Stochastic collocation and MLMC methods for elliptic PDEs with random coefficients

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R. Tempone, (KAUST), J. Beck (UCL)

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Center for Advanced Modeling and Science

Outline

1. Model problem: elliptic PDEs with random coefficients
2. Polynomial approximation by sparse grid collocation
   - Quasi optimal sparse grid construction
   - Convergence result for elliptic PDEs with random inclusions
   - Numerical results
3. Combined MLMC / Sparse grid method
   - MLMC with Sparse Grid Control Variate
   - Variance analysis and algorithm tuning
   - Numerical results
4. Conclusions

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Model problem: elliptic PDE with random coeffs

Let $(\Omega, \mathcal{F}, P)$ be a complete probability space and $D \subset \mathbb{R}^d$ and open bounded domain.

$$\begin{cases} -\operatorname{div}(a(\omega, x)\nabla u(\omega, x)) = f(x) & x \in D, \quad \omega \in \Omega, \\ u(\omega, x) = 0 & x \in \partial D, \quad \omega \in \Omega \end{cases}$$

with $f \in L^2(D)$ and $a(\omega, x) : \Omega \times D \to \mathbb{R}$ an almost surely bounded random field.

Coercivity assumption: $a_{min}(\omega) = \operatorname{essinf}_{x \in D} a(\omega, x) > 0$ almost surely and $\mathbb{E}[a_{min}^{-\bar{p}}] < \infty$ for some $\bar{p} \geq 2$.

Then $u \in V = H_0^1(D)$ almost surely and

$$\|u(\omega, \cdot)\|_V \leq \frac{C_P}{a_{min}(\omega)} \|f\|_{L^2(D)}, \quad \text{a.s. in } \Omega$$

Therefore, $u \in L_P^p(\Omega, V)$ for all $p \leq \bar{p}$. In particular, $u \in L_P^2(\Omega, V)$.

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Random field parametrization

In view of polynomial approximation we parametrize the random field $a(\omega, x)$ by a finite or countable sequence of random variables $\mathbf{y}(\omega) = (y_1(\omega), \ldots, y_N(\omega))$ with range $\Gamma = \mathbf{y}(\Omega) \subset \mathbb{R}^N$ and probability density function $\rho : \Gamma \to \mathbb{R}_+$:

$$a(\omega, x) = a(\mathbf{y}(\omega), x)$$

Then the stochastic solution u depends on ω only through the vector $\mathbf{y}(\omega)$: $u(\omega, x) = u(\mathbf{y}(\omega), x)$

parameter-to-solution map: $u(\mathbf{y}) : \Gamma \to V, \quad u \in L^2_\rho(\Gamma, V).$

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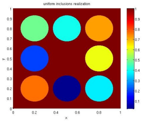
Examples of random diffusion coefficients

Inclusions problem

y describes the conductivity in each inclusion



$$a(\mathbf{y},x) = a_0 + \sum_{n=N}^{N} y_n \mathbb{1}_{D_n}(x)$$

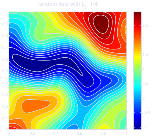
with $y_n \sim \mathcal{U}([y_{min}, y_{max}])$ and $y_{min} > -a_0$.

Therefore $a_{min}(\mathbf{y}) \in L^p_\rho(\Gamma)$ for any $1 \leq p \leq \infty$.

$$\Longrightarrow \quad u \in L^p_\rho(\Gamma, H^1_0(D)),\ \forall 1 \leq p \leq \infty$$

Random fields problem

$a(\mathbf{y},x)$ is a random field, e.g. lognormal: $a(\mathbf{y},x) = e^{\gamma(\mathbf{y},x)}$ with γ expanded e.g. in Karhunen-Loève series



$$\gamma(\mathbf{y},x) = \sum_{n=1}^{\infty} \sqrt{\lambda_n} y_n b_n(x), \quad y_n \sim N(0,1)\ i.i.d.$$

If $Cov[\gamma]$ is Holder continuous, then $a_{min} \in L^p_\rho(\Gamma)$ for any $1 \leq p < \infty$ (see e.g. [Charrier, 2011])

$$\Longrightarrow \quad u \in L^p_\rho(\Gamma, H^1_0(D)),\ \forall 1 \leq p < \infty$$

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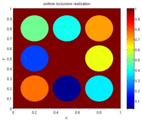

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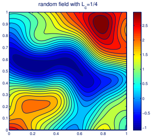

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Stochastic multivariate polynomial approximation

- The parameter-to-solution map $u(\mathbf{y}) : \Gamma \to V$ is often smooth (even analytic for the elliptic diffusion model). It is therefore sound to approximate it by global multivariate polynomials.
- Let $\Lambda \subset \mathbb{N}^N$ be an index set of cardinality $|\Lambda| = M$, and consider the multivariate polynomial space

$$\mathbb{P}_\Lambda(\Gamma) = span\left\{\prod_{n=1}^N y_n^{p_n}, \quad \text{with } \mathbf{p} = (p_1, \dots, p_N) \in \Lambda\right\}$$

We seek an approximation $P_\Lambda u \in \mathbb{P}_\Lambda(\Gamma) \otimes V$.

Collocation approaches

Construct a polynomial approximation of $u(\mathbf{y}) : \Gamma \to V$ using only point evaluations $u_i = u(\mathbf{y}_i)$ where $\{\mathbf{y}_i\}_{i=1}^{\tilde{M}}$ is a set of suitable collocation points, with $\tilde{M} \geq M$.

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Collocation on a (generalized) Sparse Grid

Let $\mathbf{i} = [i_1, \dots, i_N] \in \mathbb{N}_+^N$ and $m(i) : \mathbb{N}_+ \to \mathbb{N}_+$ an increasing function

1. 1D polynomial interpolant operators: $\mathscr{U}_n^{m(i_n)}$ on $m(i_n)$ abscissas. We use either
   - Clenshaw-Curtis (extrema on Chebyshev polynomials)
   - Gauss points w.r.t. the weight ρ_n, assuming that the probability density factorizes as $\rho(\mathbf{y}) = \prod_{n=1}^N \rho_n(y_n)$
2. Detail operator: $\Delta_n^{m(i_n)} = \mathscr{U}_n^{m(i_n)} - \mathscr{U}_n^{m(i_n-1)}$, $\mathscr{U}_n^{m(0)} = 0$.
3. Hierarchical surplus: $\Delta^{m(\mathbf{i})} = \bigotimes_{n=1}^N \Delta_n^{m(i_n)}$.
4. Sparse grid approximation: on an index set $\mathcal{I} \subset \mathbb{N}^N$

$$\mathcal{S}_{\mathcal{I}} u = \sum_{\mathbf{i} \in \mathcal{I}} \Delta^{m(\mathbf{i})}[u]$$

Assumption: The set $\mathcal{I}$ is downward closed:
$\mathbf{i} \in \mathcal{I} \;\Rightarrow\; \mathbf{i} - \mathbf{e}_n \in \mathcal{I}$, $n = 1, \dots, N$.

