Monte Carlo Methods for Uncertainty Quantification

Mike Giles

Mathematical Institute, University of Oxford

Contemporary Numerical Techniques

Lecture outline

Lecture 4: PDE applications

- PDEs with uncertainty
- examples
- multilevel Monte Carlo
- details of MATLAB code

PDEs with Uncertainty

Looking at the history of numerical methods for PDEs, the first steps were about improving the modelling:

- 1D → 2D → 3D
- steady → unsteady
- laminar flow → turbulence modelling → large eddy simulation → direct Navier-Stokes
- simple geometries (e.g. a wing) → complex geometries (e.g. an aircraft in landing configuration)
- adding new features such as combustion, coupling to structural / thermal analyses, etc.

. . . and then engineering switched from analysis to design.

PDEs with Uncertainty

The big move now is towards handling uncertainty:

- uncertainty in modelling parameters
- uncertainty in geometry
- uncertainty in initial conditions
- uncertainty in spatially-varying material properties
- inclusion of stochastic source terms

Engineering wants to move to "robust design" taking into account the effects of uncertainty.

Other areas want to move into Bayesian inference, starting with an *a priori* distribution for the uncertainty, and then using data to derive an improved *a posteriori* distribution.

PDEs with Uncertainty

Examples:

- Long-term climate modelling:

  Lots of sources of uncertainty including the effects of aerosols, clouds, carbon cycle, ocean circulation (`http://climate.nasa.gov/uncertainties`)

- Short-range weather prediction

  Considerable uncertainty in the initial data due to limited measurements

PDEs with Uncertainty

- Engineering analysis

  Perhaps the biggest uncertainty is geometric due to manufacturing tolerances

- Nuclear waste repository and oil reservoir modelling

  Considerable uncertainty about porosity of rock

- Astronomy

  "Random" spatial/temporal variations in air density disturb correlation in signals received by different antennas

- Finance

  Stochastic forcing due to market behaviour

PDEs with Uncertainty

In the past, Monte Carlo simulation has been viewed as impractical due to its expense, and so people have used other methods:

- stochastic collocation
- polynomial chaos

Because of Multilevel Monte Carlo, this is changing and there are now several research groups using MLMC for PDE applications

The approach is very simple, in principle:

- use a sequence of grids of increasing resolution in space (and time)
- as with SDEs, determine the optimal allocation of computational effort on the different levels
- the savings can be much greater because the cost goes up more rapidly with level

MLMC Theorem

If there exist independent estimators $\widehat{Y}_\ell$ based on N_ℓ Monte Carlo samples, each costing C_ℓ, and positive constants $\alpha, \beta, \gamma, c_1, c_2, c_3$ such that $\alpha \geq \frac{1}{2} \min(\beta, \gamma)$ and

i) $\left| \mathbb{E}[\widehat{P}_\ell - P] \right| \leq c_1 \, 2^{-\alpha \, \ell}$

ii) $\mathbb{E}[\widehat{Y}_\ell] = \begin{cases} \mathbb{E}[\widehat{P}_0], & \ell = 0 \\ \mathbb{E}[\widehat{P}_\ell - \widehat{P}_{\ell-1}], & \ell > 0 \end{cases}$

iii) $\mathbb{V}[\widehat{Y}_\ell] \leq c_2 \, N_\ell^{-1} 2^{-\beta \, \ell}$

iv) $\mathbb{E}[C_\ell] \leq c_3 \, 2^{\gamma \, \ell}$

MLMC Theorem

then there exists a positive constant c_4 such that for any $\varepsilon < 1$ there exist L and N_ℓ for which the multilevel estimator

$$\widehat{Y} = \sum_{\ell=0}^{L} \widehat{Y}_\ell,$$

has a mean-square-error with bound $\mathbb{E}\left[\left(\widehat{Y} - \mathbb{E}[P]\right)^2\right] < \varepsilon^2$

with a computational cost C with bound

$$C \leq \begin{cases} c_4\, \varepsilon^{-2}, & \beta > \gamma, \\ c_4\, \varepsilon^{-2} (\log \varepsilon)^2, & \beta = \gamma, \\ c_4\, \varepsilon^{-2-(\gamma-\beta)/\alpha}, & 0 < \beta < \gamma. \end{cases}$$

