Multilevel Monte Carlo methods for random partial differential equations

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Outline

1. Uncertainty Quantification in PDE models
2. Parametric Uncertainty in Diffusion Problems
3. (Multilevel) Monte Carlo Methods
4. Multilevel Monte Carlo Methods for Multi-scale Problems

Uncertainty Quantification in PDE models

- Modelling and simulation with partial differential equations are routinely used to inform decisions and assess risk.
- Physical quantities appearing in the models are often not fully known, and hence subject to uncertainty.

Uncertainty Quantification in PDE models

- Modelling and simulation with partial differential equations are routinely used to inform decisions and assess risk.
- Physical quantities appearing in the models are often not fully known, and hence subject to uncertainty.
- Uncertainty Quantification is a broad methodology for incorporating this uncertainty in simulations.
- The uncertainty can come from a variety of sources:
  - geometric uncertainties (e.g. diffusion on a cell membrane)
  - uncertainty about values of physical parameters (e.g. incomplete knowledge of sub-surface geology)
  - model-form uncertainty (e.g. a set of suitable scales and models)
- Uncertainty quantification is frequently based on stochastic modelling.

Parametric Uncertainty in Diffusion Problems

A Simple Model for Groundwater Flow

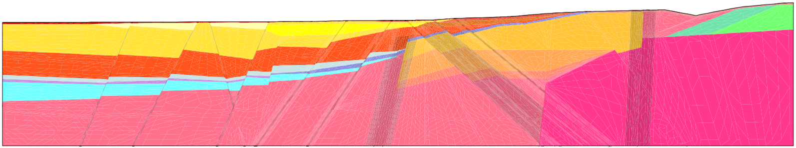
- Darcy's law for an incompressible fluid leads to the diffusion equation

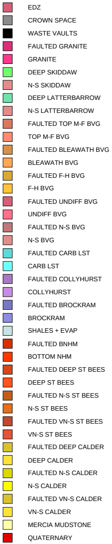
$$-\nabla \cdot (k(x)\nabla p(x)) = g(x), \qquad x \in D \subseteq \mathbb{R}^d,$$

  with

  - the hydraulic conductivity k of the sub-surface,
  - source/sink terms g,
  - the resulting pressure field p of groundwater.

- Lack of data leads to uncertainty in the conductivity k.





Parametric Uncertainty in Diffusion Problems

General Formulation

- The uncertainty in k is expressed in a probabilistic formulation: k is modelled as a random process (field, function $\ldots$) $k(x, \omega)$ with
  - $k(\cdot, \omega) \in L^\infty(D)$ for all $\omega \in \Omega$,
  - $k(x, \cdot)$ a random variable, for all $x \in D$.
- The uncertainty in k propagates through the model to the solution p, with $p(x, \omega)$ now a random process.

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- The uncertainty in k propagates through the model to the solution p, with $p(x, \omega)$ now a random process.
- The model for k is chosen to incorporate knowledge about properties of k: continuity/differentiability, typical length scales, contrast, positive-valued ...
- A popular and flexible approach to define a distribution on k is a parametric approach.

Parametric Uncertainty in Diffusion Problems

Parametric Uncertainty [Dashti, Stuart '17]

- Suppose we want to define a probability distribution on $L^2(D)$, the space of square integrable functions $f : D \to \mathbb{R}$.
- Since $L^2(D)$ is separable, there exists a *basis* $\{\phi_n\}_{n\in\mathbb{N}}$ such that any function $f \in L^2(D)$ can be written in the form

$$f(x) = \sum_{n=1}^{\infty} c_n \phi_n(x), \qquad c_n \in \mathbb{R}, \quad \sum_{n=1}^{\infty} \|\phi_n\|_{L^2(D)} < \infty.$$

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- A common way to define a distribution on $f \in L^2(D)$ is the following:

$$f(x,\omega) = m(x) + \sum_{n=1}^{\infty} \xi_n(\omega)\phi_n(x),$$

where

  - $\{\xi_n\}_{n\in\mathbb{N}}$ is an i.i.d. sequence of mean zero random variables,
  - $m(x) = \mathbb{E}[f(x)]$ is a chosen mean function.

Parametric Uncertainty in Diffusion Problems

- The parametrisation is very flexible, since you are free to choose $\{\phi_n\}_{n\in\mathbb{N}}$ and $\{\xi_n\}_{n\in\mathbb{N}}$.
- It includes Gaussian measures on $L^2(D)$, in which case we have the Karhunen-Loève expansion of the Gaussian field f, with $\{\xi_n\}_{n\in\mathbb{N}}$ i.i.d. $\mathrm{N}(0,1)$ and $\{\phi_n\}_{n\in\mathbb{N}}$ determined by the covariance operator.

