

Novel Monte Carlo type methods for elliptic PDEs with random coefficients

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“Uncertainty Quantification”

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Motivation: Uncertainty in Groundwater Flow

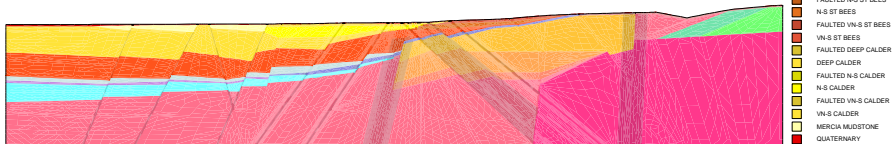
(e.g. risk analysis for radioactive waste disposal ©NIREX UK Ltd.)

Darcy's Law: $\vec{q} + k \nabla p = f$

Incompressibility: $\nabla \cdot \vec{q} = 0$

+ **Boundary Conditions**

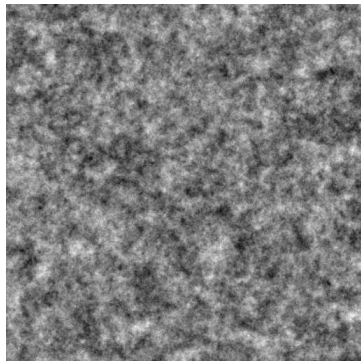
More advanced: multiphase flow in porous media, e.g. oil reservoir simulation or CO₂ sequestration



Stochastic Modelling of Uncertainty:

Log-normal random field $k(x, \omega)$ (here with $n = 512^2$, $\lambda = 1/64$ and $\sigma^2 = 8$)

Typical Realisation



$\log k(x, \omega)$ = Gaussian with mean 0 & covariance function

$$R(x, y) := \sigma^2 \exp\left(-\frac{\|x - y\|}{\lambda}\right)$$

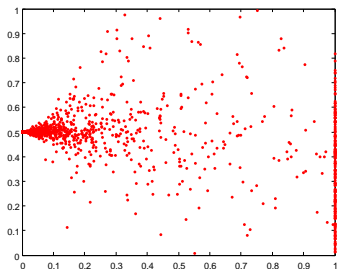
(Field data suggests that this is a reasonable representation of reality, e.g. [Gelhar, 1975], [Hoeksema et al, 1985])

Variance σ^2 determines “contrast”

Correlation length λ determines “roughness”

Quantities of Interest

Leaking repository at $(0, \frac{1}{2})$



$\lambda = 0.3, \sigma^2 = 4, t = 0.2$

- flow field \vec{q}
- particle position at time t
- breakthrough time (to right)
- **effective permeability:**

$$k_{\text{eff},1} := \frac{\int_D q_1 d\vec{x}}{\int_D -\frac{\partial p}{\partial x_1} d\vec{x}}$$

Elliptic PDEs with Random Coefficients

Key Computational Challenges

$$-\nabla \cdot (k(x, \omega) \nabla p(x, \omega)) = f(x, \omega), \quad x \in \Omega \subset \mathbb{R}^d$$

Elliptic PDEs with Random Coefficients

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- **Discretise** with respect to ω :
 - ▶ stochastic Galerkin (+ sparse versions)
 - ▶ stochastic collocation (+ anisotropic versions)
 - ▶ **Monte Carlo** (+ variants)
 - ▶ etc...

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- **Sample** or **approximate** the random field $k(x, \omega)$:
 - ▶ **truncated Karhunen-Loève expansion**
 - ▶ Matrix factorisation, e.g. **circulant embedding (FFT)**
 - ▶ etc...

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- **Solve** a **huge** number of deterministic PDEs
(with very rough coefficients and very fine mesh resolution)

Truncated Karhunen-Loève Expansion

$$\log k(x, \omega) \approx \sum_{j=1}^K \sqrt{\mu_j} \phi_j(x) Y_j(\omega)$$

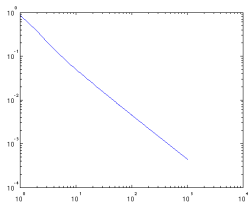
$(\mu_j, \phi_j(x))$ orthonormal eigenpairs of $\int_{\Omega} R(x, y) \phi(y) dy$; $Y_j(\omega)$ i.i.d. $N(0, \sigma^2)$

Truncated Karhunen-Loève Expansion

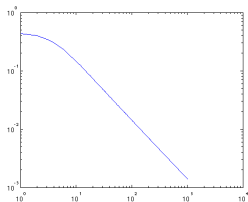
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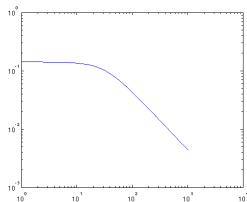
- Small $\lambda \implies$ Large number of KL-modes $\gg 100$:



