Sparse Tensor Methods for PDEs with Stochastic Data

I: MLMC and FoSM

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Numerical models in engineering can be solved with high accuracy

if input data are known exactly.

Often, however,

input data are not known exactly

and

accurate numerical solutions are of limited use.

- Mathematical description of uncertainty in input data and solution?
- How to *propagate* data uncertainty through an engineering FEM simulation?
- How to process statistical information in FEM?

Goal:

given statistics of input data, compute (deterministic) solution statistics.

Tool:

Formulation and solution of *Stochastic Partial Differential Equation (SPDE)*

1. Deterministic operator w. stochastic data:

   $u : \Omega \ni \omega \to X$ such that

   $$Au = f(\cdot, \omega), \qquad f : \Omega \ni \omega \to Y'$$

2. Stochastic operator $A(\omega) \in L(X, Y')$ and deterministic data $f \in Y'$:
   $u : \Omega \ni \omega \to X$ such that

   $$A(\omega)u = f \ .$$

Choices of X and Y: elliptic PDEs $X = Y$, parabolic/hyperbolic PDEs: $X \neq Y$.

Examples

$(\Omega, \Sigma, \mathbb{P})$ P.-space, $\quad \omega \in \Omega, \quad x \in D \subset \mathbb{R}^d$ bounded Lipschitz domain

1. Diffusion (random medium, random source term) (Dettinger & Wilson (1985), ...)

$$-\nabla \cdot (a(x;\omega)\nabla u(x;\omega)) = f(x;\omega) \quad \text{in} \quad D, \qquad u(\cdot;\omega)|_{\partial D} = 0 \ .$$

2. Random Eigenvalue Problem (R. Andreev & CS (2010))

$$-\nabla \cdot (a(x;\omega)\nabla w(x;\omega)) = \lambda(\omega) w(x;\omega) \quad \text{in} \quad D, \qquad w(\cdot;\omega)|_{\partial D} = 0 \ .$$

3. Diffusion in Random Medium

$$\rho(x,t;\omega)\partial_t u - \nabla \cdot (a(x,t;\omega)\nabla u(x,t;\omega)) = f(x,t;\omega) \quad \text{in} \quad D, \qquad u(\cdot,\cdot;\omega)|_{\partial D} = 0 \ ,$$

$$u(x,0;\omega) = u_0(x;\omega) \quad \text{in} \quad D \ .$$

4. Wave Propagation in Random Medium

$$\rho(x,t;\omega)\partial_{tt}^2 u - \nabla \cdot (a(x,t;\omega)\nabla u(x,t;\omega)) = f(x,t;\omega) \quad \text{in} \quad D, \qquad u(\cdot,\cdot;\omega)|_{\partial D} = 0 \ ,$$

$$u(x,0;\omega) = u_0(x;\omega) \ , \quad \partial_t u(x,0;\omega) = u_1(x;\omega) \quad \text{in} \quad D \ .$$

References

Monte Carlo FEM
Sampling Methods w. *Sparse Tensor Estimation* of Correlations (CS and von Petersdorff (2006)) ,
Multilevel Monte Carlo: (Heinrichs (2000), Giles (2006))
Diffusion (Barth, CS & Zollinger (2010)) , SCL (Mishra & CS (2010)) .

Perturbation Methods "First Order Second Moment" (FOSM)
Asymptotics: J. B. Keller (1964), L. Borcea, G. Papanicolau et al., M. Kleiber, T.D. Hien (1992)
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Outline

Random fields, statistics

$$D \subset \mathbb{R}^d \quad \text{bounded domain,} \quad \Gamma = \partial D = \Gamma_0 \cup \Gamma_1 \quad \text{Lipschitz,}$$
$$(\Omega, \Sigma, \mathbb{P}) \quad \text{probability space}$$

Random fields on Γ, D:

X separable Hilbert space. $u(x, \omega)$ *random field* iff

$$u \in L^0(\Omega, X) := \{u(x,\omega) : \quad \Omega \to X | \quad \Omega \ni \omega \to \|u(\cdot,\omega)\|_X \text{ is } \mathbb{P}\text{-measurable } \}$$

A random field $u \colon \Omega \to X$ is in $L^1(\Omega, X)$ if $\omega \mapsto \|u(\omega)\|_X$ is integrable so that

$$\|u\|_{L^1(\Omega,X)} := \int_\Omega \|u(\omega)\|_X \, d\mathbb{P}(\omega) < \infty$$

In this case the Bochner integral

$$\mathbb{E}u := \int_\Omega u(\omega) d\mathbb{P}(\omega) \in X$$

exists and we have

$$\|\mathbb{E}u\|_X \leq \|u\|_{L^1(\Omega,X)} \,. \tag{1}$$

$B : X \to Y$ continuous, linear.

$u \in L^k(\Omega, X)$ random field in $X \implies v(\omega) = Bu(\omega) \in L^k(\Omega, Y)$

$$\|Bu\|_{L^k(\Omega,Y)} \leq C \|u\|_{L^k(\Omega,X)}$$

and

$$B \int_\Omega u \, d\mathbb{P}(\omega) = \int_\Omega Bu \, d\mathbb{P}(\omega).$$

Statistical moments of u: for any $k \in \mathbb{N}$ need k-fold tensor product spaces

$$X^{(k)} = \underbrace{X \otimes \cdots \otimes X}_{k\text{-times}},$$

equipped with a cross norm $\| \circ \|_{X^{(k)}}$ (Schatten (TAMS 1943), Grothendieck (MAMS 1955))

$$\forall u_1, \ldots, u_k \in X \qquad \|u_1 \otimes ... \otimes u_k\|_{X^{(k)}} = \|u_1\|_X ... \|u_k\|_X$$

For $u \in L^k(\Omega, X)$ consider random field

$$u^{(k)} = u(\omega) \otimes \cdots \otimes u(\omega) \in L^1(\Omega, X^{(k)})$$

and

$$\begin{aligned} \left\| u^{(k)} \right\|_{L^1(\Omega, X^{(k)})} &= \int_\Omega \|u(\omega) \otimes \cdots \otimes u(\omega)\|_{X^{(k)}} \, d\mathbb{P}(\omega) \\ &= \int_\Omega \|u(\omega)\|_X \cdots \|u(\omega)\|_X \, d\mathbb{P}(\omega) = \|u\|^k_{L^k(\Omega,X)} \end{aligned} \tag{2}$$

Define k-th moment (k-point correlation function) $\mathcal{M}^k u$ as expectation of $u \otimes \cdots \otimes u$:

Definition 1

For $u \in L^k(\Omega, X)$ for some integer $k \geq 1$, the k-th moment of $u(\omega)$ is defined by

$$\mathcal{M}^k u = \mathbb{E}[\underbrace{u \otimes ... \otimes u}_{k-times}] = \int_{\omega \in \Omega} \underbrace{u(\omega) \otimes \; ... \otimes u(\omega)}_{k-times} \, d\mathbb{P}(\omega) \in X^{(k)} \tag{3}$$

Application: Covariance of $u \in L^2(\Omega, V)$, V separable and reflexive (e.g. $V = H_0^1(D)$)

$$\mathrm{C}[u] = \mathbb{E}\left[(u - \mathbb{E}u) \otimes (u - \mathbb{E}u)\right] \in V \otimes V$$

