Multilevel Monte Carlo

Robert Scheichl

Department of Mathematical Sciences

UNIVERSITY OF BATH

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Plain vanilla Monte Carlo for large scale problems

$$\mathbf{Z}(\omega) \in \mathbb{R}^s \xrightarrow{\text{Model}(M)} \mathbf{U}(\omega) \in \mathbb{R}^M \xrightarrow{\text{Output}} Q_{M,s}(\omega) \in \mathbb{R}$$

random input — intermediate variables — quantity of interest

- s large, M **very** large; e.g. $\mathbf{Z}$ multivariate Gaussian; $\mathbf{X}$ numerical solution of a DE; $Q_{M,J}$ a (non)linear functional of $\mathbf{X}$

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- Typically, problem above is already an approximation of the real problem (e.g. SDE or PDE with uncertain coefficient field):
  - $\mathbf{Z}$ approximation of an infinite dimensional (or v. large) object, e.g. W_t (Wiener process) or the s dominant modes in Karhunen-Loève expansion of (spatially) correlated random field
  - $\mathbf{U}$ FD or FE approximation of a time- or space dependent function $u(t)$ or $u(x)$ on a grid with M vertices.
  - $Q_{M,s}(\omega)$ approximation of an inaccessible random variable $Q(\omega)$

Monte Carlo for large scale problems (ctd.)

- Often we can assume something like $\mathbb{E}[Q_{M,s}] \stackrel{M,s\to\infty}{\longrightarrow} \mathbb{E}[Q]$ and

$$|\mathbb{E}[Q_{M,s} - Q]| = \mathcal{O}(M^{-\alpha}) + \mathcal{O}(s^{-\alpha'})$$

(but exact asymptotics irrelevant, provided there is some decay;
∞ can also be simply "unfeasibly huge")

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- **Standard Monte Carlo** estimator for $\mathbb{E}[Q]$:

$$\hat{Q}^{\mathrm{MC}} := \frac{1}{N} \sum_{i=1}^{N} Q_{M,s}^{(i)}$$

where $\{Q_{M,s}^{(i)}\}_{i=1}^{N}$ are i.i.d. samples computed with Model(M).

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- Convergence typically quantified via **mean square error**

$$\mathrm{MSE} := \mathbb{E}\left[\left(\hat{Q}^{\mathrm{MC}} - \mathbb{E}[Q]\right)^2\right] = \underbrace{\frac{\mathbb{V}[Q_{M,s}]}{N}}_{\textbf{sampling error}} + \underbrace{\left(\mathbb{E}[Q_{M,s} - Q]\right)^2}_{\textbf{model error ("bias")}}$$

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Complexity Theorem for (plain vanilla) Monte Carlo

Assume that $Q_{M,s} \to Q$ with $\mathcal{O}(M^{-\alpha})$ and cost per sample is $\mathcal{O}(M)$. Then

$$\text{Cost}(\hat{Q}^{\text{MC}}) \;=\; \mathcal{O}\left(\text{TOL}^{-2-\frac{1}{\alpha}}\right) \;\text{ to obtain }\; \text{MSE} < \text{TOL}^2.$$

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- SDEs for atmos. dispersion: typically $\alpha = 1 \;\Rightarrow\; \text{Cost}(\hat{Q}^{\text{MC}}) = \mathcal{O}\left(\text{TOL}^{-3}\right)$
- UQ for subsurface flow: typically $\alpha = 1/3 \;\Rightarrow\; \text{Cost}(\hat{Q}^{\text{MC}}) = \mathcal{O}\left(\text{TOL}^{-5}\right)$

Example: Uncertainty Quantification in Subsurface Flow
(eg. risk analysis of radiocative waste disposal or oil reservoir simulation)

$$\begin{array}{lrcl} \textbf{Darcy's Law:} & \vec{q} + k\,\nabla u & = & f \\ \textbf{Incompressibility:} & \nabla \cdot \vec{q} & = & 0 \end{array}$$

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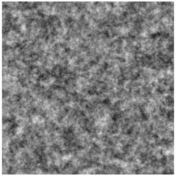
Typical simplified model:

