Stochastic Simulation: Lecture 11

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PDEs with Uncertainty

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

- 1D $\rightarrow$ 2D $\rightarrow$ 3D
- steady $\rightarrow$ unsteady
- laminar flow $\rightarrow$ turbulence modelling $\rightarrow$ large eddy simulation $\rightarrow$ direct Navier-Stokes
- simple geometries (e.g. a wing) $\rightarrow$ 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

- Finance

  Stochastic forcing due to market behaviour

PDEs with Uncertainty

In the past, Monte Carlo simulation was 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 many 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
- in comparison, cost is $O(\varepsilon^{-3/2})$ for a single calculation with ε accuracy

SPDEs

- great MLMC application – better cost savings than SDEs due to higher dimensionality
- range of applications
  - Graubner & Ritter (Darmstadt) – 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

Non-geometric MLMC

Most (95-99%?) MLMC applications have a geometric structure, with the accuracy improving geometrically, and the cost increasing geometrically, as the level increases.

In some situation (e.g. SDEs) you can argue that a geometric sequence is near-optimal – e.g. you don't get significantly better overall performance by using $h_\ell \sim 1/\ell^2$.

But there are a few applications with a different structure, and one good example is by Vidal-Codina, Nguyen, G, Peraire (2014).

Application: high-frequency Helmholtz PDE

$$-\nabla \cdot (\kappa(x)\nabla u) - \rho(x)\,\Omega^2 u = f(x)$$

in a domain with random piecewise uniform properties.

Non-geometric MLMC

A standard finite element approximation leads to a very large set of discrete equations of the form

$$A(\omega)\, u = f(\omega)$$

where u is a huge (10^7) vector of nodal values, $A(\omega)$ is a large sparse matrix, and ω represents the stochastic sample.

Standard geometric MLMC doesn't work well for this application because the high-frequency waves need to be adequately resolved.

(Similarly, there are major challenges with developing a good multigrid solver.)

Instead, they used a reduced-basis approach.

Non-geometric MLMC

First, they solve

$$A(\omega_k)\, u_k = f(\omega_k)$$

for a set of M samples ω_k.

Then, for other samples they define

$$u \approx \sum_{k=1}^{K} v_k\, u_k$$

to obtain a low-dimensional reduced system

$$A_r(\omega)\, v = f_r(\omega)$$

- larger $K \Longrightarrow$ greater accuracy at greater cost
- in multilevel treatment, K_ℓ varies with level
- brute force optimisation determines the optimal number of levels, and reduced basis size on each level

Parabolic SPDE

Unusual parabolic SPDE arises in CDO modelling (Bush, Hambly, Haworth & Reisinger)

$$\mathrm{d}p = -\mu \frac{\partial p}{\partial x}\,\mathrm{d}t + \frac{1}{2}\frac{\partial^2 p}{\partial x^2}\,\mathrm{d}t + \sqrt{\rho}\frac{\partial p}{\partial x}\,\mathrm{d}W$$