If u "sufficiently regular":
Covariance function:

$$\mathrm{C}[u](x, x') = \int_\Omega (u(x,\omega) - \mathbb{E}u(x))(u(x',\omega) - \mathbb{E}u(x'))d\mathbb{P}(\omega), \qquad x, x' \in D.$$

k-th Moment (k-point correlation function): if $u \in L^k(\Omega, V)$, then

$$\begin{cases} \mathcal{M}^{(k)} u = \mathbb{E}[u \otimes ... \otimes u] \in V^{(k)} := V \otimes ... \otimes V \; : \\ \mathcal{M}^{(k)} u(x_1, ..., x_k) := \displaystyle\int_\Omega u(x_1, \omega) \otimes ... \otimes u(x_k, \omega) \, d\mathbb{P}(\omega) \end{cases}$$

Linear Operator Equation with Stochastic Data

Given $A : V \to V'$ linear, bounded, $f \in L^1(\Omega, V')$, find $u \in L^1(\Omega, V)$:

$$Au = f$$

Assume ex. $\alpha > 0$ and $T : V \to V'$ compact such that

$$\forall v \in V : \left\langle (A + T)\, v, v \right\rangle \geq \alpha \, \|v\|_V^2 \tag{4}$$

and

$$\ker A = \{0\} \tag{5}$$

Proposition 2

Assume (4) and (5). Then

- for every $f \in L^0(\Omega, V')$ exists a unique $u \in L^0(\Omega, V)$ solution of $Au = f$,
- for every $f \in L^k(\Omega, V')$ holds $u \in L^k(\Omega, V)$.

Example: Time harmonic waves w. random incident field

$D \subset \mathbb{R}^3$ bounded, $\Gamma = \partial D$ Lipschitz, $\kappa \in \mathbb{R}$ wavenumber

$$-\Delta U - \kappa^2 U = 0 \text{ in } D^c := \mathbb{R}^3 \backslash \overline{D}$$

subject to Dirichlet boundary conditions

$$\gamma_0 U = U|_\Gamma = u_{inc}(\cdot;\omega) \text{ on } \Gamma, \quad \text{Radiation Condition at } \infty \,.$$

Given random incident field

$$u_{inc} \in L^k(\Omega, H^{\frac{1}{2}}(\Gamma)), \qquad k \geq 0,$$

ex. unique solution (scattered wave)

$$U(x,\omega) \in L^k(\Omega, H^1(D)) \qquad \text{(Sch. \& Todor 2003).}$$

Time harmonic waves w. random incident field: BEM (Harbrecht & CS)

$$U(x,\omega) = (SL_\kappa \sigma)(x;\omega) := \int_\Gamma e(\kappa; x, y)\, \sigma(y;\omega) ds_y .$$

$$V = H^{-1/2}(\Gamma), \quad \sigma(x;\omega) : \Omega \to H^{-1/2}(\Gamma) \quad \text{random flux}$$

Fubini: SL_κ and $\mathcal{M}^{(1)}$ commute. Hence

$$\mathbb{E}[U] = \mathcal{M}^{(1)}[U] = \mathcal{M}^{(1)}[SL_\kappa \sigma] = SL_\kappa \left[\mathcal{M}^{(1)}[\sigma] \right] = SL_\kappa \left[\mathbb{E}[\sigma] \right]$$

where the mean field $\mathbb{E}[\sigma] = \mathcal{M}^{(1)}[\sigma] \in H^{-\frac{1}{2}}(\Gamma)$ satisfies first kind deterministic integral equation

$$S_\kappa \mathbb{E}[\sigma] = \mathbb{E}[u_{inc}] \in H^{\frac{1}{2}}(\Gamma) \,. \tag{6}$$

Unique Solvability (Nédélec and Planchard (1973)): under assumption of nonresonance,

$$\kappa^2 \not\in \Sigma \,.$$

w. Σ set of eigenfreq. of int. Dirichlet problem, ex. $c_S > 0$ such that

$$\forall \sigma \in H^{-1/2}(\Gamma) : \quad \langle \sigma, S_\kappa \sigma \rangle \geq c_S \, \|\sigma\|^2_{H^{-1/2}(\Gamma)}$$

$$!! \;\; c_S \simeq \mathrm{dist}(\kappa^2, \Sigma)$$

Time harmonic waves w. random incident field: BEM (Harbrecht & CS)

If in the stochastic Dirichlet problem $u \in L^2\big(\Omega, H^{\frac{1}{2}}(\Gamma)\big)$ and $\mathbb{E}[u] = 0$, then $U \in L^2\big(\Omega, H^1(D)\big)$ and

$$C[U] = \mathcal{M}^{(2)}U = \mathcal{M}^{(2)}(SL_\kappa \sigma) = (SL_\kappa \otimes SL_\kappa)\mathcal{M}^{(2)}\sigma = \int_\Gamma \int_\Gamma e(\kappa; x, z)\, e(\kappa; y, w)\, C[\sigma](z, w) ds_z\, ds_w\,,$$

where

$$C[\sigma] \in H^{-\frac{1}{2},-\frac{1}{2}}(\Gamma \times \Gamma) := H^{-\frac{1}{2}}(\Gamma) \otimes H^{-\frac{1}{2}}(\Gamma)$$

satisfies the first kind BIE

$$(S_\kappa \otimes S_\kappa)\, C[\sigma] = C[u_{inc}] \in H^{\frac{1}{2},\frac{1}{2}}(\Gamma \times \Gamma)\,.$$

Solvability:

$$\forall C[\sigma] \in H^{-\frac{1}{2},-\frac{1}{2}}(\Gamma \times \Gamma): \quad \langle (S_\kappa \otimes S_\kappa)C[\sigma], C[\sigma]\rangle \geq c_S^2 \|C[\sigma]\|^2_{H^{-\frac{1}{2},-\frac{1}{2}}(\Gamma\times\Gamma)}$$

Stability: Condition of second (k-th) moment equation is c_S^2 (c_S^k) !!!!

Example: SCL in $\mathbb{R}^d$ (Mishra & CS (2010))

$$\frac{\partial u}{\partial t} + \sum_{j=1}^{d} \frac{\partial}{\partial x_j} (f_j(u)) = 0, \quad x = (x_1, \ldots, x_d) \in \mathbb{R}^d,\ t > 0 \quad u(x,t;\omega)|_{t=0} = u_0(x;\omega)\ . \tag{7}$$

For every $0 < T < \infty$, ex. unique *random entropy solution* $u : \Omega \ni \omega \mapsto C_b((0,T); L^1(\mathbb{R}^d))$ given by

$$u(\cdot, t; \omega) = S(t) u_0(\cdot, \omega)\ , \quad t > 0,\ \omega \in \Omega \tag{8}$$

such that for every $k \geq m \geq 1$ and for every $0 \leq t \leq T < \infty$ holds $\mathbb{P}$-a.s.

$$\|u\|_{L^k\left(\Omega; C(0,T;L^1(\mathbb{R}^d))\right)} \leq \ \|u_0\|_{L^k\left(\Omega; L^1(\mathbb{R}^d)\right)}\ , \tag{9}$$

$$\|S(t)\, u_0(\cdot, \omega)\|_{(L^1 \cap L^\infty)(\mathbb{R}^d)} \leq \ \|u_0(\cdot, \omega)\|_{(L^1 \cap L^\infty)(\mathbb{R}^d)} \tag{10}$$

Example: SCL in $\mathbb{R}^d$ (Mishra & CS (2010))