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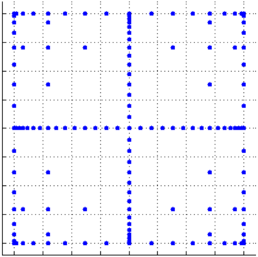
Equivalent formulation

$$\mathcal{S}_{\mathcal{I}} u = \sum_{\mathbf{i} \in \mathcal{I}} c(\mathbf{i}) \mathscr{U}_1^{m(i_1)} \otimes \cdots \otimes \mathscr{U}_N^{m(i_N)} u.$$

with $\quad c(\mathbf{i}) = \sum_{\substack{\mathbf{j} \in \{0,1\}^N \\ (\mathbf{i}+\mathbf{j}) \in \mathcal{I}}} (-1)^{j_1 + \ldots + j_N}, \quad$ and $\quad c(\mathbf{i}) = 0 \quad$ if $\quad \mathbf{i} + \mathbf{1} \in \mathcal{I}$

- linear combination of tensor grids (each with relatively few points!)



Theorem ([Back-Nobile-Tamellini-Tempone, 2010])

Let $\Lambda(\mathcal{I}, m) = \{\mathbf{p} \in \mathbb{N}^N : \ \mathbf{p} \leq m(\mathbf{i}) - 1, \ \mathbf{i} \in \mathcal{I}\}$. Then

- $\mathcal{S}_{\mathcal{I}} : C^0(\Gamma) \to \mathbb{P}_{\Lambda(\mathcal{I},m)}(\Gamma)$
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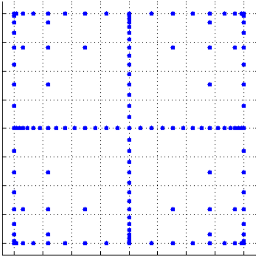

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Quasi-optimal sparse grid construction

$$\mathcal{S}_{\mathcal{I}} u = \sum_{\mathbf{i}\in\mathcal{I}} \Delta^{m(\mathbf{i})}[u] \implies \|u - \mathcal{S}_{\mathcal{I}} u\| = \|\sum_{\mathbf{i}\notin\mathcal{I}} \Delta^{m(\mathbf{i})}[u]\| \leq \sum_{\mathbf{i}\notin\mathcal{I}} \|\Delta^{m(\mathbf{i})}[u]\|$$

One can use a knapsack problem-approach [Griebel-Knapek '09, Gerstner-Griebel '03, Bungartz-Griebel '04] to select the best $\mathcal{I}$: for each multiindex $\mathbf{i}$:

- Estimated error contribution (how much error decreases if $\mathbf{i}$ is added to $\mathcal{I}$)

$$\Delta E(\mathbf{i}) \geq \|\Delta^{m(\mathbf{i})}[u]\|_V$$

- Estimated work contribution (how much the work, i.e. number of evaluations, increases if $\mathbf{i}$ is added to $\mathcal{I}$)

$$\Delta W(\mathbf{i}) \quad \text{such that} \quad \sum_{\mathbf{i}\in\mathcal{I}} \Delta W(\mathbf{i}) \geq W(\mathcal{I})$$

where $W(\mathcal{I})$ is the total number of points in the sparse grid

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One can use a knapsack problem-approach [Griebel-Knapek '09, Gerstner-Griebel '03, Bungartz-Griebel '04] to select the best $\mathcal{I}$: for each multiindex $\mathbf{i}$:

- Estimated error contribution (how much error decreases if $\mathbf{i}$ is added to $\mathcal{I}$)

$$\Delta E(\mathbf{i}) \geq \|\Delta^{m(\mathbf{i})}[u]\|_V$$

- Estimated work contribution (how much the work, i.e. number of evaluations, increases if $\mathbf{i}$ is added to $\mathcal{I}$)

$$\Delta W(\mathbf{i}) \quad \text{such that} \quad \sum_{\mathbf{i}\in\mathcal{I}} \Delta W(\mathbf{i}) \geq W(\mathcal{I})$$

where $W(\mathcal{I})$ is the total number of points in the sparse grid

Quasi-optimal sparse grid construction

Then estimate the profit of each $\mathbf{i}$ as

$$P(\mathbf{i}) = \frac{\Delta E(\mathbf{i})}{\Delta W(\mathbf{i})}$$

and build the sparse grid using the set $\mathcal{I}_M$ of the M indices with the largest estimated profit.

$$\mathcal{I}_M := \{\mathbf{i} \in \mathbb{N}^N \quad P(\mathbf{i}) \geq P_M^{ord}\}$$

where $\{P_j^{ord}\}_j$ is the ordered sequence of profits.

If the set $\mathcal{I}_M$ is not downward closed (lower), take the smallest lower set $\tilde{\mathcal{I}}_M \supset \mathcal{I}_M$. This is equivalent to consider the modified profits $\tilde{P}(\mathbf{i}) = \max_{\mathbf{j} > \mathbf{i}} P(\mathbf{j})$. (see [Chkifa-Cohen-DeVore-Schwab M2AN '13])

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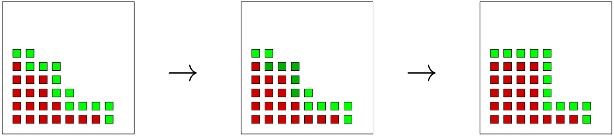
- A posteriori approach [Gerstner-Griebel '03, Klimke, PhD '06]. Given a set Λ, explore all the neighbor multi-indices (margin) and pick up those corresponding to the largest profits.



- A priori approach [Back-Nobile-Tamellini-Tempone '11]. Whenever possible, use *a-priori/a-posteriori* information to build the optimal set. Avoids the "exploration" cost that can be expensive in high dimension.

  The estimate of $\Delta E(\mathbf{i})$ can be related to the decay of the coefficients of the gPC expansion $u = \sum_{\mathbf{p}} u_{\mathbf{p}} \psi_{\mathbf{p}}$ of the solution onto an orthonormal polynomial basis (Legendre, Chebyshev, Hermite, ...) and to the Lebesgue constant of the interpolation scheme.