with absorbing boundary $p(0,t) = 0$

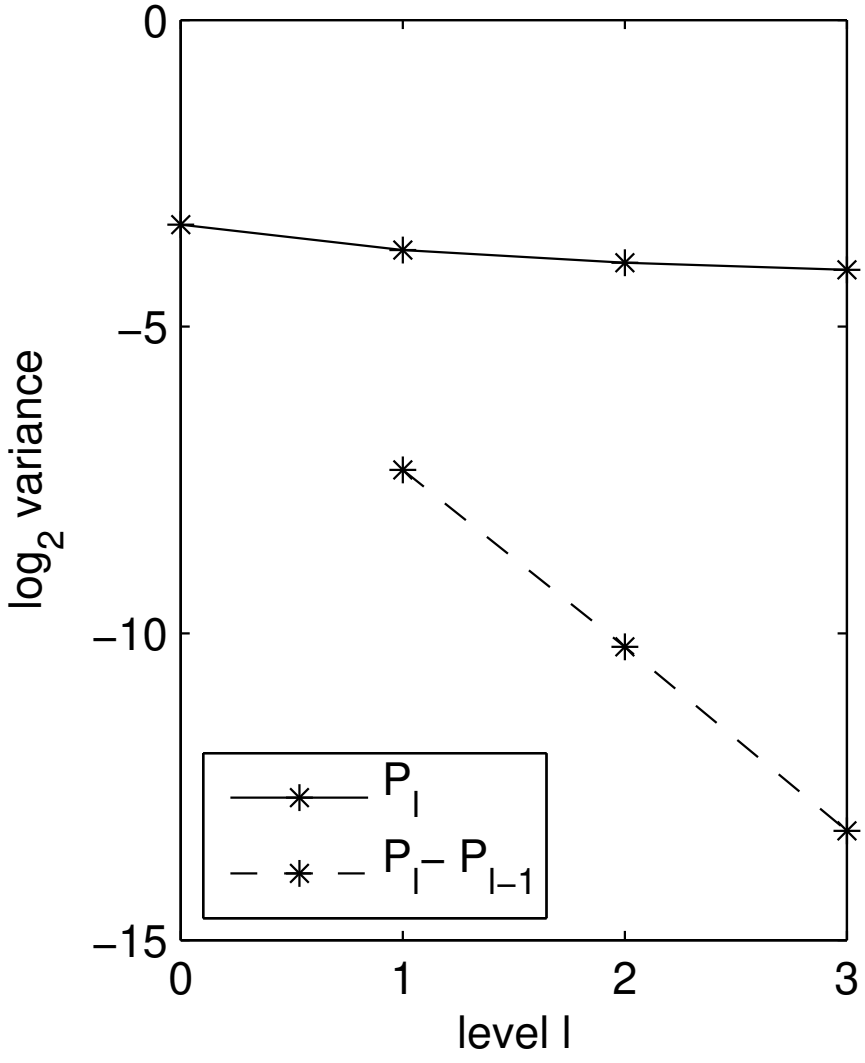
- derived in limit as number of firms $\longrightarrow \infty$
- x is distance to default
- $p(x,t)$ is probability density function
- $\mathrm{d}W$ term corresponds to systemic risk
- $\partial^2 p/\partial x^2$ comes from idiosyncratic risk

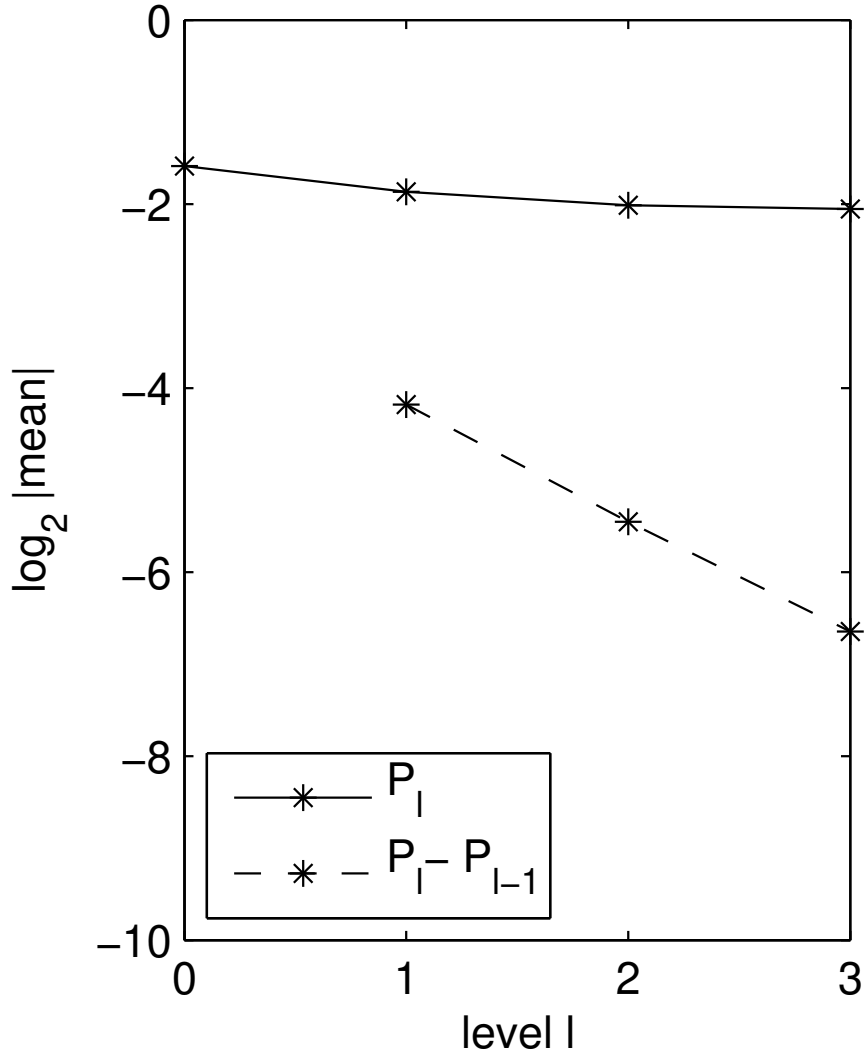
Parabolic SPDE

- numerical discretisation combines Milstein time-marching with central difference approximations
- coarsest level of approximation uses 1 timestep per quarter, and 10 spatial points
- each finer level uses four times as many timesteps, and twice as many spatial points – ratio is due to numerical stability constraints
- mean-square stability theory, with and without absorbing boundary
- computational cost $C_\ell \propto 8^\ell$
- numerical results suggest variance $V_\ell \propto 8^{-\ell}$
- can prove $V_\ell \propto 16^{-\ell}$ when no absorbing boundary