Assume further that for some $k \in \mathbb{N}$ and for some real number $r \geq 1$

$$u_0 \in L^{rk}(\Omega; L^1(\mathbb{R}^d))\,. \tag{11}$$

Then, for every $0 < T < \infty$ and every

$$0 < t_1, t_2, \ldots, t_k \leq T < \infty \tag{12}$$

the spatial k-point correlation function

$$u(x_1, t_1; \omega) \otimes \cdots \otimes u(x_k, t_k; \omega) \tag{13}$$

is well-defined as an element of $L^r(\Omega; L^1(\mathbb{R}^{kd}))$. In particular, the k-th moment

$$(\mathcal{M}^k u)(t_1, \ldots, t_k) := \mathbb{E}[u(\cdot, t_1; \omega) \otimes \cdots \otimes u(\cdot, t_k; \omega)] \tag{14}$$

is well-defined for any choice of t_j as in (12) as an element of $L^1(\mathbb{R}^{kd})$, and it satisfies

$$\left\| \left(\mathcal{M}^k u\right)(t_1, ..., t_k) \right\|_{(L^1(\mathbb{R}^d))^{(k)}} \leq \left\| \bigotimes_{j=1}^{k} u(\cdot, t_j; \cdot) \right\|_{L^1(\Omega; (L^1(\mathbb{R}^d))^{(k)})} \leq \|u_0\|^k_{L^k(\Omega; L^1(\mathbb{R}^d))}\,. \tag{15}$$

Goal of Computation

For the operator equation

$$Au = f$$

with $f \in L^k(\Omega, V)$,

$$\text{given } \mathcal{M}_f^{(k)}, \quad \text{find } \mathcal{M}_u^{(k)}.$$

$$\text{given law of } f, \quad \text{find law of } u\ .$$

Approaches:

- Monte-Carlo FEM ("Collocation in ω"):
  1. multilevel MC
  2. sparse tensor approximation of higher moments
- Sparse Wavelet FEM for deterministic approximation of $\mathcal{M}^{(k)}$

Monte Carlo - I

Given data ensemble

$$\{f(\omega_j), \quad j = 1, ..., M\} \subset V'$$

generate (in parallel) solution ensemble

$$\{u(\omega_j), \quad j = 1, ..., M\} \subset V$$

Theorem 3

Assume (4) and (5) and that $f \in L^{2k}(\Omega, V')$.
Estimate $\mathcal{M}^{(k)}u$ by the k-th moment of ensemble $\{u(\omega_j) : j = 1, ..., M\}$, i.e. by

$$\bar{E}^M[\mathcal{M}^{(k)}u] := \overline{u \otimes \cdots \otimes u}^M = \frac{1}{M}\sum_{j=1}^{M} u(\omega_j) \otimes ... \otimes u(\omega_j) \in V^{(k)}.$$

Then ex. $C(k) > 0$ such that for every $M \geq 1$ and every $0 < \varepsilon < 1$ holds

$$\mathbb{P}\left(\|\mathcal{M}^{(k)}u \ - \bar{E}^M[\mathcal{M}^{(k)}u]\|_{V\otimes...\otimes V} \leq C\frac{\|\mathcal{M}^{2k}(f)\|^{1/2}_{V'^{(2k)}}}{\sqrt{\varepsilon M}}\right) \geq 1 - \varepsilon \qquad (16)$$

Monte Carlo - II

Lemma (Law of iterated logarithm in Hilbert spaces):

V separable Hilbert and $X \in L^2(\Omega, V)$. Then

$$\limsup_{M\to\infty} \frac{\left\| \overline{X}^M - E(X) \right\|_V}{(2M^{-1}\log\log M)^{1/2}} \le \|X - E(X)\|_{L^2(\Omega,V)} \quad \text{with probability 1.}$$

Proof: Classical law of iterated logarithm: for real valued $Y(\omega)$ holds

$$\limsup_{M\to\infty} \frac{\left| \overline{Y}^M - E(Y) \right|^2}{2M^{-1}\log\log M} = \mathrm{Var}Y \quad \text{with probability 1.} \tag{17}$$

Let $Z := X - E(X)$. V separable $\Rightarrow$ w.l.o.g $V = \ell^2 = \mathrm{span}\{e_j\}_{j=1}^\infty$ and $Y := (e^j, Z) = Z_j \in \mathbb{R}$. Apply (17) with

$$\mathrm{VarY} = (e^j \otimes e^j, \mathcal{M}^2 Z) = (\mathcal{M}^2 Z)_{j,j}.$$

Add estimates for $j = 1, 2, \ldots$ and obtain

$$\limsup_{M\to\infty} \frac{\sum_{j=1}^\infty |Z_j|^2}{2M^{-1}\log\log M} \le \sum_{j=1}^\infty (\mathcal{M}^2 Z)_{j,j} \quad \text{with probability 1.}$$

Monte Carlo - III

$\mathbb{P}$-a.s. convergence of MCM (*Semidiscrete Case !*).

Convergence of MCM without Second Moments?

Theorem 4

Consider Moments of order $k \in \mathbb{N}$ and assume

$$f \in L^{\alpha k}(\Omega, V') \quad \text{for some} \quad \alpha \in (1, 2].$$

Then ex. C such that for every $M \geq 1$ and every $0 < \varepsilon < 1$

$$\mathbb{P}\left(\|\mathcal{M}^k u - \bar{E}^M[\mathcal{M}^k u]\|_{V^{(k)}} \leq C \frac{\|f\|^k_{L^{\alpha k}(\Omega, V')}}{\varepsilon^{1/\alpha} M^{1-1/\alpha}} \right) \geq 1 - \varepsilon \tag{18}$$

So far: MCM assuming that $Au = f$ solved exactly ("Semidiscrete MCM").

Next: Galerkin FEM in V.

Galerkin FEM

Dense sequence of subspaces:

$$S_0 \subset S_1 \subset S_2 \subset \cdots \subset S_\ell \subset S_{\ell+1} \subset \ldots V$$

Galerkin FEM: given $f \in L^k(\Omega, V')$, find

$$u_L(\omega) \in L^k(\Omega, S_L) \text{ such that } \quad \langle v_L, Au_L(\omega)\rangle = \langle v_L, f(\omega)\rangle \qquad \forall v_L \in S_L$$

Galerkin Projection: $G_L : V \to S_L$ defined by

$$\forall v_L \in S_L : \quad \langle AG_L u, v_L\rangle = \langle f, v_L\rangle$$

is stable: ex. $L_0 > 0$ s.t.

$$\forall L \geq L_0 : \qquad \|G_L u\|_V \leq C\|u\|_V$$

and converges quasioptimally:

$$\forall L \geq L_0 \quad \forall v_L \in S_L : \qquad \|u(\omega) - u_L(\omega)\|_V \leq C\|u(\omega) - v\|_V \quad \mathbb{P} - \text{a.e.}\,\omega \in \Omega.$$

Convergence Rates

Smoothness Spaces:

$$\{X_s\}_{s\geq 0}, \quad X_0 = V, \quad X_s \subseteq V, \qquad \{Y_s\}_{s\geq 0}, \quad Y_0 = V', \quad Y_s \subseteq V'$$

Regularity:

$$A^{-1} : Y_s \ni f \to u \in X_s, \quad s \geq 0.$$

Convergence Rate:

$$\|u(\omega) - u_L(\omega)\|_V \leq C\Phi(s, N_L)\,\|f\|_{Y_s} \quad \text{where} \quad \Phi(s, N_\ell) := \sup_{v\in X_s} \inf_{v_\ell \in S_\ell} \frac{\|v - v_\ell\|_V}{\|v\|_{X_s}} \quad .$$

MC Galerkin: given $\{f(\omega_j) : j = 1, ..., M\}$, compute $\{u_L(\omega_j) : j = 1, ..., M\}$ and sample average

$$\bar{E}^{M,L}_{\mathcal{M}^k u} := \frac{1}{M} \sum_{j=1}^{M} \underbrace{u_L(\omega_j) \otimes ... \otimes u_L(\omega_j)}_{k-\text{times}} \in S_L^{(k)}.$$

Work:

$O(MN_L^k)$ where $N_L = \dim S_L$ DOFs for "mean field" problem.