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- The approach is not restricted to $L^2(D)$, and works for any separable Banach space X $(\Rightarrow X = \overline{\mathrm{span}\{\phi_n\}_{n\in\mathbb{N}}})$.
- We can also take non-linear transformations of the parametric expansion, e.g. to ensure positiveness.

Parametric Uncertainty in Diffusion Problems

Typical set-up [Barth, Schwab, Zollinger '11], [Charrier, Scheichl, T. '13]

- The most commonly used parametrisations are:
  - a log-normal distribution, i.e. $k(x, \omega) = \exp\left(\sum_{n=1}^{\infty} \xi_n(\omega)\phi_n(x)\right)$, with $\xi_n \sim N(0, 1)$ and $\{\phi_n\}_{n=1}^{\infty}$ given functions in $L^{\infty}(D)$, or
  - a uniform distribution, i.e. $k(x, \omega) = m(x) + \sum_{n=1}^{\infty} \xi_n(\omega)\phi_n(x)$, with $\xi_n \sim U[-1, 1]$ and $\{\phi_n\}_{n=1}^{\infty}$ given functions in $L^{\infty}(D)$.

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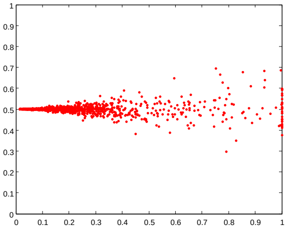
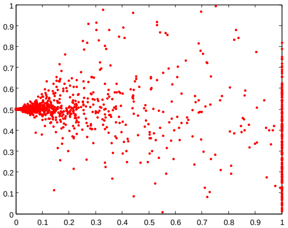
- Both parametrisations ensure positiveness of k. (In the uniform case, this requires assumptions on the relative size of m and $\{\phi_n\}_{n=1}^{\infty}$.)
- Common choices for the basis functions are:
  - indicator functions on sub-domains $\bigcup_{i=1}^{s} \overline{D_i} = D \Rightarrow$ piece-wise constant
  - Fourier-like bases $\Rightarrow$ frequency increasing with n

Parametric Uncertainty in Diffusion Problems

Goal of simulations

- The end goal is usually to estimate the expected value of a quantity of interest (QoI) $\phi(p)$ or $\phi(k,p)$.
  - point values or local averages of the pressure p
  - point values or local averages of the Darcy flow $-k\nabla p$
  - outflow over parts of the boundary
  - travel times of contaminant particles





(Multilevel) Monte Carlo Methods

Monte Carlo Methods [Robert, Casella '99]

The standard Monte Carlo estimator for $Q = \mathbb{E}[\phi(p)]$ is

$$\widehat{Q}^{\mathrm{MC}}_{h,N} := \frac{1}{N}\sum_{i=1}^{N} \phi(p_h^{(i)})$$

where $\phi(p_h^{(i)})$ is the ith sample of $\phi(p)$ approximated on grid $\mathcal{T}_h$.

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The mean square error can be shown to equal

$$\begin{aligned}
\mathbb{E}\big[\big(\widehat{Q}^{\mathrm{MC}}_{h,N} - \mathbb{E}[\phi(p)]\big)^2\big] &= \mathbb{V}[\widehat{Q}^{\mathrm{MC}}_{h,N}] + \big(\mathbb{E}[\widehat{Q}^{\mathrm{MC}}_{h,N}] - \mathbb{E}[\phi(p)]\big)^2 \\
&= \underbrace{\mathbb{V}[\phi(p_h)]\, N^{-1}}_{\textbf{sampling error}} + \underbrace{\Big(\mathbb{E}[\phi(p_h) - \phi(p)]\Big)^2}_{\textbf{FE error (``bias'')}}
\end{aligned}$$

$\Rightarrow$ need to solve a large number of PDEs on a fine grid!

(Multilevel) Monte Carlo Methods

Multilevel Monte Carlo Methods [Heinrich '01], [Giles '08]

The multilevel method works on a sequence of levels, s.t. $h_\ell = 2^{-\ell} h_0$, $\ell = 0, 1, \dots, L$.

