A practical Multilevel quasi-Monte Carlo method for simulating elliptic PDEs with random coefficients

Pieterjan Robbe
(pieterjan.robbe@cs.kuleuven.be)

Co-Authors: D. Nuyens, S. Vandewalle

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KU LEUVEN

Faculteit Ingenieurswetenschappen

Overview

Model Problem

Model Problem

- steady-state flow through porous media: Darcy's law
- second-order elliptic PDE

$$-\nabla \cdot (k(\boldsymbol{x};\omega)\nabla p(\boldsymbol{x};\omega)) = f(\boldsymbol{x})$$

- consider simple 3D flow cell

Representation of Uncertainty

Representation of Uncertainty

- model $k(\boldsymbol{x};\omega)$ as a lognormal field
- use KL-expansion to take samples of $Z := \log(k)$:

$$Z(\boldsymbol{x};\omega) = \bar{Z} + \sum_{n=1}^{\infty} \sqrt{\theta_n} f_n(\boldsymbol{x}) \xi(\omega)$$

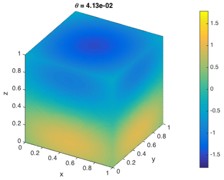
where θ_n and f_n are eigenvalues and eigenfunctions of covariance operator

$$C(\boldsymbol{x},\boldsymbol{y}) := \sigma^2 \exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{y}\|_p}{\lambda}\right) \quad \boldsymbol{x},\boldsymbol{y} \in D = [0,1]^3$$

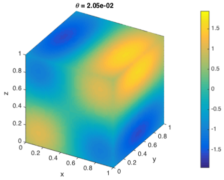
- in practice, truncate sum after s terms

Representation of Uncertainty

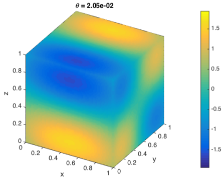
Eigenfunctions in three dimensions



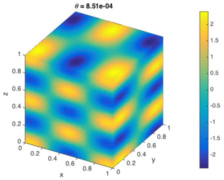
f_2



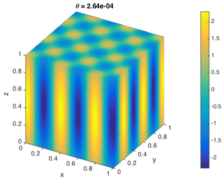
f_5



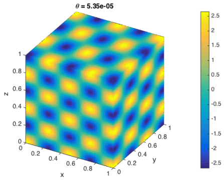
f_6



f_{101}



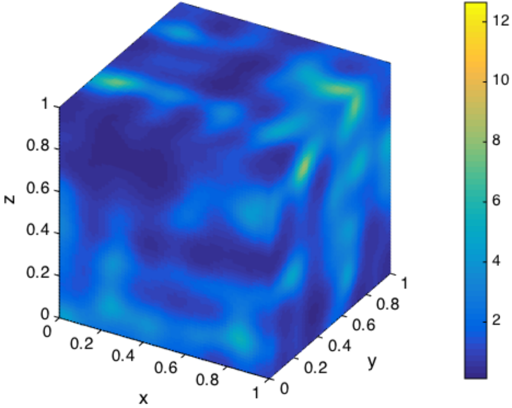
f_{156}



f_{200}

Representation of Uncertainty

A typical sample of k



Multilevel Monte Carlo methods

Multilevel Monte Carlo methods

- we are interested in some functional $Q := \mathcal{G}(p(\boldsymbol{x};\omega))$
- what is the expected value of the functional $\mathbb{E}[Q]$?

taking a sample of $Q(\omega)$ consists of 3 steps:

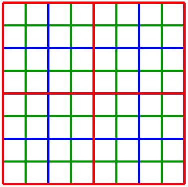
(i) take a sample from the random field,