Wavelet FEM (Cohen, Dahmen, Kunoth, Schneider, ...)

Wavelet Scale:

$$W_0 := S_0, \qquad S_\ell = S_{\ell-1} \oplus W_\ell,\ \ell = 1, 2, \ldots,$$

Sparse Tensor Product Space (Smol'yak, Teml'yakov, Zenger, Griebel,...):

$$\widehat{V}_L^{(k)} = \sum_{\substack{\vec{\ell} \in \mathbb{N}_0^k \\ |\vec{\ell}| \le L}} W_{\ell_1} \otimes W_{\ell_2} \otimes \cdots \otimes W_{\ell_k}\,.$$

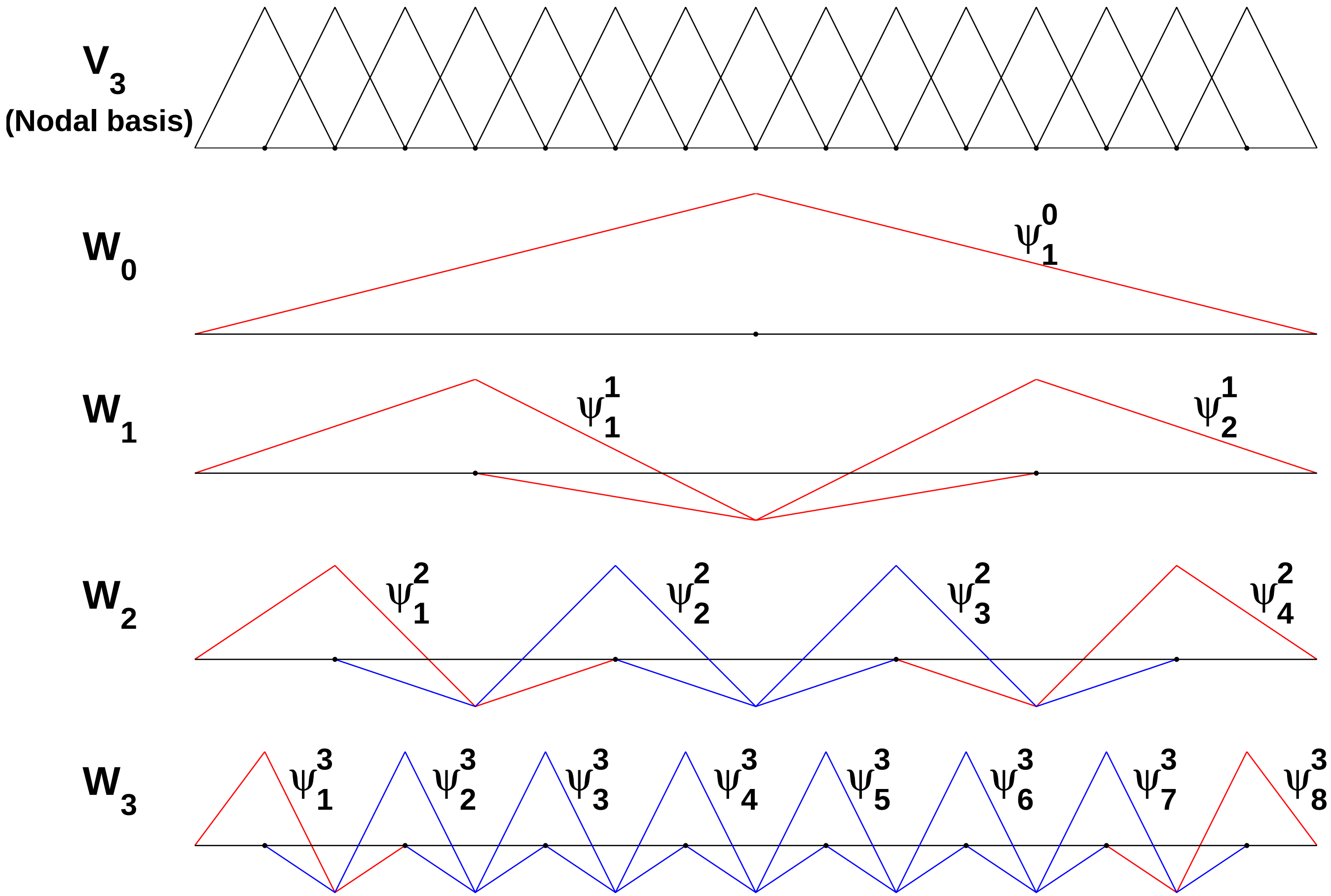
Sparse Projection (quasi-interpolation):

$$\widehat{P}_L^{(k)} : V^{(k)} \to \hat{V}_L^{(k)} \text{ given by } (\widehat{P}_L^{(k)} v)(x) := \sum_{\substack{0 \le \ell_1 + \cdots + \ell_k \le L \\ 1 \le j_\nu \le n_{\ell_\nu}, \nu = 1, \ldots, k}} v_{j_1 \cdots j_k}^{\ell_1 \ldots \ell_j}\, \psi_{j_1}^{\ell_1}(x_1) \ldots \psi_k^{\ell_k}(x_k)$$