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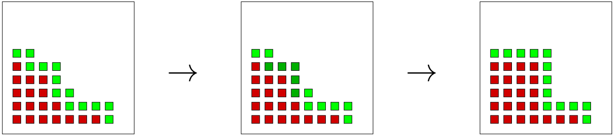

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General convergence result

Theorem [Tamellini PhD thesis '12], [Nobile-Tamellini-Tempone, in preparation]

Let $\mathcal{S}_{\tilde{\mathcal{I}}_M} u$ be the quasi-optimal sparse grid approximation and $W_{\tilde{\mathcal{I}}_M}$ the total number of points in the sparse grid.

If $C(\tau) := \left(\sum_{\mathbf{i}\in\mathbb{N}^N} \tilde{P}(\mathbf{i})^\tau \Delta W(\mathbf{i})\right)^{\frac{1}{\tau}} < \infty$ for some $\tau < 1$

Then $\|u - \mathcal{S}_{\tilde{\mathcal{I}}_M} u\|_{L^2_\rho(\Gamma,V)} \leq C(\tau) W_{\tilde{\mathcal{I}}_M}^{1-\frac{1}{\tau}}$

Proof

The proof uses

- Stechkin lemma: given a non-negative descreasing sequence $\{a_k\}_k$, then

$$\sum_{k=N+1}^{\infty} a_k \leq N^{1-\frac{1}{\tau}} \left(\sum_{k=1}^{\infty} a_k^{\tau} \right)^{\frac{1}{\tau}}, \quad 0 < \tau < 1.$$

- ordered repeated sequence of profits $\{\hat{P}_k\}_k = \{\underbrace{\tilde{P}_1, \ldots, \tilde{P}_1}_{\Delta W_1 \text{ times}}, \underbrace{\tilde{P}_2, \ldots, \tilde{P}_2}_{\Delta W_2 \text{ times}}, \ldots\}$.
- Let $W_M = \sum_{j=1}^{M} \Delta W_j$ and observe that $W_M \geq W_{\tilde{\mathcal{I}}_M}$. Then

$$\|u - \mathcal{S}_{\tilde{\mathcal{I}}_M} u\|_{L^2_\rho(\Gamma,V)} \leq \sum_{k=M+1}^{\infty} \Delta E_k \leq \sum_{k=W_M+1}^{\infty} \hat{P}_k \quad \text{[apply Stechkin]}$$

$$\leq \|\{\hat{P}_k\}_k\|_{l^\tau} W_M^{1-\frac{1}{\tau}} \leq C(\tau) W_{\tilde{\mathcal{I}}_M}^{1-\frac{1}{\tau}}$$

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How to estimate ΔW and ΔE

1. $\Delta W(\mathbf{i})$: number of new points in $\bigotimes_{n=1}^N \Delta_n^{m(i_n)}$
   Count all points in $\mathscr{U}_1^{m(i_1)} \otimes \cdots \otimes \mathscr{U}_N^{m(i_N)}$ (non-nested case) or just the extra points added (nested case)
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   E.g. for Chebyshev expansion ($\|\psi_{\mathbf{p}}\|_\infty = 1$)

$$\Delta E(\mathbf{i}) \leq 2\, \mathbb{L}_{m(\mathbf{i})} \sum_{\mathbf{p} \geq m(\mathbf{i}-1)} \|u_{\mathbf{p}}\|_V,$$

where $\mathbb{L}_{m(\mathbf{i})} = \prod_{n=1}^N \mathbb{L}_{m(i_n)}$ and $\mathbb{L}_{m(i_n)} := \|\mathscr{U}_n^{m(i_n)}\|_{\mathcal{L}(C^0, L^2_\rho)}$ is the Lebesgue constant form C^0 to L^2_ρ.

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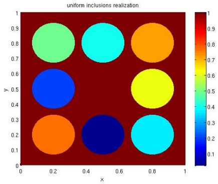
Elliptic equation with random inclusions



- $Y_i \sim \mathcal{U}[a_i, b_i]$, independent
- $\Gamma = \prod_{i=1}^{N} [a_i, b_i]$
- $u(\mathbf{y}) : \Gamma \to H_0^1(D)$

- The solution $u(\mathbf{y}) : \Gamma \to H_0^1(D)$ is analytic in a polydisk in the complex plane $\mathbb{C}^N$
- The solution can be expanded in Chebyshev series $u(\mathbf{y}) = \sum_{\mathbf{p}} u_{\mathbf{p}} \psi_{\mathbf{p}}(\mathbf{y})$ with $\|\psi_{\mathbf{p}}\|_\infty \leq 1$. Estimates on Chebyshev coefficients are available [Babuska-Nobile-Tempone '07] [Nobile-Tamellini-Tempone '13]

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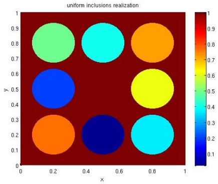

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Quasi-optimal sparse grid construction using (nested) Clenshaw-Curtis points

- $m(i) = 2^{i-1} + 1$ (doubling the points). $\Delta W(\mathbf{i}) \approx \prod_{n=1}^{N} 2^{i_n - 2}$
- Decay of Chebyshev coefficients: $\|u_{\mathbf{p}}\|_V \leq C e^{-g \sum_{n=1}^{N} p_n}$
- Lebesgue constant: $\mathbb{L}(i) \leq \frac{2}{\pi} \log(i+1) + 1$
- Error estimate: $\Delta E(\mathbf{i}) = C \prod_{n=1}^{N} e^{-\hat{g} m(i_n - 1)}$
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Theorem [Nobile-Tamellini-Tempone '13]

$$\left(\sum_{\mathbf{i} \in \mathbb{N}^N} P(\mathbf{i})^{\tau} \Delta W(\mathbf{i})\right)^{\frac{1}{\tau}} < \infty \quad \text{for all } 0 < \tau < 1$$

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By optimizing with respect to τ one can get the estimate

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Quasi-optimal sparse grid construction using (non-nested) Legendre points

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Quasi optimal sparse grid in practice

We have the theoretical bound $\|u_{\mathbf{p}}\|_V \approx Ce^{-\sum_{n=1}^{N} g_n p_n}$, hence, in particular, for $\mathbf{p} = \mathbf{e}_j = (0, \ldots, 0, 1, 0, \ldots, 0)$, $\|u_{\mathbf{e}_j}\|_V \approx Ce^{-g_j p_j}$ which implies that a 1D polynomial interpolation in the variable y_j only converges exponentially with rate g_j.