$\lambda = 1$



$\lambda = 0.1$



$\lambda = 0.01$

- Very high-dimensional problem \implies Monte Carlo !!
- Very fine mesh width $h \ll 1$!! (FVM or Mixed FEs)

Quantity of interest: Expected value of $Q := \mathcal{G}(\vec{q})$

Standard Monte Carlo estimate for this is

$$\hat{Q}_h^{\text{MC}} := \frac{1}{N_h} \sum_{i=1}^{N_h} Q_h^{(i)} \quad \text{with} \quad \mathbb{V}[\hat{Q}_h^{\text{MC}}] = \frac{\mathbb{V}[Q_h]}{N_h}$$

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Complexity of Standard Monte Carlo

Assuming

$$\text{(A1)} \quad |\mathbb{E}[\hat{Q}_h^{\text{MC}} - Q]| = \mathcal{O}(h^\alpha) \quad (\text{FE error})$$

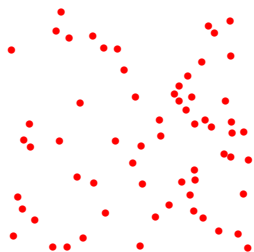
$$\text{(A2)} \quad \text{Cost}(Q_h^{(i)}) = \mathcal{O}(h^{-\gamma}) \quad (\text{PDE solver})$$

Then the **total cost** to obtain **mean square error**

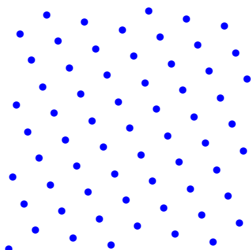
$$\mathbb{E}[(\hat{Q}_h^{\text{MC}} - \mathbb{E}[Q])^2] = \mathcal{O}(\varepsilon^2) \quad \text{is} \quad \mathcal{O}(\varepsilon^{-2-\frac{\gamma}{\alpha}})$$

Quasi-Monte Carlo (Reducing Number of Samples)

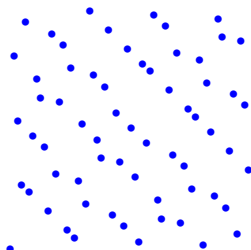
random $\omega^{(i)}$ \longrightarrow deterministically chosen $\tilde{\omega}^{(i)}$



64 random points



64 lattice points



64 Sobol' points

Equal weighted sum $\frac{1}{N_h} \sum_{i=1}^{N_h} \tilde{Q}_h^{(i)}$ as in standard MC

(for details see [Ian Sloan's](#) and [Ivan Graham's](#) talks)

Now, numerically observed:

(and theoretically shown under certain smoothness assumptions)

$$\mathbb{V}[\hat{Q}_h^{\text{QMC}}] = \frac{\mathbb{V}[Q_h]}{N_h^{2\delta}},$$

with $0.5 \leq \delta < 1$

(0.5 is standard MC rate)

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Complexity of Quasi-Monte Carlo

Assuming **(A1)**, **(A2)** for \hat{Q}_h^{QMC} and

$$\text{(A3) } \mathbb{V}[\hat{Q}_h^{\text{QMC}}] = \mathcal{O}(N_h^{-2\delta})$$

Then the **total cost** to obtain **mean square error**

$$\mathbb{E}[(\hat{Q}_h^{\text{QMC}} - \mathbb{E}[Q])^2] = \mathcal{O}(\varepsilon^2) \quad \text{is} \quad \mathcal{O}(\varepsilon^{-\frac{1}{\delta} - \frac{\gamma}{\alpha}})$$

Multilevel Monte Carlo (Reducing Cost per Sample)

Exploit

$$\mathbb{E}[Q_L] = \mathbb{E}[Q_0] + \sum_{\ell=1}^L \mathbb{E}[Q_\ell - Q_{\ell-1}]$$

(where $h_\ell = h_{\ell-1}/2$ and $Q_\ell = Q_{h_\ell}$)

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Define following **multilevel MC** estimator for $\mathbb{E}[Q]$:

$$\hat{Q}_L^{\text{ML}} := \hat{Q}_0^{\text{MC}} + \sum_{\ell=1}^L (\widehat{Q_\ell - Q_{\ell-1}})^{\text{MC}}$$