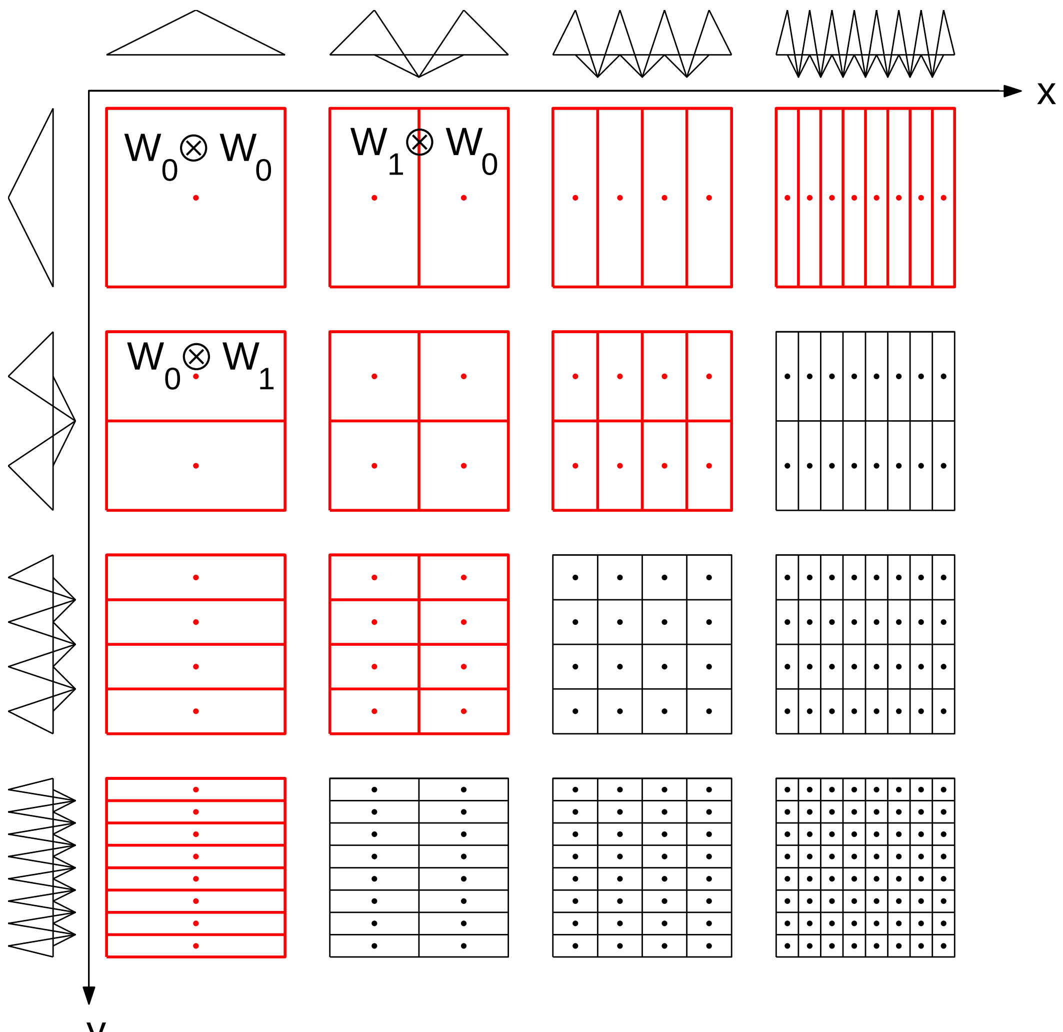
or

$$\widehat{P}_L^{(k)} = \sum_{0 \le \ell_1 + \cdots + \ell_k \le L} Q_{\ell_1} \otimes \cdots \otimes Q_{\ell_k} \quad \text{where} \quad Q_\ell := P_\ell - P_{\ell-1}, \ell = 0, 1, \ldots \text{ and } P_{-1} := 0.$$

Biorthogonal Spline Wavelets in $1-d$, degree $p=1$.



Sparse Tensor Product Space
(Zenger 1990, Griebel & Bungartz Acta Numerica 2004)



Monte Carlo IV – Sparse Monte Carlo FEM

Sparse Tensor Product MC estimate of $\mathcal{M}^k u$:

$$\hat{E}^{M,L}[\mathcal{M}^k u] := \frac{1}{M}\sum_{j=1}^{M} \widehat{P}_L^{(k)}\left[u_L(\omega_j)\otimes \ldots \otimes u_L(\omega_j)\right] \in S_L^{(k)}.$$

Work:

$$O(MN_L(\log_2 N_L)^{k-1}) \quad \text{operations and} \quad N_L(\log_2 N_L)^{k-1} \quad \text{memory}$$

Theorem 5

Assume $1 < \alpha \leq 2$ and

$$f \in L^k(\Omega, Y_s) \cap L^{\alpha k}(\Omega, V') \text{ for some } 0 \leq s < s_0.$$

Then

$$\mathcal{M}^k u \in X_s \otimes \ldots \otimes X_s =: X_s^{(k)}$$

and there is $C(k) > 0$ such that for all $M \geq 1$, $L \geq L_0$ and all $0 < \varepsilon < 1$ holds

$$P\left(\|\mathcal{M}^k u - \hat{E}^{M,L}[\mathcal{M}^k u]\|_{V^{(k)}} < \lambda\right) \geq 1 - \varepsilon$$

$$\text{with } \lambda = C(k)\left[\Phi(s, N_L)(\log N_L)^{(k-1)/2}\,\|f\|^k_{L^k(\Omega,Y_s)} + \varepsilon^{-1/\alpha} M^{-(1-1/\alpha)}\,\|f\|^k_{L^{\alpha k}(\Omega,V')}\right].$$

Sparse Tensor FEM

Idea: A *linear and deterministic* allows to

Compute $\mathcal{M}^k u$ directly, *without* MC

Proposition 6

Assume A satisfies (4), (5) and that $f \in L^k(\Omega, V')$ for $k > 1$.

Then

$$(A \otimes ... \otimes A)Z = \mathcal{M}^k f \, , \tag{19}$$

has a unique solution $Z \in V^{(k)}$ and

$$Z = \mathcal{M}^k u.$$

For $f \in L^k(\Omega, Y_s)$, $s > 0$, holds

$$\|\mathcal{M}^k u\|_{X_s \otimes ... \otimes X_s} \leq C_{k,s} \, \|\mathcal{M}^k f\|_{Y_s \otimes ... Y_s}, \qquad 0 \leq s < s_0, \quad k \geq 1$$

Regularity of $\mathcal{M}^k u$ in spaces of mixed highest derivative!

Sparse Tensor FEM

Theorem 7

Then for all $L \geq kL_0$ sparse Galerkin approximation $\widehat{Z}_L$ of $\mathcal{M}^k u$ is uniquely defined and

$$\|\mathcal{M}^k u - \widehat{Z}_L\|_{V\otimes\ldots\otimes V} \leq C(k) h_L^s |\log h_L|^{(k-1)/2} \|f\|_{L^k(\Omega,Y_s)} \sim N_L^{-s} \log^b N_L \|f\|_{L^k(\Omega,Y_s)} \qquad 0 \leq s < s_0.$$

$\widehat{Z}_L$ can be computed in $O(N_L(\log N_L)^{k+1})$ work and memory.

Note: Full Tensor Galerkin FEM gives

$$\|\mathcal{M}^k u - Z_L\|_{V\otimes\ldots\otimes V} \leq C(k) h_L^s \|f\|_{L^k(\Omega,Y_s)} \sim N_L^{-s/k} \|f\|_{L^k(\Omega,Y_s)} \qquad 0 \leq s < s_0$$

Z_L can be computed in $O(N_L^k)$ work and memory.

Multilevel MC (for Hyperbolic Conservation Laws)

$\mathbf{FVM}$: based on $\{\mathcal{T}_\ell\}_{\ell=0}^\infty$ *nested triangulations* of $D \subset \mathbb{R}^d$ such that mesh width

$$\Delta x_\ell = \Delta x(\mathcal{T}_\ell) = \sup\{\operatorname{diam}(K) : \ K \in \mathcal{T}_\ell\} = O(2^{-\ell}\Delta x_0), \quad \ell \in \mathbb{N}_0 \tag{20}$$

Assume shape regular cells, CFL condition and

$$S_\ell := S(\mathcal{T}_\ell), \quad P_\ell := P_{\mathcal{T}_\ell}, \qquad \mathcal{T}_\ell \in \mathfrak{M}, \quad \ell = 0, 1, \dots . \tag{21}$$

generate a sequence of stable FV approximations, $\{v_\ell(\cdot, t)\}_{\ell=0}^\infty$ on $\mathcal{T}_\ell$ for a number of time steps of sizes Δt_ℓ adapted to grid $\mathcal{T}_\ell \in \mathfrak{M}$. Set in what follows $v_{-1}(\cdot, t) := 0$.