Engineering Uncertainty Quantification

- consider 3D elliptic PDE, with uncertain boundary data
- use grid spacing proportional to $2^{-\ell}$ on level ℓ
- cost is $O(2^{+3\ell})$, if using an efficient multigrid solver
- 2nd order accuracy means that

$$\begin{aligned} \widehat{P}_\ell(\omega) - P(\omega) &\approx c(\omega)\, 2^{-2\ell} \\ \Longrightarrow \quad \widehat{P}_{\ell-1}(\omega) - \widehat{P}_\ell(\omega) &\approx 3\, c(\omega)\, 2^{-2\ell} \end{aligned}$$

- hence, $\alpha = 2, \;\; \beta = 4, \;\; \gamma = 3$
- cost is $O(\varepsilon^{-2})$ to obtain ε RMS accuracy

SPDEs

- great MLMC application – better cost savings than SDEs due to higher dimensionality
- range of applications
  - Graubner & Ritter (Darmstadt → Kaiserslautern) – parabolic
  - G, Reisinger (Oxford) – parabolic
  - Cliffe, G, Scheichl, Teckentrup (Bath/Nottingham) – elliptic
  - Barth, Jenny, Lang, Meyer, Mishra, Müller, Schwab, Sukys, Zollinger (ETHZ) – elliptic, parabolic, hyperbolic
  - Harbrecht, Peters (Basel) – elliptic
  - Efendiev (Texas A&M) – numerical homogenization
  - Vidal-Codina, G, Peraire (MIT) – reduced basis approximation
  - G, Hou, Zhang (Caltech) – numerical homogenization

PDEs with Uncertainty

I worked with Rob Scheichl (Bath) and Andrew Cliffe (Nottingham) on multilevel Monte Carlo for the modelling of oil reservoirs and groundwater contamination in nuclear waste repositories.

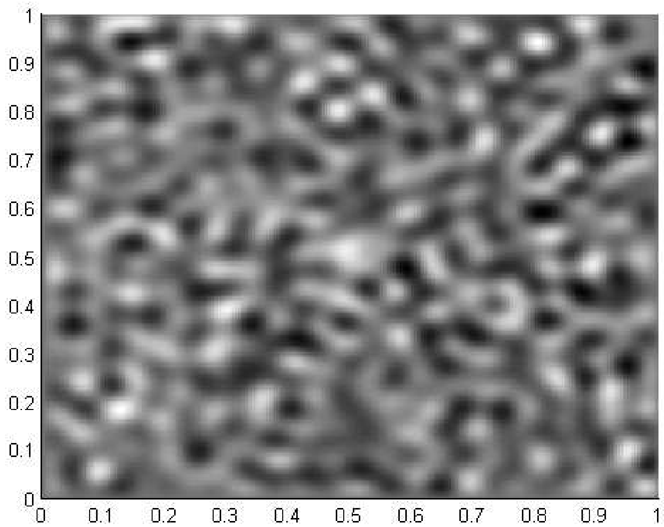
Here we have an elliptic SPDE coming from Darcy's law:

$$\nabla \cdot \Big(\kappa(x)\, \nabla p \Big) = 0$$

where the permeability $\kappa(x)$ is uncertain, and $\log \kappa(x)$ is often modelled as being Normally distributed with a spatial covariance such as

$$\mathrm{cov}(\log \kappa(x_1), \log \kappa(x_2)) = \sigma^2 \exp(-\|x_1 - x_2\|/\lambda)$$

Elliptic SPDE



A typical realisation of κ for $\lambda = 0.01$, $\sigma = 1$.