- The rates g_j can be estimated numerically by "1D analyses". (increase the polynomial degree in one variable at the time and fit the convergence rate).
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When working with random fields instread of inclusion problmes a good estimate for the Legendre/Chebyshev coefficients is (see [Bech-N.-Tamellini-Tempone M3AS '12, Cohen-DeVore-Schwab FoCM '10])

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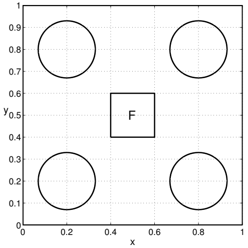
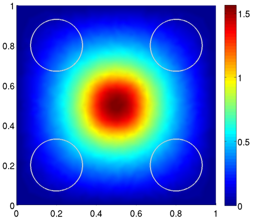
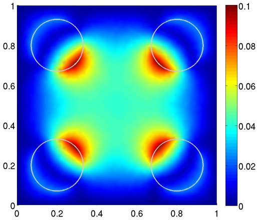
Isotropic test case – 4 random inclusions



- Conductivity coefficient: matrix k=1
  circular inclusions: $k|_{\Omega_i} \sim \mathcal{U}(0.01, 1.99)$
  $\rightarrow$ 4 iid uniform random variables
- forcing term $f = 100\mathbb{1}_F$
- zero boundary conditions
- quantity of interest $\psi(u) = \int_F u$



mean



std

Isotropic test case – 4 random inclusions

convergence plot for $\|\psi(u) - \mathcal{S}_{\mathcal{I}}\psi(u)\|_{L^2_\rho(\Gamma)}$ versus # pts sparse grid

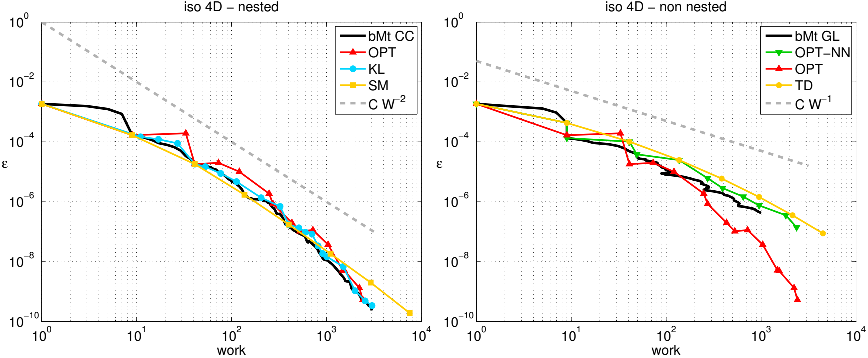


Figure: Results for the isotropic problem. **Left**: (nested) CC points **Right**: (non-nested) Gauss-Legendre points

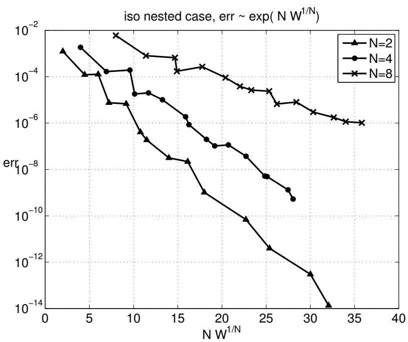
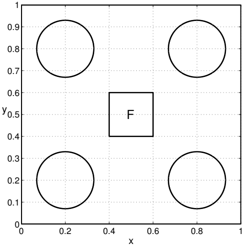
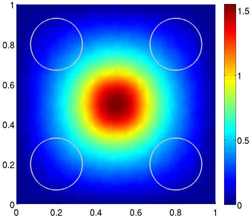


Figure: Results for the isotropic problem. Optimal sparse grids and their predicted convergence rates. **Top**: Nested CC points. **Bottom**: Non-nested Gauss Legendre points.

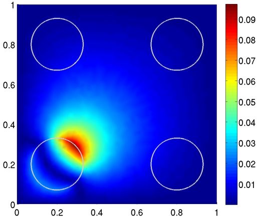
Anisotropic test case – 4 random inclusions



- Conductivity coefficient: matrix k=1 circular inclusions: $k|_{\Omega_i} \sim \gamma_i \mathcal{U}(-0.99, 0.99) \to$ 2 iid uniform random variables
- $\gamma_{1,2,3,4} = 1,\ 0.06,\ 0.0035,\ 0.0002$



mean



std

Anisotropic test case – 4 random inclusions

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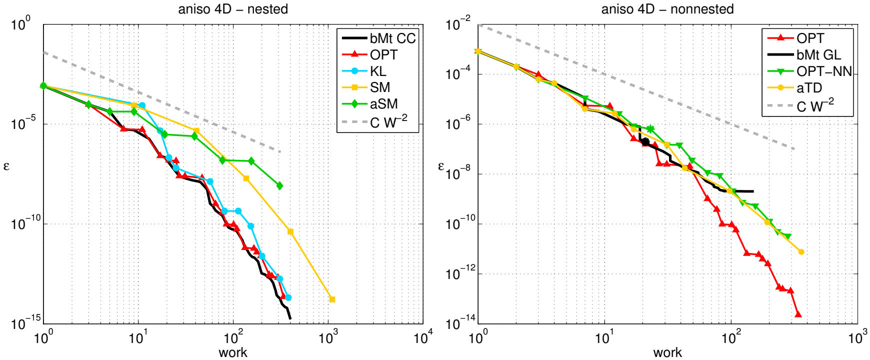

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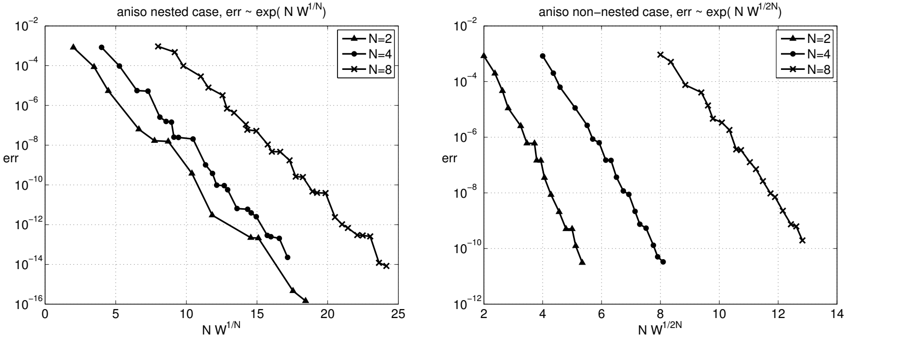
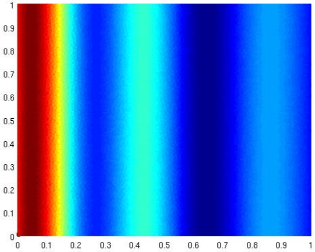


Figure: Results for the anisotropic problem. Optimal sparse grids and their predicted convergence rates. **Top**: Nested CC points. **Bottom**: Non-nested Gauss Legendre points.