(ii) solve the resulting deterministic PDE, and

(iii) apply the functional $\mathcal{G}$ to the discretized solution

Multilevel Monte Carlo methods

- hierarchy of nested grids $\{h_\ell\}_{\ell=0}^{L}, h_\ell = h_0 2^{-\ell}$, called levels
- basic idea = take samples not from one approximation Q_M for Quantity of Interest but from multiple $Q_\ell, \ell = 0 \dots L$



$$
\begin{aligned}
\mathbb{E}[Q_1] &= \mathbb{E}[Q_0] + (\mathbb{E}[Q_1] - \mathbb{E}[Q_0]) \\
&= \mathbb{E}[Q_0] + \mathbb{E}[Q_1 - Q_0] \\
\mathbb{E}[Q_2] &= \mathbb{E}[Q_1] + \mathbb{E}[Q_2 - Q_1] \\
&= \mathbb{E}[Q_0] + \mathbb{E}[Q_1 - Q_0] + \mathbb{E}[Q_2 - Q_1] \\
&\vdots \\
\mathbb{E}[Q_L] &= \mathbb{E}[Q_0] + \sum_{\ell=1}^{L} \mathbb{E}[Q_\ell - Q_{\ell-1}] \coloneqq \sum_{\ell=0}^{L} \mathbb{E}[Y_\ell]
\end{aligned}
$$

Multilevel Monte Carlo methods

Error analysis

- 2 unknowns: # samples at each level N_ℓ and # levels L
- total error = stochastic error + discretization error

$$\Downarrow \qquad\qquad\qquad \Downarrow$$

$$N_\ell \qquad\qquad\qquad L$$

Multilevel Monte Carlo methods

Practical details

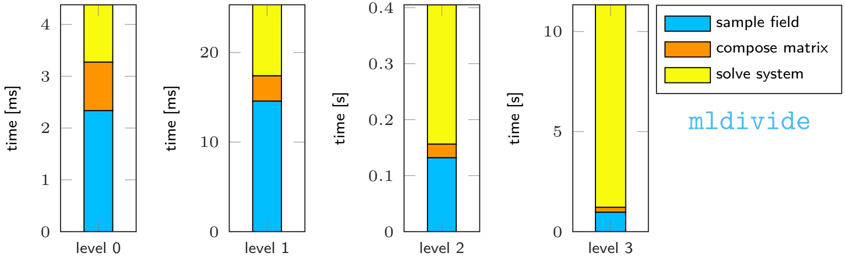
- choose $\lambda = 0.3$, $\sigma = 1$, $s = 100$, $h_0 = 1/4$, no source term
- geometry of simple 3D flow cell with $p(0, \boldsymbol{y}, \boldsymbol{z}) = 1$ and $p(1, \boldsymbol{y}, \boldsymbol{z}) = 0$, no outflow through other boundaries
- Quantity of Interest (QoI) is pressure head at point $\boldsymbol{x}^* = (0.12564, 0.12564, 0.12564)$
- assume cost per level $\mathcal{C}_\ell$ is proportional to $\left(h_\ell^{-3}\right)^\gamma$
- for MATLAB's `mldivide`, $\gamma \approx 1.653$ hence

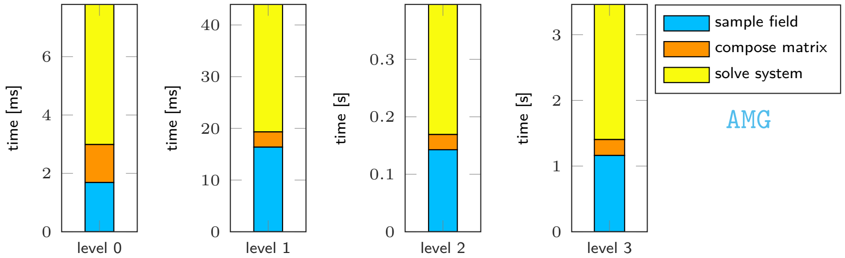
$$\frac{\mathcal{C}_{\ell+1}}{\mathcal{C}_\ell} = 2^{3\gamma} \approx 31.103$$