Then, given level $L \in \mathbb{N}$ of spatial resolution, by the linearity of the expectation

$$\mathbb{E}[v_L(\cdot, t)] = \mathbb{E}\Big[\sum_{\ell=0}^{L} (v_\ell(\cdot, t) - v_{\ell-1}(\cdot, t))\Big] . \tag{22}$$

Multilevel MC (for Hyperbolic Conservation Laws)

Estimate each term in (22) statistically by a MCM with a level-dependent number of samples, M_ℓ; this gives the MLMC estimator

$$E^L[u(\cdot,t)] = \sum_{\ell=0}^{L} E_{M_\ell}[v_\ell(\cdot,t) - v_{\ell-1}(\cdot,t)] \tag{23}$$

where $E_M[v_\ell(\cdot,t)]$ is defined by

$$\mathcal{M}^1(u(\cdot,t)) \approx E_M[v_\ell(\cdot,t)] := \frac{1}{M} \sum_{i=1}^{M} \widehat{v}_\ell^i(\cdot,t)\,, \tag{24}$$

and, for $k > 1$, the kth moment (or k point correlation function) $\mathcal{M}^k(u(\cdot,t)) = \mathbb{E}[(u(\cdot,t))^{(k)}]$ is estimated by the sparse tensor MLMC estimate of $\mathcal{M}^k[u(\cdot,t)]$ defined by

$$\widehat{E^{L,(k)}}[u(\cdot,t)] := \sum_{\ell=0}^{L} E_{M_\ell}[\widehat{P}_\ell^{(k)}(v_\ell(\cdot,t))^{(k)} - \widehat{P_{\ell-1}}^{(k)}(v_{\ell-1}(\cdot,t))^{(k)}]\;. \tag{25}$$

Multilevel MC (for Hyperbolic Conservation Laws)

Error Bounds: Assume

$$u_0 \in L^{2k}(\Omega; W^{s,1}(\mathbb{R}^d)) \quad \text{for some } 0 < s < 1 \; .$$

The MLMC-FVM estimate $\widehat{E^{L,(k)}}[u(\cdot,t)]$ in (25) satisfies, for every sequence $\{M_\ell\}_{\ell=0}^L$ of MC samples,

$$\|\mathcal{M}^k u(\cdot,t) - \widehat{E^{L,(k)}}[u(\cdot,t;\omega)]\|_{L^2(\Omega;L^1(\mathbb{R}^{kd}))}$$

$$\lesssim (1 \vee t)\Delta x_L^s |\log \Delta x_L|^{k-1} \left\{ \|\mathrm{TV}(u_0(\cdot,\omega))\|^k_{L^k(\Omega;d\mathbb{P})} + \|u_0(\cdot\,;\omega)\|^k_{L^\infty(\Omega;W^{s,1}(\mathbb{R}^d))} \right\}$$

$$+ \left\{ \sum_{\ell=0}^{L} \frac{\Delta x_\ell^s |\log \Delta x_\ell|^{k-1}}{M_\ell^{1/2}} \right\} \left\{ \|u_0(\cdot\,;\omega)\|^k_{L^{2k}(\Omega;W^{s,1}(\mathbb{R}^d))} + t\|\mathrm{TV}(u_0(\cdot\,;\omega))\|^k_{L^{2k}(\Omega;d\mathbb{P})} \right\} \; .$$

The total work to compute the MLMC estimates $\widehat{E^{L,(k)}}[u(\cdot\,;t)]$ on compact domains $D \subset \mathbb{R}^d$ is therefore (with $O(\cdot)$ depending on the size of D)

$$\widehat{\mathrm{Work}}_L^{MLMC} = O\left(\sum_{\ell=0}^{L} M_\ell \Delta x_\ell^{-(d+1)} |\log \Delta x|^{k-1} \right) \; .$$

Multilevel MC (for Hyperbolic Conservation Laws)

Choice of samples?

$$M_\ell^{-\frac{1}{2}}\,\Delta x_l^s \stackrel{!}{=} \hat{C}\Delta x_L^s, \quad \ell = 0, \ldots, L\,.$$

Then

$$\|\mathcal{M}^k u(\cdot,t) - \widehat{E^{L,(k)}}[u(\cdot,t;\omega)]\|_{L^2(\Omega;L^1(D^k))} \leq C(\widehat{\mathrm{Work}}_L^{MLMC})^{-s'/(d+1)}$$

for any $0 < s' < s$ with the constant depending on D and growing as $0 < s' \to s \leq 1$.

Same accuracy vs. Work as a single deterministic FVM run.

FoSM on Domains with Stochastic Boundaries

Dirichlet Problem:

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

How does u depend on D?

Boundary Perturbation of amplitude $\varepsilon > 0$ in direction $\mathbf{U}$:

$$\mathbf{U}(\mathbf{x}) : \partial D \to \mathbb{R}^3, \qquad ||\mathbf{U}||_2 = 1, \quad \mathbf{U}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) > 0$$

$$\partial D_\varepsilon := \{\mathbf{x} + \varepsilon \mathbf{U}(\mathbf{x}) : \mathbf{x} \in \partial D\}, \qquad D_\varepsilon := \mathrm{interior} \partial D_\varepsilon$$

Specifically:

$$\mathbf{U}(\mathbf{x}) = \kappa(\mathbf{x})\mathbf{n}(\mathbf{x})$$

with $\kappa(\mathbf{x}) \in C^4(\partial D, \mathbb{R})$

Dirichlet Problem on perturbed domain:

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

Idea: for $\varepsilon > 0$ sufficiently small

$$u_\varepsilon = \bar{u} + \varepsilon du[\mathbf{U}] + \frac{\varepsilon^2}{2} d^2 u[\mathbf{U}, \mathbf{U}] + O(\varepsilon^3)$$

FoSM on Domains with Stochastic Boundaries

Thm (Hadamard 1909, F. Murat & J. Simon (1976), J. Sokolowski & P. Zolesio,J. Simon (1980)):

$$u \text{ depends Fréchet-differentiably on } D.$$

The first derivative of u w.r. to D, the *local shape derivative* $du[\mathbf{U}]$, is solution of the Dirichlet problem

$$\Delta du = 0 \text{ in } D, \qquad du = \langle \nabla(g - \bar{u}), \mathbf{U} \rangle = \langle \mathbf{U}, \mathbf{n} \rangle \frac{\partial(g - \bar{u})}{\partial \mathbf{n}} \text{ on } \partial D$$

where $\bar{u}$ is the solution of the Dirichlet Problem on D.

Shape Hessian: bilinear form on pairs of boundary perturbation fields $(\mathbf{U}, \mathbf{U}')$, denoted by

$$d^2 u = d^2 u[\mathbf{U}, \mathbf{U}'].$$

It is obtained from the Dirichlet problem (Hettlich & Rundell SINUM 2000, Eppler 2003):

$$\Delta d^2 u = 0 \text{ in } D,$$

$$d^2 u = \langle \mathbf{H}[g - \bar{u}])\mathbf{U}', \mathbf{U} \rangle - \langle \nabla du[\mathbf{U}], \mathbf{U}' \rangle - \langle \nabla du[\mathbf{U}'], \mathbf{U} \rangle \text{ on } \partial D.$$

FoSM on Domains with Stochastic Boundaries

Random domain variation:

$$\mathbf{U}(\mathbf{x},\omega) = \kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x}),$$

where κ is $\mathbb{P}$-measurable and

$$\kappa(\mathbf{x},\omega) : \Omega \to X = C^k(\partial D, \mathbb{R}), k = 4.$$

Finite second moments of $\kappa(\mathbf{x},\omega)$ in X with respect to P:

$$\mathbb{E}_\kappa(\mathbf{x}) := \int_\Omega \kappa(\mathbf{x},\omega) d\mathbb{P}(\omega) = \mathbb{E}\big(\kappa(\mathbf{x},\omega)\big) = 0, \quad \mathbf{x} \in \partial D,$$

and

$$\mathrm{Covar}_\kappa(\mathbf{x},\mathbf{y}) := \int_\Omega \kappa(\mathbf{x},\omega)\kappa(\mathbf{y},\omega) d\mathbb{P}(\omega) = \mathbb{E}\big(\kappa(\mathbf{x},\omega)\kappa(\mathbf{y},\omega)\big), \quad \mathbf{x},\mathbf{y} \in \partial D,$$

of $\kappa(\mathbf{x},\omega)$ exist and are known:

$$\mathbb{E}_\kappa = 0 \quad \Longrightarrow \quad \mathrm{Covar}_\kappa = \mathcal{M}^2[\kappa].$$