Numerical test - 1D stationary lognormal field



$L = 1,\ D = [0, L]^2.$

$$\begin{cases} -\nabla \cdot a(\mathbf{y}, \mathbf{x}) \boldsymbol{\nabla} u(\mathbf{y}, \mathbf{x}) = 0 \\ u = 1 \text{ on } x = 0,\ h = 0 \text{ on } x = 1 \\ \text{no flux otherwise} \end{cases}$$

$$a(\mathbf{x}, \mathbf{y}) = e^{\gamma(\mathbf{x}, \mathbf{y})},\ \mu_\gamma(\mathbf{x}) = 0,$$

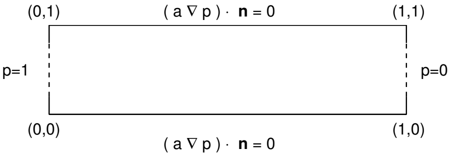
$$Cov_\gamma(\mathbf{x}, \mathbf{x}') = \sigma^2 e^{-\frac{|\mathbf{x}_1 - \mathbf{x}_1'|^2}{LC^2}}$$

We approximate γ as

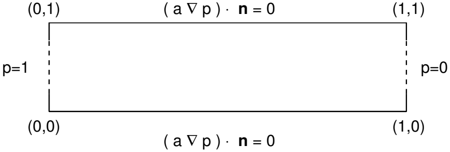
$$\gamma(\mathbf{y}, \mathbf{x}) \approx \mu(\mathbf{x}) + \sigma a_0 y_0 + \sigma \sum_{k=1}^{K} a_k \left[y_{2k-1} \cos\left(\frac{\pi}{L} k \mathbf{x}_1\right) + y_{2k} \sin\left(\frac{\pi}{L} k \mathbf{x}_1\right) \right]$$

with $y_i \sim \mathcal{N}(0, 1)$, i.i.d.

Given the Fourier series $\sigma^2 e^{-\frac{|z|^2}{LC^2}} = \sum_{k=0}^{\infty} c_k \cos\left(\frac{\pi}{L} kz\right)$, $a_k = \sqrt{c_k}$.



- Quantity of interest: effective permeability $\mathbb{E}[\Phi(u)]$, with $\Phi = \left[\int_0^L k(\cdot,x)\frac{\partial u(\cdot,x)}{\partial x}dx\right]$
- Convergence: $|\mathbb{E}[\Phi(\mathcal{S}_{\tilde{\mathcal{I}}_M} u)] - \mathbb{E}[\Phi(u)]|$
- We compare Monte Carlo estimate with quasi-optimal sparse grids based on Gauss-Hermite-Patterson points (nested Gauss-Hermite)
- Estimate of Hermite coefficients decay:
  - for the simpler problem $\nabla \cdot a(\mathbf{y})\nabla u(\mathbf{y},\mathbf{x}) = f$, $a(\mathbf{y}) = e^{b_0 + \sum_{n=1}^N y_n b_n}$, we have $\|u_{\mathbf{i}}\|_V = C\frac{b_n^{i_n}}{\sqrt{i_n!}}$.
  - Heuristic: use the same ansatz $\|u_{\mathbf{i}}\|_V \approx C\prod_{n=1}^N \frac{e^{-g_n i_n}}{\sqrt{i_n!}}$ but estimate the rates g_n numerically.



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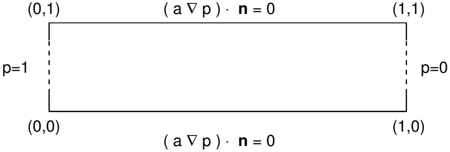

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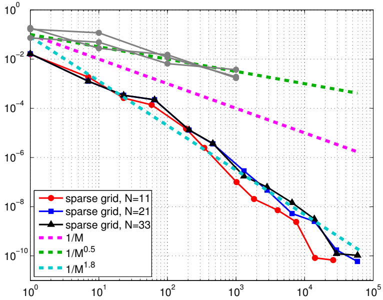
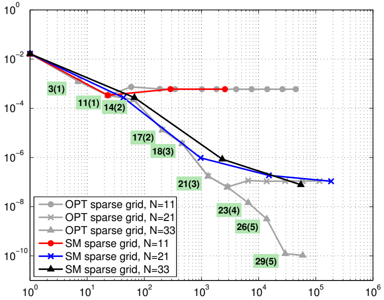
Correlation length: $LC = 0.2$, Std: $\sigma = 0.3$ (c.o.v. $\sim 30\%$)



(a) Convergence of quasi-optimal sparse grid approximations.



(b) Convergence with respect to the reference solution with $N = 33$ r.vs.

- The quasi optimal construction automatically adds new variables when needed.
- No need to truncate a-priori the random field

"A quasi-optimal sparse grids procedure for groundwater flows" by J. Beck, F. Nobile, L. Tamellini and R. Tempone. To appear, LNCSE, Springer, 2013.

Partial conclusions

- Sparse grid polynomial approximation works well for elliptic problems with random coefficients for
  - inclusion type problems with few inclusions
  - smooth random fields with long correlation length
- On the other hand, these techniques suffer in the cases of
  - rough fields even with long correlation lenght; e.g. exponential covariance: $Cov_a(x,y) = \sigma^2 e^{|x-y|/l_c}$

$$a(\omega, x) = \bar{a}(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n} y_n(\omega) b_n(x), \qquad \lambda_n \sim n^{-2}$$

  - fields with short correlation length:

$$\lambda_n = O(1) \quad \text{for} \quad n \leq diam(D)/l_c$$

Idea. In the case of rough longly correlated fields, combine sparse grid polynomial approximation with Multi Level Monte Carlo.