Linearity of expectation gives us

$$\mathbb{E}\left[\phi(p_{h_L})\right] = \mathbb{E}\left[\phi(p_{h_0})\right] + \sum_{\ell=1}^{L} \mathbb{E}\left[\phi(p_{h_\ell}) - \phi(p_{h_{\ell-1}})\right]$$

We define the multilevel MC estimator

$$\widehat{Q}^{\mathrm{ML}}_{\{h_\ell, N_\ell\}} = \frac{1}{N_0} \sum_{i=1}^{N_0} \phi(p_{h_0}^{(i,0)}) \; + \sum_{\ell=1}^{L} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} \phi(p_{h_\ell}^{(i,\ell)}) - \phi(p_{h_{\ell-1}}^{(i,\ell)})$$

Terms are estimated independently, with N_ℓ samples on level ℓ.

(Multilevel) Monte Carlo Methods

Multilevel Monte Carlo Methods [Heinrich '01], [Giles '08]

The mean square error of the this estimator is

$$\mathbb{E}\Big[\big(\widehat{Q}^{\mathrm{ML}}_{\{h_\ell,N_\ell\}} - \mathbb{E}[\phi(p)]\big)^2\Big] = \underbrace{\mathbb{V}[\widehat{Q}^{\mathrm{ML}}_{\{h_\ell,N_\ell\}}]}_{\text{sampling error}} + \underbrace{\big(\mathbb{E}[\widehat{Q}^{\mathrm{ML}}_{\{h_\ell,N_\ell\}}] - \mathbb{E}[\phi(p)]\big)^2}_{\text{FE error}}$$

$$= \frac{\mathbb{V}[\phi(p_{h_0})]}{N_0} + \sum_{\ell=1}^{L} \frac{\mathbb{V}[\phi(p_{h_\ell}) - \phi(p_{h_{\ell-1}})]}{N_\ell} + \big(\mathbb{E}[\phi(p_{h_L}) - \phi(p)]\big)^2$$

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- N_0 still needs to be large, but samples are much cheaper to obtain on coarser grid
- N_ℓ $(\ell > 0)$ much smaller, since $\mathbb{V}[\phi(p_{h_\ell}) - \phi(p_{h_{\ell-1}})] \to 0$ as $h_\ell \to 0$

$\Rightarrow$ need to solve a large number of PDEs on a coarse grid and a small number of PDEs on a fine grid!

(Multilevel) Monte Carlo Methods

Complexity of Multilevel Monte Carlo ([Giles, '08], [Cliffe et al, '11])

Assume that

(A1) $\left|\mathbb{E}[\phi(p) - \phi(p_{h_\ell})]\right| = \mathcal{O}(h_\ell^\alpha)$ (FE error)

(A2) $\mathbb{V}[\phi(p_{h_\ell}) - \phi(p_{h_{\ell-1}})] = \mathcal{O}(h_\ell^\beta)$ (FE difference)

(A3) $\text{Cost}(\phi(p_{h_\ell}^{(i)})) = \mathcal{O}(h_\ell^{-\gamma})$ (PDE solver)

with $2\alpha \geq \min(\beta, \gamma)$. Then there exist L and $\{N_\ell\}$ such that the total cost to obtain a mean square error

$$\mathbb{E}\left[(\widehat{Q}^{\text{ML}}_{\{h_\ell, N_\ell\}} - \mathbb{E}[Q])^2\right] = \mathcal{O}(\varepsilon^2)$$

is

$$\text{Cost}(\widehat{Q}^{\text{ML}}_{\{h_\ell, N_\ell\}}) = \begin{cases} \mathcal{O}(\varepsilon^{-2}) & \text{if } \beta > \gamma \\ \mathcal{O}(\varepsilon^{-2} \log(\varepsilon)^2) & \text{if } \beta = \gamma \\ \mathcal{O}(\varepsilon^{-2-(\gamma-\beta)/\alpha}) & \text{if } \beta < \gamma \end{cases}$$

- $\text{Cost}(\widehat{Q}^{\text{MC}}_{h,N}) = \mathcal{O}(\varepsilon^{-2-\gamma/\alpha})$!

(Multilevel) Monte Carlo Methods

Proving assumption (A3)

- Assumption (A3) is an assumption on the PDE solver. This typically involves solving a sparse, linear system of dimension $n \sim h_\ell^{-d}$, so with an optimal solver we have $\gamma \approx d$: Cost$(\phi(p_{h_\ell}^{(i)})) = \mathcal{O}(h_\ell^{-d})$.
  - The cost of producing a sample $k^{(i)}$ has to be included as well, but this is typically an order of magnitude cheaper and can easily be made to have $\mathcal{O}(h_\ell^{-d})$ cost by choosing a suitable sampling scheme.