Parabolic SPDE

Fractional loss on equity tranche of a 5-year CDO:





Parabolic SPDE

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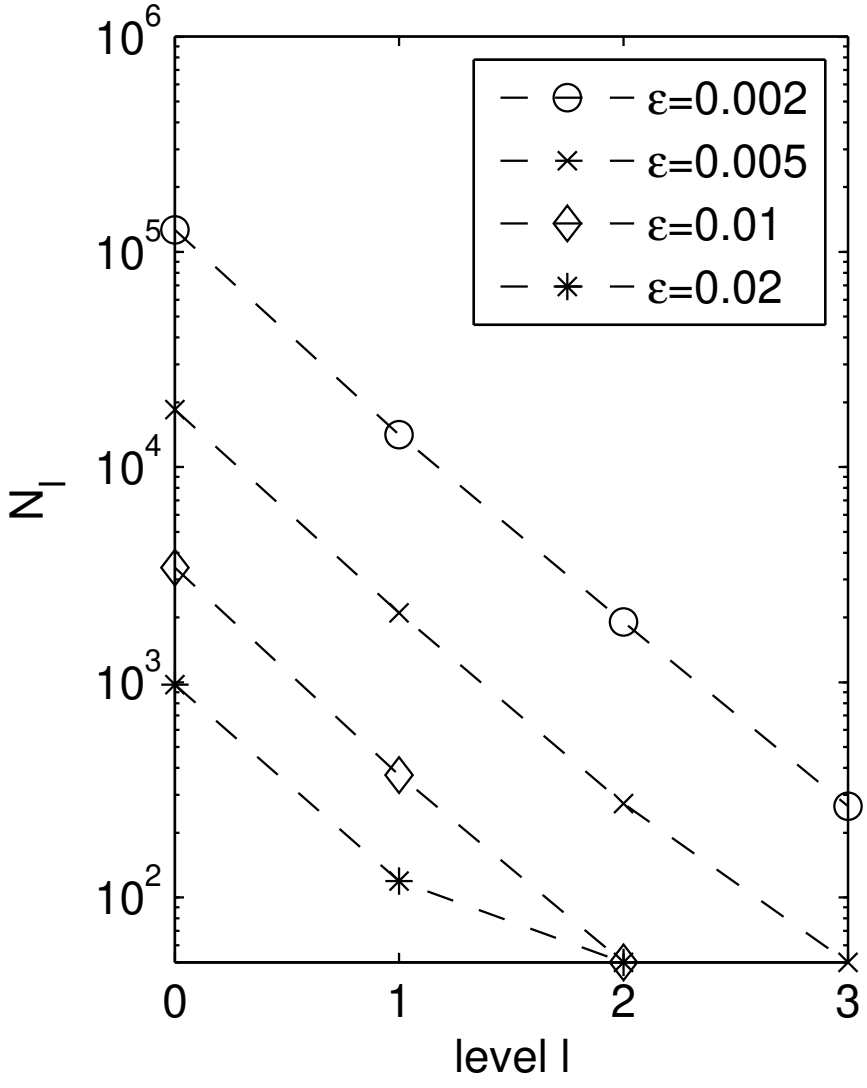