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Outline

1 Model problem: elliptic PDEs with random coefficients

2 Polynomial approximation by sparse grid collocation
- Quasi optimal sparse grid construction
- Convergence result for elliptic PDEs with random inclusions
- Numerical results

3 Combined MLMC / Sparse grid method
- MLMC with Sparse Grid Control Variate
- Variance analysis and algorithm tuning
- Numerical results

4 Conclusions

Darcy Problem with log-normal permeability

find $\mathbf{u}(x,\omega) : \overline{D} \times \Omega \to \mathbb{R}^d$ and $p(x,\omega) : \overline{D} \times \Omega \to \mathbb{R}$ such that almost everywhere in $\omega \in \Omega$ it holds :

$$\begin{cases} \mathbf{u}(x,\omega) = -a(x,\omega)\nabla p(x,\omega) & in \quad D, \\ \mathrm{div}(\mathbf{u}(x,\omega)) = f(x) & in \quad D, \\ + \text{boundary conditions} & on \quad \partial D. \end{cases}$$

- D is the bounded physical domain and $(\Omega, \mathcal{F}, P)$ is the probability space
- $\mathbf{u}$ and p are the Darcy velocity and pressure, respectively
- $a(x,\omega)$ is the permeability field modeled as a lognormally distributed random field $a(x,\omega) = e^{\gamma(x,\omega)}$
- $\gamma(x,\omega)$ is a Gaussian stationary random field

Matérn Covariance Function

Matérn Family

$$\mathrm{cov}_\gamma(x_1 - x_2) = \frac{\sigma^2}{\Gamma(\nu)2^{\nu-1}} \left(\sqrt{2\nu} \frac{\|x_1 - x_2\|}{L_c} \right)^\nu K_\nu \left(\sqrt{2\nu} \frac{\|x_1 - x_2\|}{L_c} \right)$$

- L_c is a correlation length
- Γ is the gamma function
- K_ν is the modified Bessel function of the second kind

- $\nu = 0.5$: $\mathrm{cov}_\gamma(x_1 - x_2) = \sigma^2 e^{-\frac{\|x_1 - x_2\|}{L_c}}$ (exponential covariance)
- $\nu \to \infty$: $\mathrm{cov}_\gamma(x_1 - x_2) = \sigma^2 e^{-\frac{\|x_1 - x_2\|^2}{L_c^2}}$ (Gaussian covariance)

Matérn Covariance Function: Regularity issues

Let $\nu = s + \alpha$ with $s = \lceil \nu - 1 \rceil \in \mathbb{N}$ and $\alpha = \nu - \lceil \nu - 1 \rceil \in (0, 1]$. Then the realizations of the random field are almost surely Hölder continuous, $\gamma(x, \omega) \in \mathcal{C}^{s,\beta}(\bar{D})$ with $\beta < \alpha$.

- For $\nu = 0.5$ the covariance function is only Lipschitz continuous and the field is almost surely Hölder continuous $\gamma(x, \omega) \in \mathcal{C}^{0,\alpha}(\bar{D})$ with $\alpha < 0.5$.
- For $\nu \to \infty$ the covariance function as well as the field are continuous with all their derivates, namely $\mathrm{cov}_\gamma(x), \gamma(x, \omega_i) \in C^\infty(\bar{D})$ $\forall \omega \in \Omega$

(see [Graham, Kuo, Nichols, Scheichl, Schwab, Sloan '13])

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MLMC

$Q = Q(p)$: QoI related to the solution of the PDE
$\mathcal{T}_{h_0}, \dots, \mathcal{T}_{h_L}$: sequence of increasingly fine triangulations
$Y_{h_l} = Q_{h_l} - Q_{h_{l-1}}$: difference of the QoI between two consecutive grids.

Telescopic sum + Linearity of expectation:

$$\mathbb{E}[Q_{h_L}] = \sum_{l=0}^{L} \mathbb{E}[Y_{h_l}], \quad Q_{h_{-1}} = 0$$

MLMC Estimator:

$$\hat{Q}^{MLMC}_{L,\{M_l\}} = \sum_{l=0}^{L} \frac{1}{M_l} \sum_{i=1}^{M_l} \left(Q_{h_l}(\omega_i) - Q_{h_{l-1}}(\omega_i) \right)$$

see [Teckentrup, Scheichl, Giles, Ullmann '12], [Charrier, Scheichl, Teckentrup '11]

MLMC – Mean Square Error (MSE)

$$e(\hat{Q}^{MLMC}_{L,\{M_l\}})^2 = \underbrace{\sum_{l=0}^{L} \frac{\mathbb{V}\mathrm{ar}(Y_{h_l})}{M_l}}_{(i)} + \underbrace{\mathbb{E}[Q_{h_L} - Q]^2}_{(ii)}$$

M_l: number of samples on each level. A good choice of M_l, for $l = 0, ..., L$, represents a crucial issue for the effectiveness of the method (see [Cliffe, Giles, Scheichl, Teckentrup, '11], [Barth, Schwab, Zollinger, '11])

(i): represents the variance of the estimator, i.e. the statistical error: it is expected to be significantly smaller than the variance of the standard MC estimator

(ii): represents the bias of the error, due to the finite element (FE) discretization

Control Variate

Idea: use the solution of an auxiliary problem with regularized coefficient as control variate

Problem: we do not know exactly the expected value of the control variate. However this can be computed efficiently by a Stochastic Collocation (SC) technique

Original Problem

$$\begin{cases} -\mathrm{div}(a\nabla p) = f & \text{in } D, \\ + \text{ boundary conditions} & \text{on } \partial D. \end{cases}$$

Auxiliary Problem

$$\begin{cases} -\mathrm{div}(a^\epsilon\nabla p^\epsilon) = f & \text{in } D, \\ + \text{ boundary conditions} & \text{on } \partial D. \end{cases}$$

- $a = e^{\gamma}$: random field obtained starting from the Matérn covariance function with parameter ν
- $a^\epsilon = e^{\gamma^\epsilon}$: regularized version of a

Control Variate

Regularized Gaussian random field obtained via convolution with a Gaussian kernel

$$\gamma^{\epsilon} = \gamma * \phi_{\epsilon}(x), \text{ where } \phi_{\epsilon} = \frac{1}{(2\pi\epsilon^2)^{\frac{d}{2}}} e^{-\frac{\|x\|^2}{2\epsilon^2}}$$