$\Rightarrow$ use algebraic multigrid method (AMG) with $\gamma \approx 1.070$

Multilevel Monte Carlo methods

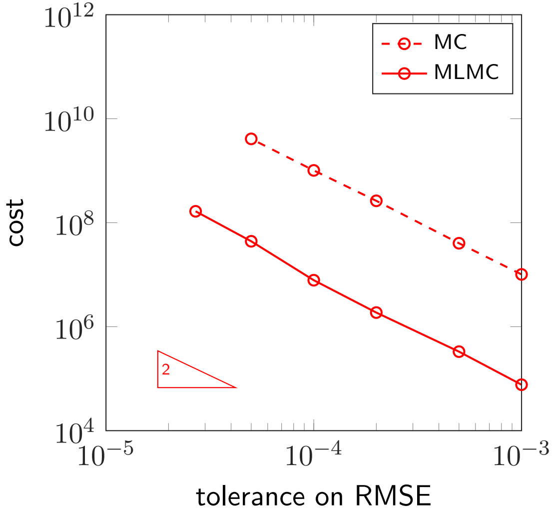
mldivide vs AMG





Multilevel Monte Carlo methods

Performance



Multilevel quasi-Monte Carlo methods

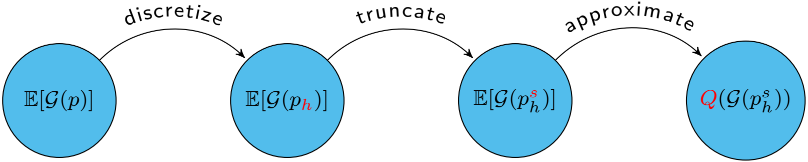
Multilevel quasi-Monte Carlo methods

- basic idea: use quasi-Monte Carlo points for faster convergence
- here, we use randomly shifted rank-1 lattice rules:

$$\xi_n = \text{frac}\left(\frac{n\boldsymbol{z}}{N} + \boldsymbol{\Delta}_\ell\right)$$

Multilevel quasi-Monte Carlo methods

Error analysis



contributions in mean-square-error (MSE):

$$\text{discretization error} = \mathbb{E}[\mathcal{G}(p - p_h)]^2 \qquad \to L$$

$$\text{truncation error} = \mathbb{E}[\mathcal{G}(p_h - p_h^s)]^2$$

$$\text{stochastic error} = \sum_{\ell=0}^{L} \mathbb{E}_{\boldsymbol{\Delta}} \left[\left| (I_s - Q_{\boldsymbol{\Delta}_\ell})(\mathcal{G}(p_\ell^s) - \mathcal{G}(p_{\ell-1}^s)) \right|^2 \right] \quad \to N_\ell$$

Multilevel quasi-Monte Carlo methods

Error analysis

- randomly shifted lattice rule: take q shifts at each level
- worst-case analysis of stochastic error yields

$$\text{stochastic error} \leq \sum_{\ell=0}^{L} \frac{1}{q} \|\mathcal{G}(p_\ell^s) - \mathcal{G}(p_{\ell-1}^s))\|_{H^1_{\text{mix}}}^2 \frac{C_{s,\alpha}^2}{N_\ell^{2\alpha}}$$

