand side $f_{\text{ref}}(\mathbf{x}, \mathbf{y})$ satisfy

$$\left\| \partial_{\mathbf{y}}^{\alpha} f_{\text{ref}} \right\|_{L^{\infty}(\square; L^{\infty}(D_{\text{ref}}))} \leq 2(|\alpha|!)^2 c_f \bar{\sigma}^d \left(\frac{d}{\underline{\sigma} \rho \log 2} \right)^{|\alpha|} \gamma^{\alpha}.$$

Theorem

It holds for the univariate derivatives of the right hand side $f_{\text{ref}}(\mathbf{x}, \mathbf{y})$ that

$$\left\| \partial_{y_i}^{\alpha} f_{\text{ref}} \right\|_{L^{\infty}(\square; L^{\infty}(D_{\text{ref}}))} \leq (\alpha + 1)! c_f \bar{\sigma}^d \left(\frac{2d}{\underline{\sigma} \rho \log 2} \right)^{\alpha} \gamma_i^{\alpha}.$$

- ▶ The univariate results are sufficient to show the applicability of the stochastic collocation method, cf. [Babuška et al. 07]. Here, we obtain rates of convergence in terms of the particular decay of the perturbation field's Karhunen-Loève expansion.

- ▶ Incorporating all the constants provided by the theorems (and the following one), leads to the modified sequence

$$\{\tilde{\gamma}_k\}_k := \left\{ \gamma_k \max \left(\frac{4d\bar{\sigma}^d}{\underline{\sigma}\rho \log^2 2}, \frac{8d\bar{\sigma}^d(1+c_\gamma)}{\underline{\sigma}^4 \log^2 2} \right) \right\}_k.$$

Theorem

For the derivatives of the solution \hat{u} to the transported model problem, it holds

$$\|\partial_{\mathbf{y}}^\alpha \hat{u}(\mathbf{y})\|_{H^1(D_{\text{ref}})} \leq \frac{\bar{\sigma}^2}{\underline{\sigma}^d} (|\alpha|!)^3 c_f c_D \tilde{\gamma}^\alpha,$$

where c_D is a constant dependent on the domain D_{ref} .

- ▶ For all proofs in this paragraph, see [Harbrecht,P.,Siebenmorgen14b].

Quasi-Monte Carlo quadrature

- ▶ The quasi-Monte Carlo quadrature is a *sampling method* for the approximation of high-dimensional integrals. For a given set of *quasi-random points* $\{\mathbf{y}_1, \dots, \mathbf{y}_N\}$, e.g. Halton points, we have

$$\mathbb{E}[u](\mathbf{x}) \approx \frac{1}{N} \sum_{i=1}^N \hat{u}(\mathbf{x}, \mathbf{y}_i)$$

- ▶ Our regularity results imply that the Quasi-Monte Carlo quadrature based on Halton points for the mean $\mathbb{E}[u]$ is strongly tractable, i.e. convergence independent of M , if the sequence $\{\tilde{\gamma}_k\}_k$ is bounded by

$$\tilde{\gamma}_k \lesssim k^{-5-\varepsilon}$$

for arbitrary $\varepsilon > 0$.

- ▶ More precisely, we have for the quadrature error based on N points the estimate

$$\left\| \mathbb{E}[u] - \frac{1}{N} \sum_{i=1}^N \hat{u}(\cdot, \mathbf{y}_i) \right\|_{H^1(D_{\text{ref}})} \lesssim \frac{\bar{\sigma}^2}{\underline{\sigma}^d} c_f N^{\delta-1}$$

for all $\delta > 0$ with a constant only dependent on δ .

- ▶ Notice that we can obtain similar approximation results for the moments of \hat{u} , i.e. for \hat{u}^p with $p \in \mathbb{N}$, possibly with worse constants.

Numerical results

- ▶ For the preceding analysis, we have considered the diffusion problem for the reference domain D_{ref} .
- ▶ For the numerical solution, we exploit that $\hat{u}(\mathbf{y}) = u \circ \mathbf{V}(\mathbf{y})$.
- ▶ Thus, we may compute samples of the solution on the actual realization $\mathbf{V}(D_{\text{ref}}, \mathbf{y}_i)$. To this end, we employ parametric finite elements (here: mapped piecewise linear finite elements).
- ▶ As a consequence, we avoid the computation of the diffusion matrix $\mathbf{A}(\mathbf{x}, \mathbf{y})$.
- ▶ We have simply to solve the Laplacian equation on the parametric domain $\mathbf{V}(D_{\text{ref}}, \mathbf{y}_i)$ for each sample point \mathbf{y}_i