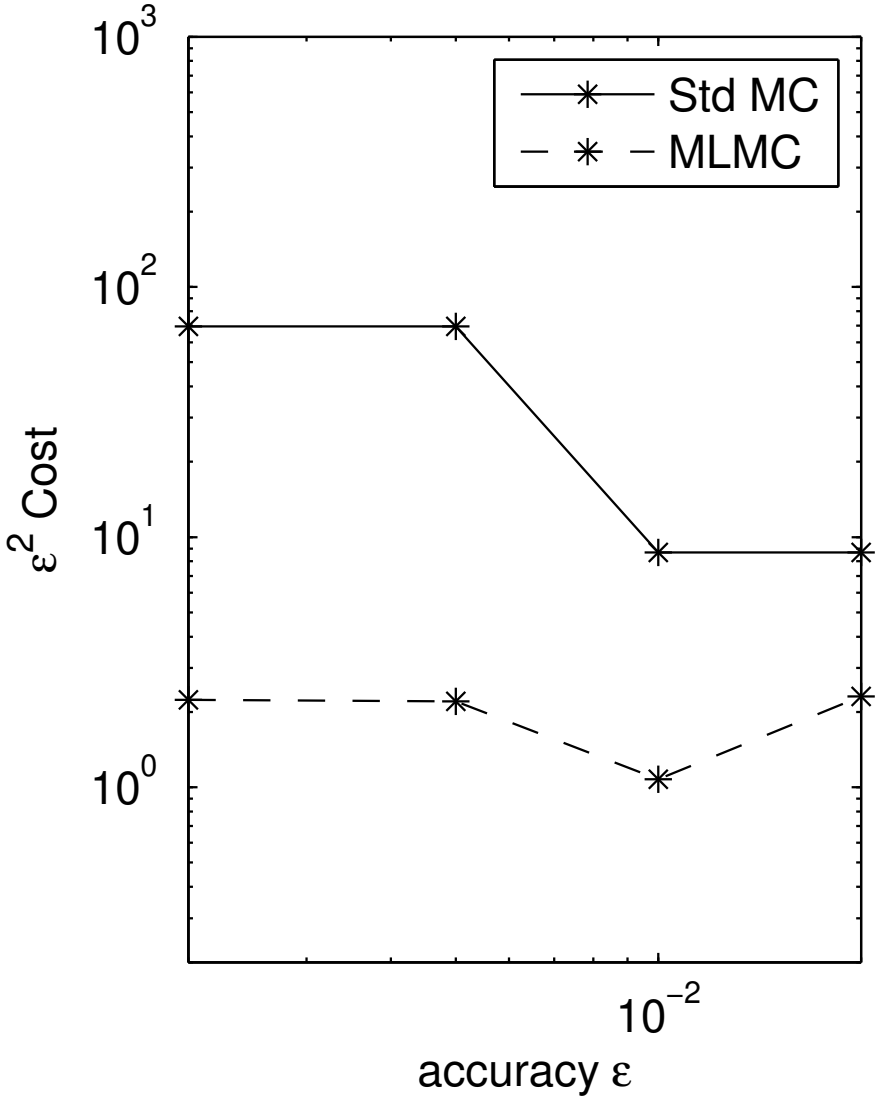

Parabolic SPDE

Milstein and central difference discretisation leads to

$$\begin{aligned} v_j^{n+1} &= v_j^n - \frac{\mu\, k + \sqrt{\rho\, k}\, Z_n}{2h}\left(v_{j+1}^n - v_{j-1}^n\right) \\ &\quad + \frac{(1-\rho)\, k + \rho\, k\, Z_n^2}{2h^2}\left(v_{j+1}^n - 2v_j^n + v_{j-1}^n\right) \end{aligned}$$

where $Z_n \sim N(0,1)$.

Considering a Fourier mode

$$v_j^n = g_n \exp(ij\theta), \quad |\theta| \leq \pi$$

leads to ...

Parabolic SPDE

$$g_{n+1} = \left(a(\theta) + b(\theta)\, Z_n + c(\theta)\, Z_n^2\right) g_n,$$

where

$$\begin{aligned}
a(\theta) &= 1 - \frac{i\,\mu\,k}{h}\,\sin\theta - \frac{2\,(1-\rho)\,k}{h^2}\,\sin^2\tfrac{\theta}{2}, \\
b(\theta) &= -\frac{i\sqrt{\rho\,k}}{h}\,\sin\theta, \\
c(\theta) &= -\frac{2\,\rho\,k}{h^2}\,\sin^2\tfrac{\theta}{2}.
\end{aligned}$$

Parabolic SPDE

Following the approach of mean-square stability analysis (e.g. see Higham)

$$\begin{aligned}\mathbb{E}[\,|g_{n+1}|^2] &= \mathbb{E}\left[(a + b\,Z_n + c\,Z_n^2)(a^* + b^* Z_n + c^* Z_n^2)\;|g_n|^2\right] \\ &= \left(\,|a+c|^2 + |b|^2 + 2|c|^2\,\right)\;\mathbb{E}\left[\,|g_n|^2\right]\end{aligned}$$

so stability requires $|a+c|^2 + |b|^2 + 2|c|^2 \;\leq\; 1$ for all θ, which leads to a timestep stability limit:

$$\begin{aligned}\mu^2 k &\leq 1 - \rho, \\ \frac{k}{h^2} &\leq (1 + 2\rho^2)^{-1}.\end{aligned}$$

Additional analysis extends this to include the effect of boundary conditions.

Key references

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