Quantity of interest defined via control variate

$$Q^{CV} = Q - (Q^{\epsilon} - \mathbb{E}[Q^{\epsilon}])$$

where $Q = Q(p)$ and $Q^{\epsilon} = Q(p^{\epsilon})$

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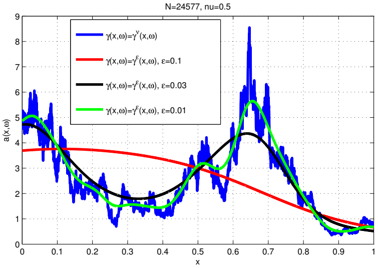
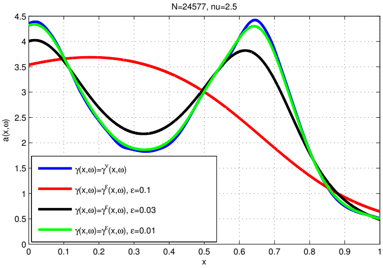


Lipschitz continuous covariance function ($\nu = 0.5$)



Twice differentiable covariance function ($\nu = 2.5$)

MLMC with Control Variate

$\mathcal{T}_{h_0}, \dots, \mathcal{T}_{h_L}$: sequence of increasingly fine triangulations;

$Y_{h_l}^{CV} = Q_{h_l}^{CV} - Q_{h_{l-1}}^{CV}$: difference of the QoI between two consecutive grids.

Telescopic sum + Linearity of expectation:

$$\mathbb{E}[Q_{h_L}^{CV}] = \sum_{l=0}^{L} \mathbb{E}[Y_{h_l}^{CV}], \quad Q_{h_{-1}}^{CV} = 0$$

MLCV Estimator

$$\hat{Q}_{h_L,\{M_l\}}^{MLCV} = \sum_{l=0}^{L} \frac{1}{M_l} \sum_{i=1}^{M_l} \left(Q_{h_l}^{i} - Q_{h_{l-1}}^{i} - (Q_{h_l}^{\epsilon,i} - Q_{h_{l-1}}^{\epsilon,i}) \right) + \mathbb{E}[Q_{h_L}^{\epsilon,SC}]$$

MLMC with Control Variate

Mean Square Error (MSE)

$$e(\hat{Q}^{MLCV}_{h_L,\{M_l\}})^2 \leq \underbrace{\sum_{l=0}^{L} \frac{\mathbb{V}\mathrm{ar}(Y^{CV}_{h_l})}{M_l}}_{(i)} + \underbrace{2\mathbb{E}[Q^{\epsilon}_{h_L} - Q^{\epsilon,SC}_{h_L}]^2}_{(ii)} + \underbrace{2\mathbb{E}[Q_{h_L} - Q]^2}_{(iii)}$$

$\mathbb{E}[Q^{\epsilon,SC}_{h_L}]$: mean of the QoI $Q^{\epsilon}_{h_L}$ computed with a SC scheme on sparse grids.

(i): variance of the estimator

(ii): bias due to the SC approximation of the mean of the control variate $\mathbb{E}[Q^{\epsilon}]$

(iii): bias due to the finite element approximation

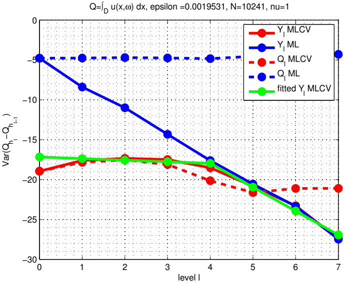
Remark: if ϵ tends to 0 the statistical error (i) vanishes; on the other hand keeping small the SC error (ii) becomes too costly.

MLMC with Control Variate

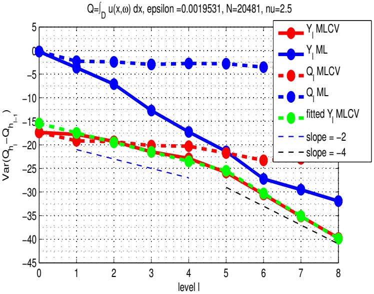
Error estimate (preliminary result)

$$\mathbb{E}\left[\left(Q - Q_{h_l} - (Q^{\epsilon} - Q^{\epsilon}_{h_l})\right)^2\right]^{\frac{1}{2}} \leq c h_l^{\min\{\nu,p\}} \min_{s=1,\dots,p} h_l^{\min\{\nu,s\}} \epsilon^{\min\{(\nu-s)_+,2\}}$$

Variance of the difference of the QoI between consecutive grids. The dashed lines represent the slopes h_l^2 and h_l^4.



$\nu = 1$, $\epsilon = 1/8^3$



$\nu = 2.5$, $\epsilon = 1/8^3$.

MLCV Algorithm

1. Given a prescribed *tol* select h_L in such a way to have $(iii) \leqslant tol^2$;
2. set $h_0 = O(|D|)$ and evaluate $(iv) = \mathbb{V}ar(Y^{CV}_{h_l})$ and $(v) = \mathbb{V}ar(Q^{CV}_{h_l})$; we can select among two basic strategies:
   Strategy 1: if $(iv) < (v)\ \forall\ l$ apply the MLCV scheme starting from level 0;
   Strategy 2: if $(iv) \approx (v)$ for $l = 0, ..., l_0$ set $h_0 = h_{l_0}$; and use the control variate only on level l_0 and a standard MLMC on subsequent levels, namely

$$\hat{Q}^{MLCV}_{h_L,\{M_l\}} = \frac{1}{M_{l_0}} \sum_{i=1}^{M_{l_0}} \left(Q^i_{h_{l_0}} - Q^{\epsilon,i}_{h_{l_0}} \right) + \sum_{l=l_0+1}^{L} \frac{1}{M_l} \sum_{i=1}^{M_l} \left(Q^i_{h_l} - Q^i_{h_{l-1}} \right) + \mathbb{E}[Q^{\epsilon,SC}_{h_{l_0}}]$$

3. according to the strategy selected compute the number of samples M_l for $l = 0, ..., L$ and the number of knots of the sparse grid M_{SG} by solving an optimization problem in such a way to have $(i) + (ii) \leqslant tol^2$

Optimization Problem

- ϵ is considered fixed
- C_l is the computational cost needed to solve one deterministic system on the grid of mesh size h_l; cost model: $C_l = 2C_{l-1} = ... = 2^l C_0 = \gamma 2^l h_0^{-1}$. For instance see [Cliffe, Giles, Scheichl, Teckentrup, '11]