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

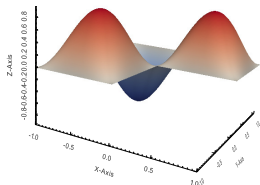


Figure: Mean (L-shape)

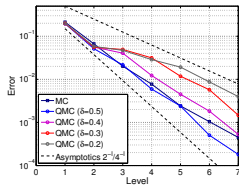
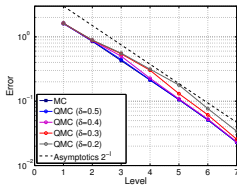
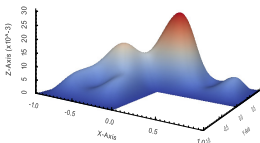
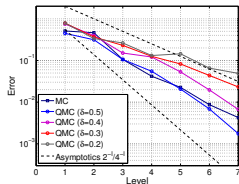
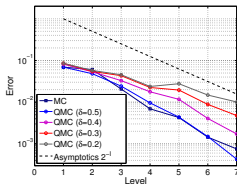

 Figure: H^1 -error (left), L^2 -error (right).


Figure: Variance (L-shape)


 Figure: $W^{1,1}$ -error (left), L^2 -error (right).

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

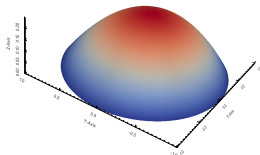


Figure: Mean (Disc)

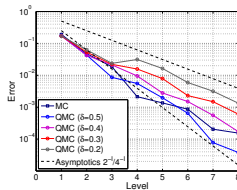
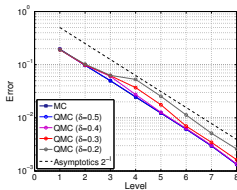
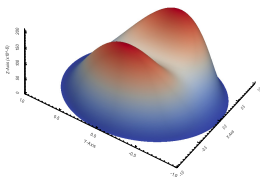
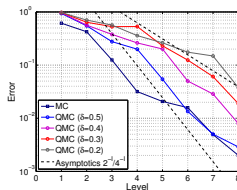
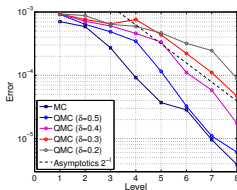

 Figure: H^1 -error (left), L^2 -error (right).


Figure: Variance (Disc)


 Figure: $W^{1,1}$ -error (left), L^2 -error (right).

$$\text{Cov}[\mathbf{V}](\mathbf{x}, \mathbf{y}) = F_0(\mathbf{x})F_0(\mathbf{y})c(\theta_x, \theta_y) \begin{bmatrix} \cos(\theta_x) \\ \sin(\theta_x) \end{bmatrix} \begin{bmatrix} \cos(\theta_y) \\ \sin(\theta_y) \end{bmatrix}^\top, \quad f(\mathbf{x}) = 1$$

$$\text{with } c(\theta_x, \theta_y) = \frac{1}{900} \sum_{k=0}^5 \cos(k\theta_x) \cos(k\theta_y) + \sin(k\theta_x) \sin(k\theta_y),$$

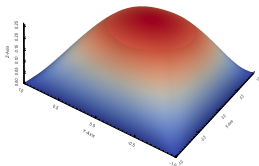


Figure: Mean (Interf.)

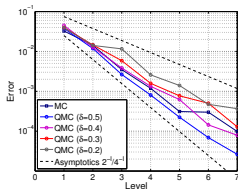
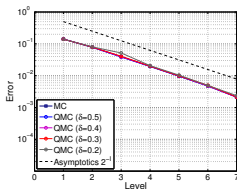
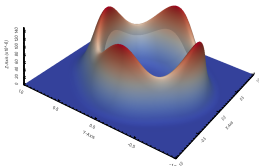
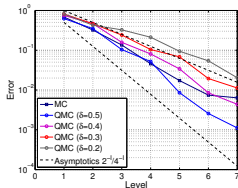
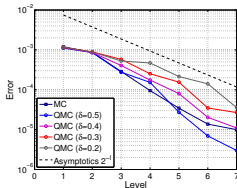

 Figure: H^1 -error (left), L^2 -error (right).


Figure: Variance (Interf.)


 Figure: $W^{1,1}$ -error (left), L^2 -error (right).

Conclusion

- ▶ Given the mean and the covariance function of a random field \mathbf{V} , we can make it feasible for numerical computations by computing its Karhunen-Loève expansion with the pivoted Cholesky decomposition.
- ▶ We have regularity results, which imply the tractability of the quasi-Monte Carlo quadrature for Halton points for the computation of $\mathbb{E}[u]$ and $\mathbb{V}[u]$ with respect to D_{ref} .
- ▶ By the application of parametric finite elements, we can compute each sample on the actual realization of the domain.



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