(Multilevel) Monte Carlo Methods

Proving assumptions (A1), (A2)

- Assumptions (A1) and (A2) are assumptions on the convergence rate of the numerical method[1].
  - This depends on smoothness properties of the problem: If $k(\cdot,\omega) \in C^t(\overline{D})$, $g \in L^2(D)$, D is Lipschitz and convex, and ϕ is Fréchet differentiable, then $p(\cdot,\omega) \in H^{1+t-\delta}(D)$ for any $\delta > 0$, and

$$\begin{aligned} \left|\mathbb{E}[\phi(p) - \phi(p_{h_\ell})]\right| &= \mathcal{O}(h_\ell^{2t-\delta}) \quad &\Rightarrow \alpha = 2t - \delta \text{ in (A1)} \\ \mathbb{V}[\phi(p_{h_\ell)} - \phi(p_{h_{\ell-1}})] &= \mathcal{O}(h_\ell^{4t-\delta}) \quad &\Rightarrow \beta = 4t - \delta \text{ in (A2)} \end{aligned}$$

    for standard, piece-wise linear finite elements.

[1] [Barth, Schwab, Zollinger '11], [Charrier, Scheichl, T. '13], [T. '12], [T., Scheichl, Giles, Ullmann '13], [T., PhD thesis '13]

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$$\left|\mathbb{E}[\phi(p) - \phi(p_{h_\ell})]\right| = \mathcal{O}(h_\ell^{2t-\delta}) \quad \Rightarrow \alpha = 2t - \delta \text{ in (A1)}$$

$$\mathbb{V}[\phi(p_{h_\ell)}) - \phi(p_{h_{\ell-1}})] = \mathcal{O}(h_\ell^{4t-\delta}) \quad \Rightarrow \beta = 4t - \delta \text{ in (A2)}$$

    for standard, piece-wise linear finite elements.
  - In the case of the log-normal distribution, the proofs are complicated by the diffusion equation not being uniformly elliptic:

$$0 < k_{\min}(\omega) = \min_{x \in \overline{D}} k(x, \omega) \leq k(x, \omega) \leq \max_{x \in \overline{D}} k(x, \omega) = k_{\max}(\omega) < \infty,$$

    where $k(x, \omega) = \exp\left(\sum_{n=1}^{\infty} \xi_n(\omega)\phi_n(x)\right)$, with $\xi_n \sim N(0, 1)$.

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(Multilevel) Monte Carlo Methods

Growth of ε-cost

The computational ε-cost is the number of FLOPS required to achieve a MSE of $\mathcal{O}(\varepsilon^2)$.

With $\gamma \approx d$, $\alpha = 1$ and $\beta = 2$, the computational ε-costs for the diffusion problem are bounded by:

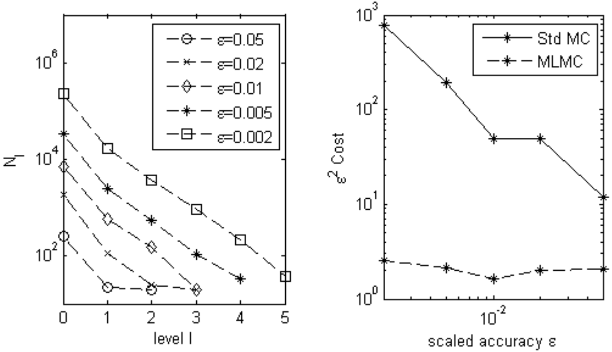
d	**MLMC**	**MC**
1	$\mathcal{O}(\varepsilon^{-2})$	$\mathcal{O}(\varepsilon^{-3})$
2	$\mathcal{O}(\varepsilon^{-2})$	$\mathcal{O}(\varepsilon^{-4})$
3	$\mathcal{O}(\varepsilon^{-3})$	$\mathcal{O}(\varepsilon^{-5})$

For $\varepsilon = 10^{-3}$ and $d = 3$, the costs of MLMC and MC are $\mathcal{O}(10^9)$ and $\mathcal{O}(10^{15})$, respectively.

(Multilevel) Monte Carlo Methods

Numerical example

- Flow cell model problem on $D = (0,1)^2$
- k a log-normal random field with $k(\cdot,\omega) \in C^{1/2-\delta}(\overline{D})$, for any $\delta > 0$
- $\phi(p) = \|p\|_{L^2(D)}$



Multilevel Monte Carlo Methods for Multi-scale Problems

Motivation

- Some physical models exhibit fine scale features that are unresolved on coarse meshes. In the context of the random diffusion problem, these are fine scale features in the coefficient k.
- In a naive implementation of multilevel Monte Carlo, the coarsest mesh size h_0 needs to be small enough to resolve all features.
  - If this is not the case, $\mathbb{V}[\phi(p_{h_\ell}) - \phi(p_{h_{\ell-1}})]$ will be large.