Elliptic SPDE

Samples of log k are provided by a Karhunen-Loève expansion:

$$\log k(\mathbf{x}, \omega) = \sum_{n=0}^{\infty} \sqrt{\theta_n}\, \xi_n(\omega)\ f_n(\mathbf{x}),$$

where θ_n, f_n are eigenvalues / eigenfunctions of the correlation function:

$$\int R(\mathbf{x}, \mathbf{y})\ f_n(\mathbf{y})\ \mathrm{d}\mathbf{y} = \theta_n\, f_n(\mathbf{x})$$

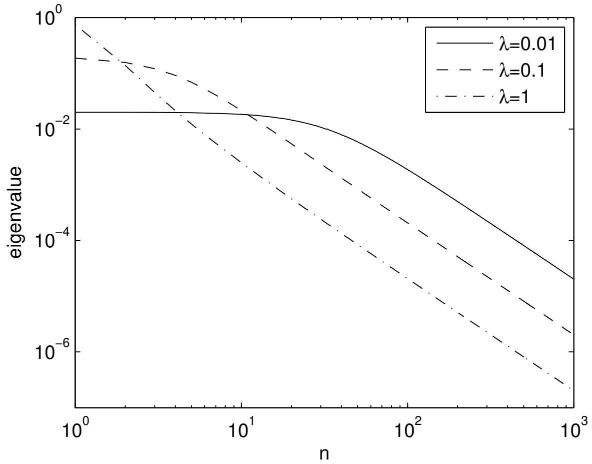
and $\xi_n(\omega)$ are standard Normal random variables.

Numerical experiments truncate the expansion.

(Latest 2D/3D work uses an efficient FFT construction based on a circulant embedding.)

Elliptic SPDE

Decay of 1D eigenvalues



When $\lambda = 1$, can use a low-dimensional polynomial chaos approach, but it's impractical for smaller λ.

Elliptic SPDE

Discretisation:

- cell-centred finite volume discretisation on a uniform grid – for rough coefficients we need to make grid spacing very small on finest grid
- each level of refinement has twice as many grid points in each direction
- current numerical experiments use a direct solver for simplicity, but in 3D will use an efficient AMG multigrid solver with a cost roughly proportional to the total number of grid points

2D Results

Boundary conditions for unit square $[0,1]^2$:
– fixed pressure: $p(0,x_2)=1,\ p(1,x_2)=0$
– Neumann b.c.: $\partial p/\partial x_2(x_1,0)=\partial p/\partial x_2(x_1,1)=0$

Output quantity – mass flux: $-\int k\, \frac{\partial p}{\partial x_1}\, \mathrm{d}x_2$

Correlation length: $\lambda = 0.2$

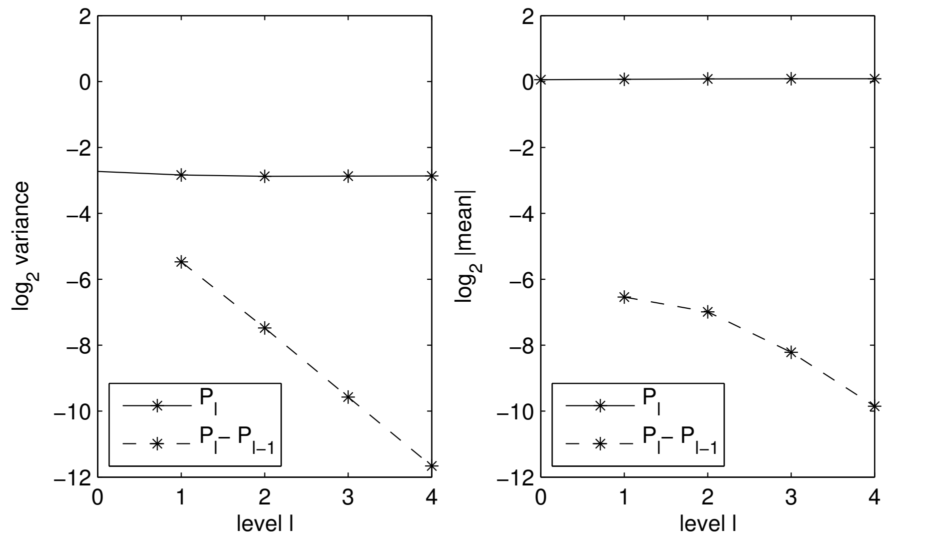
Coarsest grid: $h=1/8$ (comparable to λ)