FoSM on Domains with Stochastic Boundaries

Lemma 8

For sufficiently small $\varepsilon > 0$, $u_\varepsilon(\omega)$

$$u_\varepsilon(\mathbf{z},\omega) = \bar{u}(\mathbf{z}) + \varepsilon du(\mathbf{z},\omega) + \frac{\varepsilon^2}{2} d^2u(\mathbf{z},\omega) + \mathcal{O}(\varepsilon^3) \quad \text{for } P - a.e.\ \omega \in \Omega,$$

where $\bar{u} \in H^1(D)$ solves the deterministic Dirichlet problem

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

where

$$du(\mathbf{z},\omega) := du[\kappa(\cdot,\omega)\mathbf{n}](\mathbf{z}),$$

and

$$d^2u(\mathbf{z},\omega) := d^2u[\kappa(\mathbf{z},\omega)\mathbf{n}(\mathbf{z}), \kappa(\mathbf{z}',\omega)\mathbf{n}(\mathbf{z}')]|_{\mathbf{z}'=\mathbf{z}}.$$

The remainder term is $\mathcal{O}(\varepsilon^3)$ for P-a.e. $\omega \in \Omega$.

FoSM on Domains with Stochastic Boundaries

How to compute second moments of $u(\mathbf{x},\omega)$?
It holds

$$\mathbb{E}\big(du(\mathbf{z},\omega)\big) = 0.$$

and, for $\varepsilon > 0$ sufficiently small,

$$\mathbb{E}_u(\mathbf{z}) = \bar{u}(\mathbf{z}) + \mathcal{O}(\varepsilon^2), \qquad \mathbf{z} \in D_\varepsilon.$$

and $\mathrm{Var}_u(\mathbf{z})$ satisfies

$$\mathrm{Var}_u(\mathbf{z}) = \varepsilon^2 \,\mathrm{Var}\big(du(\mathbf{z},\omega)\big) + \mathcal{O}(\varepsilon^3) = \varepsilon^2 \mathbb{E}\,\left(du(\mathbf{z},\omega)^2\right) + \mathcal{O}(\varepsilon^3).$$

How to compute $\mathbb{E}\big(du(\mathbf{z},\omega)^2\big)$ deterministically?

Since $\mathbb{E}(du(\mathbf{x},\omega)) = 0$,

$$\mathrm{Var}\big(du(\mathbf{z},\omega)\big) = \mathrm{Covar}\big(du(\mathbf{z},\omega), du(\mathbf{z}',\omega)\big)\Big|_{\mathbf{z}=\mathbf{z}'}.$$

Approximate $\mathrm{Var}\big(du(\mathbf{z},\omega)\big)$ by trace of two-point correlation of shape gradient du in the "random" direction $\kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x})$.

FoSM on Domains with Stochastic Boundaries

Theorem 9

$$\mathrm{Covar}_{du}(\mathbf{z}, \mathbf{z}') := \mathrm{Covar}\big(du(\mathbf{z}, \omega), du(\mathbf{z}', \omega)\big)$$

is the unique solution in $H^{1,1}(D \times D)$ of the tensor product boundary value problem on $D \times D \subset \mathbb{R}^{2n}$

$$(\Delta_{\mathbf{z}} \otimes \Delta_{\mathbf{z}'})\, \mathrm{Covar}_{du}(\mathbf{z}, \mathbf{z}') = 0, \qquad \mathbf{z}, \mathbf{z}' \in D,$$

$$\mathrm{Covar}_{du}(\mathbf{x}, \mathbf{y}) = \mathrm{Covar}_{\kappa}(\mathbf{x}, \mathbf{y}) \left[\frac{\partial(g - \bar{u})}{\partial \mathbf{n}}(\mathbf{x}) \otimes \frac{\partial(g - \bar{u})}{\partial \mathbf{n}}(\mathbf{y})\right], \qquad \mathbf{x}, \mathbf{y} \in \partial D.$$

Moreover, $\mathrm{Covar}_{du} \in H^{s+1/2, s+1/2}(D \times D)$ provided that $\partial(g - \bar{u})/\partial \mathbf{n} \in H^s(\partial D)$ for some $s \geq 1/2$.

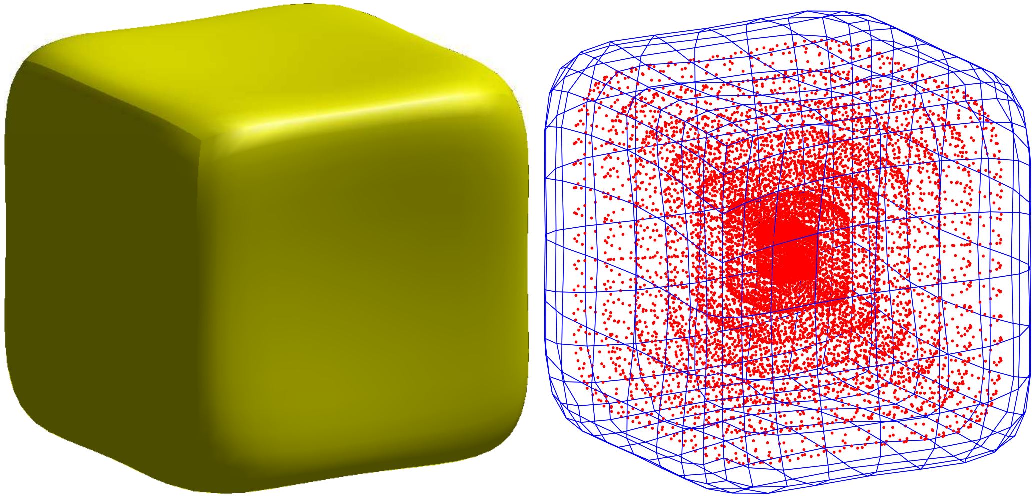


Figure 1: The domain D and the potential evaluation points.

FoSM on Domains with Stochastic Boundaries

Numerical Results

$$f = 1, \qquad g = -x^2/2, \qquad u = -x^2/2, \qquad \mathrm{Covar}_\kappa = xyz\exp(-x^2 - y^2 - z^2)$$

J	N_J	$\|\rho - \rho_J\|_{L^2(\partial D)}$	$\|\mathbf{u} - \mathbf{u}_J\|_\infty$	cpu-time
1	24	2.9e-1	5.6e-1	1
2	96	3.5e-1 (0.8)	5.1e-2 (11)	1
3	384	1.7e-1 (2.1)	2.0e-2 (2.5)	2
4	1536	8.4e-2 (2.0)	3.4e-3 (5.9)	9
5	6144	4.2e-2 (2.0)	4.4e-4 (7.9)	47
6	24576	2.1e-2 (2.0)	9.1e-5 (4.8)	413
7	98304	1.0e-2 (2.0)	1.6e-5 (5.6)	2002
8	393216	1.3e-2 (2.0)	3.7e-6 (4.3)	13097

Table 1: Numerical results with respect to the mean field equation.