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Key Observation

$$\mathbb{V} \left[(\widehat{Q_\ell - Q_{\ell-1}})^{\text{MC}} \right] \rightarrow 0 \quad \text{as} \quad h_\ell \rightarrow 0 !$$

Complexity of Multilevel Monte Carlo

Assuming **(A1)**, **(A2)** for \hat{Q}_L^{ML} and

$$\text{(A4)} \quad \mathbb{V} \left[\widehat{(Q_\ell - Q_{\ell-1})}^{\text{MC}} \right] = \mathcal{O}(N_\ell^{-1} h_\ell^\beta)$$

Then $\exists L, \{N_\ell\}$ s.t. the **total cost** to obtain **mean square error**

$$\mathbb{E} \left[(\hat{Q}_L^{\text{ML}} - \mathbb{E}[Q])^2 \right] = \mathcal{O}(\varepsilon^2)$$

is

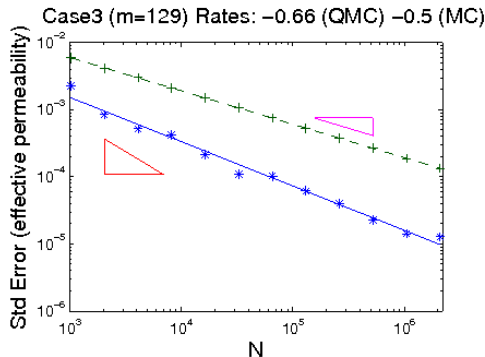
$$\mathcal{O}(\varepsilon^{-2}) \quad \text{if } \beta > \gamma$$

$$\mathcal{O}(\varepsilon^{-2} \log(\varepsilon)^2) \quad \text{if } \beta = \gamma$$

$$\mathcal{O}(\varepsilon^{-2-(\gamma-\beta)/\alpha}) \quad \text{if } \beta < \gamma$$

Numerical Example: Quasi Monte Carlo

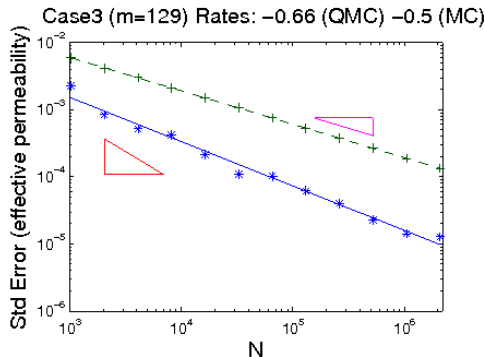
for $\Omega = [0, 1]^2$, $Q = k_{\text{eff},1}$, $\|\cdot\| = \|\cdot\|_1$, $\lambda = 0.1$, $\sigma^2 = 1$, $h = 1/129$



$$\alpha = 1.5, \gamma = 2, \delta = 0.66 \implies \text{Cost} = \mathcal{O}(\varepsilon^{-2\frac{5}{6}})$$

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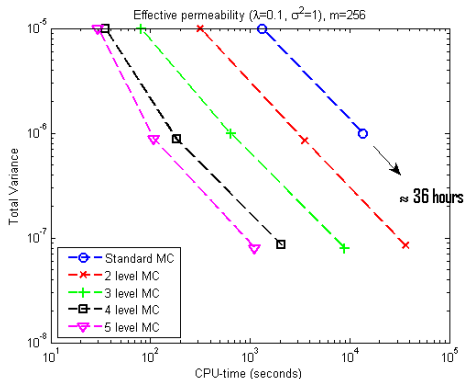
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Compare **standard Monte Carlo**: $\mathcal{O}(\varepsilon^{-3\frac{1}{3}})$

I.G. Graham Talk

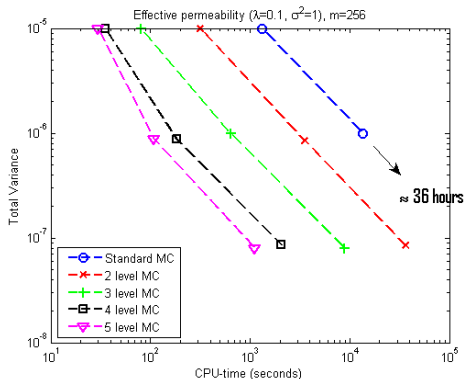
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for $\Omega = [0, 1]^2$, $Q = k_{\text{eff},1}$, $\|\cdot\| = \|\cdot\|_1$, $\lambda = 0.1$, $\sigma^2 = 1$, $h = 1/256$



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Compare **standard Monte Carlo**: $\mathcal{O}(\varepsilon^{-3\frac{1}{3}})$

A. Teckentrup Talk