Finest grid: $h=1/128$

Karhunen-Loève truncation: $m_{KL}=4000$

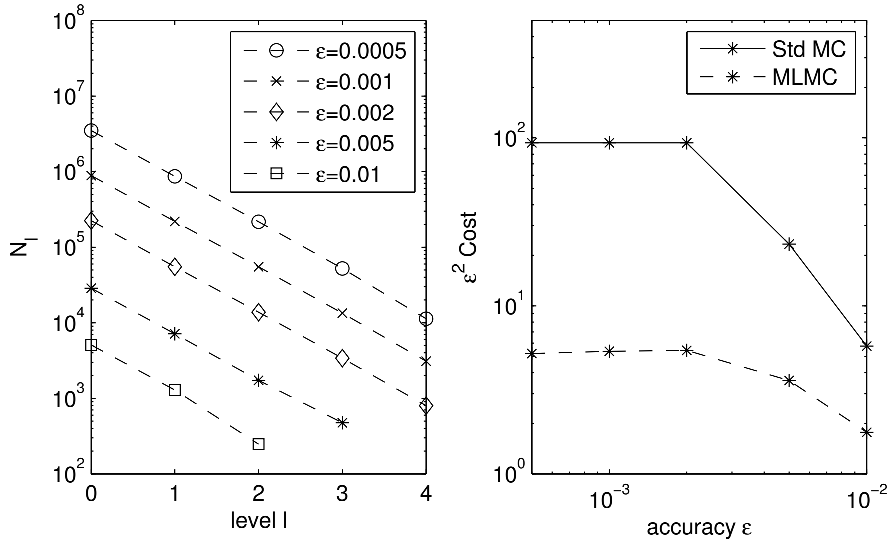
Cost taken to be proportional to number of nodes

2D Results



$\mathbb{V}[\widehat{P}_\ell - \widehat{P}_{\ell-1}] \sim h_\ell^2$ $\quad$ $\mathbb{E}[\widehat{P}_\ell - \widehat{P}_{\ell-1}] \sim h_\ell^2$

2D Results



Complexity analysis

Relating things back to the MLMC theorem:

$$\mathbb{E}[\widehat{P}_\ell - P] \sim 2^{-2\ell} \implies \alpha = 2$$
$$V_\ell \sim 2^{-2\ell} \implies \beta = 2$$
$$C_\ell \sim 2^{d\ell} \implies \gamma = d \quad \text{(dimension of PDE)}$$

To achieve r.m.s. accuracy ε requires finest level grid spacing $h \sim \varepsilon^{1/2}$ and hence we get the following complexity:

dim	MC	MLMC
1	$\varepsilon^{-2.5}$	ε^{-2}
2	ε^{-3}	$\varepsilon^{-2}(\log \varepsilon)^2$
3	$\varepsilon^{-3.5}$	$\varepsilon^{-2.5}$

Other SPDE applications

For more on multilevel for SPDEs, see the work of Christoph Schwab and his group (ETH Zurich):

`http://www.math.ethz.ch/~schwab/`

- elliptic, parabolic and hyperbolic PDEs
- stochastic coefficients, initial data, boundary data

Schwab used to work on alternative techniques such as "polynomial chaos" but has now switched to multilevel because of its superior efficiency for many applications.

For other papers on multilevel, see my MLMC community homepage:

`http://people.maths.ox.ac.uk/gilesm/mlmc_community.html`

Non-geometric multilevel

Almost all applications of multilevel in the literature so far use a geometric sequence of levels, refining the timestep (or the spatial discretisation for PDEs) by a constant factor when going from level ℓ to level $\ell+1$.

Coming from a multigrid background, this is very natural, but it is **NOT** a requirement of the multilevel Monte Carlo approach.

All MLMC needs is a sequence of levels with

- increasing accuracy
- increasing cost
- increasingly small difference between outputs on successive levels

Final comments

- Uncertainty Quantification is a hot topic, with its own conferences and journals
- Monte Carlo methods are a powerful approach to handle uncertainty in a number of different settings
- Multilevel Monte Carlo greatly reduces the cost in a lot of settings, particularly when dealing with PDEs
- for more details, can read my new *Acta Numerica* review article
- CCFE (Culham Centre for Fusion Energy) has a 10-week project on using MLMC for uncertainty quantification