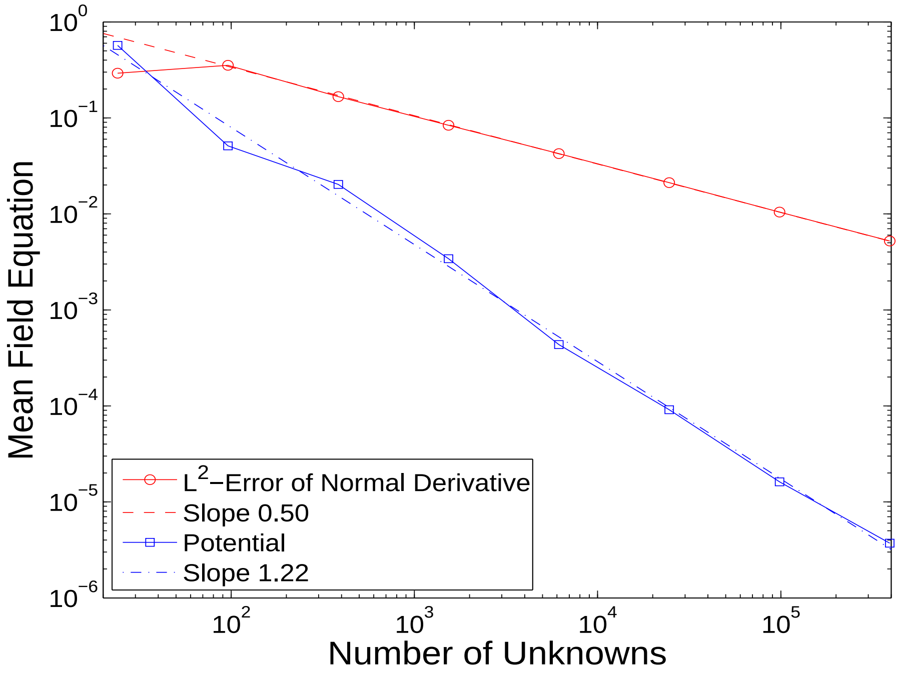


Figure 2: Asymptotic behaviour of the errors for the mean field equation.

FoSM on Domains with Stochastic Boundaries

J	$\widehat{N}_J$	$\|Q_J - \widehat{Q}_J\|_{L^2(\partial D\times\partial D)}$	$\|\Sigma_J - \widehat{\Sigma}_J\|_{L^2(\partial D\times\partial D)}$	$\|\mathbf{C}_J - \widehat{\mathbf{C}}_J\|_\infty$	cpu-time
1	252	1.2e-1	1.3e-1	1.6	1
2	1440	3.4e-1 (0.4)	7.3e-1 (0.2)	2.0e-1 (7.8)	1
3	7488	2.5e-1 (1.4)	7.2e-1 (1.0)	1.7e-1 (1.2)	3
4	36864	9.6e-2 (2.6)	5.2e-1 (1.4)	2.5e-2 (6.6)	14
5	175104	2.8e-2 (3.5)	4.2e-1 (1.2)	8.5e-3 (3.0)	124
6	811008	8.8e-3 (3.1)	3.7e-1 (1.1)	1.0e-3 (8.6)	1210
7	3.7 mio	4.2e-3 (2.1)	3.1e-1 (1.2)	1.6e-4 (6.4)	3 hrs
8	16.5 mio	2.1e-3 (2.0)	3.3e-1 (0.9)	9.4e-5 (1.6)	24 hrs

Table 2: Errors in the covariance approximation by the sparse tensor product approach.

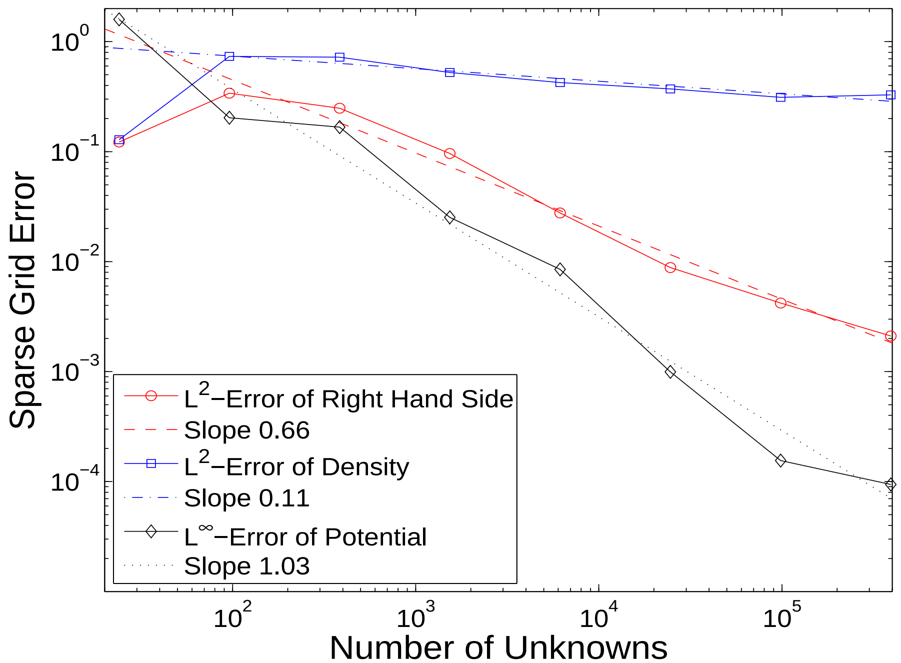


Figure 3: Asymptotic behaviour of the errors of the sparse tensor product approach.

Conclusions

- Monte-Carlo, MLMC for Galerkin FEM and FVM: framework, convergence analysis.
  Error bounds in probability (L^1), mean square (L^2) and $\mathbb{P}$-a.s.
  For low order discretizations in physical space, MLMC optimal (also vs. gpc methods).
- Sparse Tensor Galerkin FEM for k-point correlations:
  regularity in anisotropic spaces; sparse tensor product spaces,
  log-linear complexity of k-point correlation computations.
- Given data statistics, get solution statistics by deterministic computation
- trade stochasticity and MC for high-dimensionality + deterministic FEM
- Use sparse tensor products of wavelet spaces to avoid $O(N_L^k)$ complexity
- Fast Matrix Vector Multiplication (Sch. & Todor: Numer. Math. 2003)
- a-priori and a-posteriori error estimates, adaptivity: for elliptic PDEs
  $\rightarrow$ framework of Cohen, Dahmen, DeVore in tensor product Besov spaces
  (P.A. Nitsche: Constr. Approx. 2006, Stevenson and Sc.: MathComp 2008)

$$\mathcal{M}^k(u) \in B_q^\alpha(L_q(D)) \otimes_q \ldots \otimes_q B_q^\alpha(L_q(D))$$

for arbitrarily large α with

$$q = [\alpha/2 + 1/2]^{-1} < 1 \quad \text{indep. of} \quad k.$$

- nonlinear (Fréchet-differentiable) problems: First Order Second Moment (FoSM)
  - linearize around "nominal" solution,
  - get 2nd order statistics of random solution from gradient and Hessian at "nominal" solution,
  - Sparse Tensor Discretization of FoSM problems
    (H. Harbrecht, R. Schneider and Sch. Numer. Math. (2008))
- Wavelets in physical domain (e.g. D, Γ) essential?
  No, *any hierarchic basis [BPX, spectral, hp]* will work;
  for PDEs frames are sufficient... :
  H. Harbrecht, R. Schneider and Ch. Sch. (Numer. Math. (2008)),
  p-FEM, Spectral FEM: A. Chernov and Ch. Sch.: AppNum. (2009) .