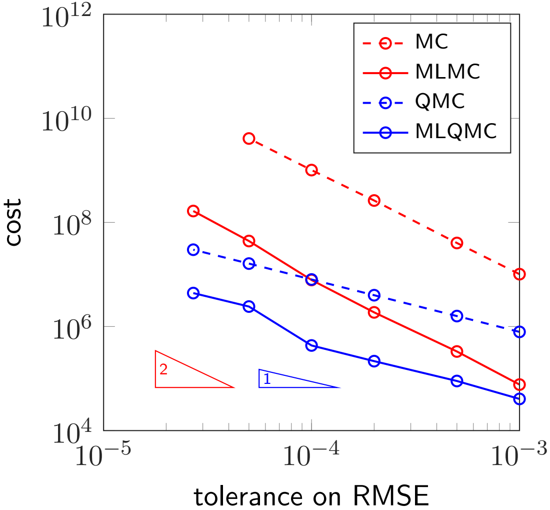
- solve optimisation problem to find

$$N_\ell \simeq \sqrt[2\alpha+1]{\frac{2\alpha C_{s,\alpha}^2 \|\cdot\|_{H^1_{\text{mix}}}^2}{q^2 \mathcal{C}_\ell}}$$

- estimate norm by variance: $\|\cdot\|_{H^1_{\text{mix}}}^2 \to \mathbb{V}[\,\cdot\,]$

Multilevel quasi-Monte Carlo methods

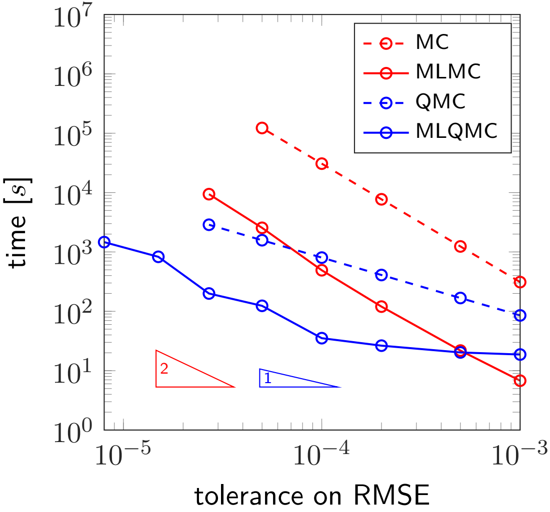
Performance



Multilevel quasi-Monte Carlo methods

Actual computation times

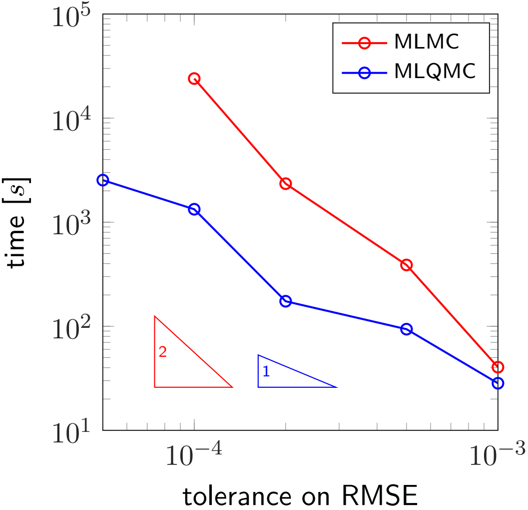
- Quantity of Interest is point evaluation of pressure at $\boldsymbol{x}^*$



Multilevel quasi-Monte Carlo methods

Other QoI's

- Quantity of Interest is outflow through rightmost face

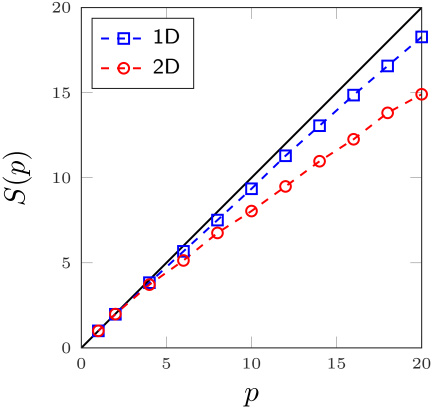


Other features

Other features

Parallelization

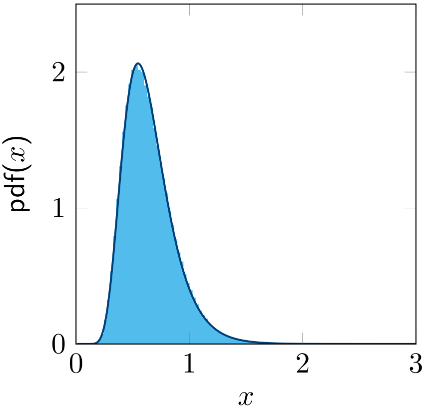
- all samples can be taken independently, as in normal MC
- speedup $S = T_{seq}/T_{par}$