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- In a naive implementation of multilevel Monte Carlo, the coarsest mesh size h_0 needs to be small enough to resolve all features.
  - If this is not the case, $\mathbb{V}[\phi(p_{h_\ell}) - \phi(p_{h_{\ell-1}})]$ will be large.
- One can circumvent this problem by choosing smoother approximations of the coefficient k on coarse grids.
- Levels in the multilevel hierarchy now correspond to different mesh sizes h_ℓ, as well as different models of coefficient k_ℓ.

Multilevel Monte Carlo Methods for Multi-scale Problems

Level-dependent truncation of parametrisation [T. et al '13]

- Assume $g = \log k$ is a Gaussian random field with mean $\mathbb{E}[g(x)] = 0$ and covariance function $\mathbb{E}[g(x)g(y)] = c(x,y) = \sigma^2 \exp\left(\frac{\|x-y\|_2}{0.1}\right)$.
  $\Rightarrow$ fine scale features for small correlation length λ
- Then we have the parametric expansion

$$k(x,\omega) = \exp\left(\sum_{n=1}^{\infty} \xi_n(\omega)\phi_n(x)\right)$$

where $\phi_n(x) = \sqrt{\sigma_n}\psi_n(x)$ with

$$c(\lambda, d)(\mathrm{Id} - \lambda^2\Delta)^{-\frac{d+1}{2}}\psi_n = \sigma_n\psi_n.$$

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- This means

  $$k_\ell(x, \omega) = \exp\left(\sum_{n=1}^{R_\ell} \xi_n(\omega)\phi_n(x)\right)$$

  is a smooth approximation of k for R_ℓ small.

Multilevel Monte Carlo Methods for Multi-scale Problems

Error Analysis [T. et al '13]

- The bias of $\widehat{Q}^{\mathrm{ML}}_{\{h_\ell, N_\ell\}}$ depends only on the accuracy of k_L.
- For the rates α and β, we need to take into account the addition to $\phi(p) - \phi(p_\ell)$.

[2] [Schwab, Todor, '06],[Charrier, '12],[Graham et al, '13]

Multilevel Monte Carlo Methods for Multi-scale Problems

- The bias of $\widehat{Q}^{\mathrm{ML}}_{\{h_\ell,N_\ell\}}$ depends only on the accuracy of k_L.
- For the rates α and β, we need to take into account the addition to $\phi(p) - \phi(p_\ell)$.
- We make use of results on the truncation error of Karhunen-Lòeve expansions [2]. We get a result of the form

$$\left|\mathbb{E}[\phi(p) - \phi(p_\ell)]\right| = \mathcal{O}(h_\ell^\alpha + R_\ell^{\alpha'}),$$
$$\mathbb{V}[\phi(p_{\ell)} - \phi(p_{\ell-1})] = \mathcal{O}(h_\ell^{2\alpha} + R_\ell^{2\alpha'}),$$

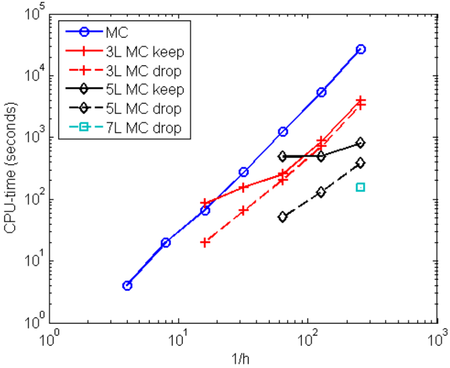
  where the rate α' depends on the decay rate of $\{\sigma_n\}_{n\in\mathbb{N}}$. For the example on the previous slide, we have $\alpha' = \frac{1}{2}$.
- We usually choose R_ℓ as a function of h_ℓ to balance the two error contributions.

[2] [Schwab, Todor, '06],[Charrier, '12],[Graham et al, '13]

Multilevel Monte Carlo Methods for Multi-scale Problems

Numerical Example

- Flow cell model problem on $D = (0,1)^2$
- k a log-normal random field with $c(x,y) = \sigma^2 \exp\left(\frac{\|x-y\|_2}{0.1}\right)$
- Truncation order $R_\ell = 4h_\ell^{-1}$



Expected value of outflow $\phi(p)$

for fixed sampling error

Conclusions

- Multilevel Monte Carlo methods are an efficient tool for uncertainty quantification in PDE models.
- The methodology is generally applicable, and is not restricted to the diffusion problem discussed here.
- The definition of the coarse levels is likewise general, and can include further simplifications in addition to a coarser mesh.

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