Computational cost

- strategy 1: $C(M_l, M_{SG}) = 2M_0 C_0 + 2\sum_{l=1}^{L} M_l(C_l + C_{l-1}) + M_{SG} C_L$
- strategy 2: $C(M_l, M_{SG}) = 2M_{l_0} C_{l_0} + \sum_{l=l_0+1}^{L} M_l(C_l + C_{l-1}) + M_{SG} C_{l_0}$

Associated Error fitted model

- strategy 1: $e(M_l, M_{SG}) = \sum_{l=0}^{L} \frac{\min\left\{c_1 h_l^{2\min\{\nu,p\}}, c_2 h_l^{4\min\{\nu,p\}}\right\}}{M_l} + c_3 M_{SG}^{\alpha}$
- strategy 2: $e(M_l, M_{SG}) = \sum_{l=l_0}^{L} \frac{c_1 h_l^{4\min\{\nu,p\}}}{M_l} + c_2 M_{SG}^{\alpha}$

Perform a Lagrange optimization by considering

$$\mathcal{L}(M_l, M_{SG}, \lambda) = C(M_l, M_{SG}) - \lambda(e(M_l, M_{SG}) - tol^2)$$

Optimization Problem

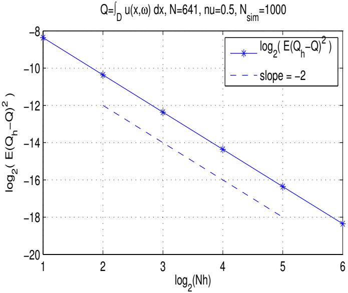
Values obtained (strategy one):

- $M_0 = \sqrt{-\lambda}\sqrt{\frac{c_1 h_0^{2\min\{\nu,p\}}}{2C_0 2^l}} = \sqrt{-\lambda}\sqrt{\frac{v_0}{2C_0}}$
- $M_l = \sqrt{-\lambda}\sqrt{\frac{\min\left\{c_1 h_l^{2\min\{\nu,p\}}, c_2 h_l^{4\min\{\nu,p\}}\right\}}{3C_0 2^l}} = \sqrt{-\lambda}\sqrt{\frac{v_l}{3C_0 2^l}}$ for $l = 1, ..., L$
- $M_{SG} = (-\lambda)^{\frac{1}{1-\alpha}} \left(-\alpha 2^{-L}\frac{c_3}{C_0}\right)^{\frac{1}{1-\alpha}}$

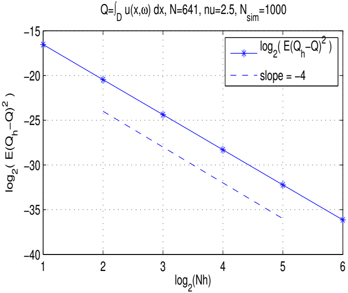
where λ has to be computed from:

$$\frac{1}{\sqrt{-\lambda}} = \frac{tol^2}{\sqrt{C_0}(\sqrt{2v_0} + \sum_{l=1}^{L}\sqrt{3v_l}2^l) + c_3(\frac{1}{\sqrt{-\lambda}})^{\frac{-1-\alpha}{1-\alpha}}(-\alpha 2^{-L}\frac{c_3}{C_0})^{\frac{\alpha}{1-\alpha}}}$$

Approximation error $\mathbb{E}[Q_{h_L} - Q]^2$

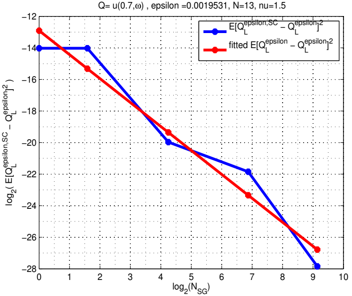


$\nu = 0.5$

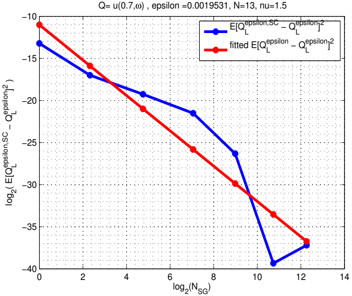


$\nu = 2.5$

SC error $\mathbb{E}[Q_{h_L}^{\epsilon,SC} - Q^{\epsilon}]^2$



$\nu = 0.5$; fitted slope $\alpha = -1.5$



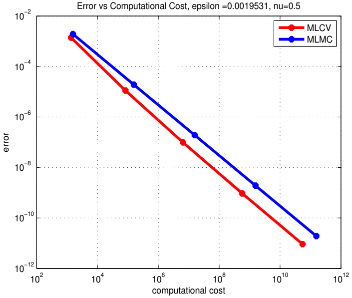
$\nu = 2.5$; fitted slope $\alpha = -2.2$

In both cases more than the 99% of the variability has been taken into account. The fitted rate is better than MC in both cases.

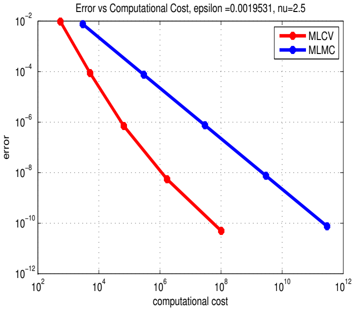
Error vs Cost : MLCV vs MLMC

Error and computational cost associated to several values of $tol = 10^{-1}, ..., 10^{-5}$. $\epsilon = 1/8^3$ in both cases.

error = statistical error + SC error



$\nu = 0.5$



$\nu = 2.5$

Outline

1. Model problem: elliptic PDEs with random coefficients
2. Polynomial approximation by sparse grid collocation
    - Quasi optimal sparse grid construction
    - Convergence result for elliptic PDEs with random inclusions
    - Numerical results
3. Combined MLMC / Sparse grid method
    - MLMC with Sparse Grid Control Variate
    - Variance analysis and algorithm tuning
    - Numerical results
4. Conclusions

Conclusions

- We have analyzed the convergence of quasi-optimal sparse grid approximations based on the selection of the M most profitable hierarchical surpluses. Convergence rates are related to summability properties of the profits, weighted by the corresponding works.
- Sharp a-priori / a-posteriori analysis of the decay of the polynomial chaos expansion of the solution allows to construct optimized sparse grids that provide effective approximations also in infinite dimensions for smooth fields.
- The "profit based" a-posteriori adaptive algorithm is also performing very efficiently, close to the best approximation.
- for rough, longly correlated fields, a good idea is to use a sparse grid polynomial approximation on a smoothed problem as a control variate in a MLMC algorith. Preliminary results show a considerable improvement of the overall complexity.

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Thank you for your attention!