Other features

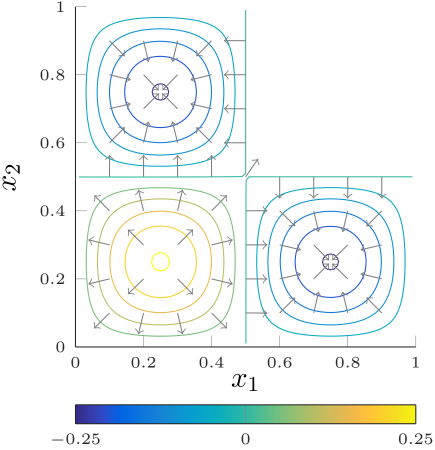
Probability density function of Quantity of Interest

- Quantity of Interest is outflow through rightmost face
- QoI $\sim \mathcal{N}(\ln x; \mu, \sigma)$ with $\mu \approx -0.4917$ and $\sigma \approx 0.3342$

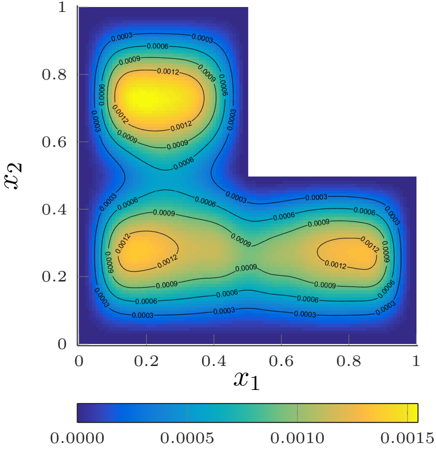


Other features

Multiple Quantities of Interest and complex geometries



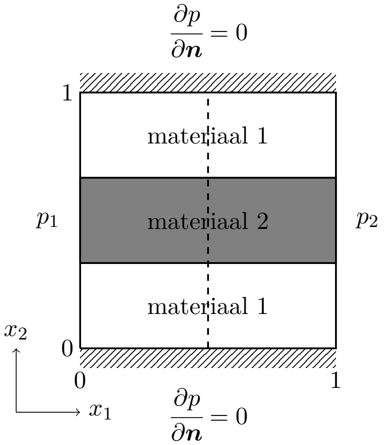
mean value

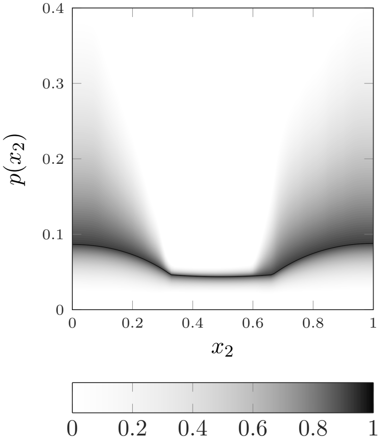


variance

Other features

Multiple Quantities of Interest and complex geometries





Other features

Weaknesses

- estimation of discretization error and finest level L is difficult
- use of multiple physical meshes is not always possible

Conclusions

- successfully applied Multilevel method to 3D problem in subsurface flow
- derivation and implementation of QMC-variant, with cost $\mathcal{O}(\epsilon^{-1.2871})$ instead of $\mathcal{O}(\epsilon^{-2})$ for MLMC
- applied MLMC to more complex problems: discontinuous diffusion coefficients, complex geometries ...
- MLMC with multiple quantities of interest