- $\log k(x,\omega)$ = isotropic, scalar **Gaussian** w. exponential covariance $R(x,y) := \sigma^2 \exp\left(-\frac{\|x-y\|}{\lambda}\right)$



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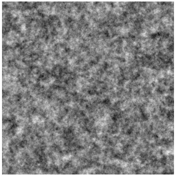
- KL expansion: $\log k(x,\omega) \approx \sum_{j=1}^{J} \sqrt{\mu_j} \phi_j(x) Z_j(\omega)$
  with $Z_j(\omega)$ i.i.d. $N(0,1)$



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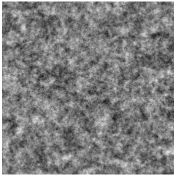

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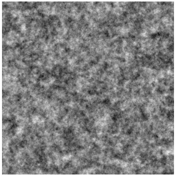
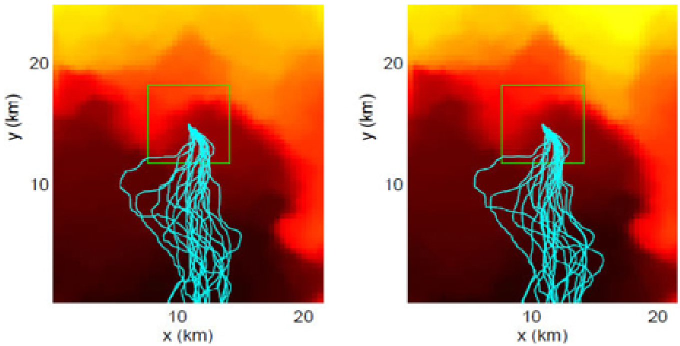


- **FE discretisation**: $A(\omega)\, \mathbf{U}(\omega) = \mathbf{b}(\omega)$
- QoI $Q(\omega)$, e.g., particle travel time from repository to boundary

Sample paths of contaminant particles

Source: K. A. Cliffe, 2012



Numerical Example

$Q = k_{\text{eff}} := \frac{1}{|\Gamma_{\text{out}}|} \int_{\Gamma_{\text{out}}} \vec{q} \cdot \vec{n}$

Case 1: $\lambda = 0.3$, $\sigma^2 = 1$

TOL	M	N	Cost
0.01	1.7×10^4	1.4×10^4	21 min
0.002	1.1×10^6	3.5×10^5	30 days

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Case 2: $\lambda = 0.1$, $\sigma^2 = 3$

TOL	M	N	Cost
0.01	2.6×10^5	8.5×10^3	4 h
0.002	**Prohibitively large!!**		

Here $\alpha \approx 3/8$ (numerically observed) $\Rightarrow$ Cost $\approx \mathcal{O}(\text{TOL}^{-14/3})$

25× more work to halve error!

Multilevel Monte Carlo [Heinrich, '01], [Giles, '07], ...

Use **hierarchy** of models w. $M_0 < M_1 < \ldots < M_L$ and note that

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

where $Q_\ell := Q_{M_\ell, s_\ell}$ (**Important:** need 'knob' to control bias error & cost)

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

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Note: $\hat{Y}_\ell^{\mathrm{MC}} = \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} (Q_\ell^{(i)} - Q_{\ell-1}^{(i)})$ with $Q_\ell^{(i)}$ and $Q_{\ell-1}^{(i)}$ from same "path"

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Key Observation: (Variance Reduction! Corrections cheaper!)

If $Q_\ell \to Q$ then $\mathbb{V}[Q_\ell - Q_{\ell-1}] \to 0$ as $\ell \to \infty$ **!**

Complexity Theorem for Multilevel Monte Carlo

Assume bias error $\mathcal{O}(M_\ell^{-\alpha})$ & cost/sample $\mathcal{O}(M_\ell)$ (as above) **as well as**

$$\mathbb{V}[Q_\ell - Q_{\ell-1}] = \mathcal{O}(M_\ell^{-\beta}) \quad \text{(requires strong convergence!)}$$

There exist L, $\{N_\ell\}_{\ell=0}^{L}$ (computable on the fly) to obtain $\text{MSE} < \text{TOL}^2$ with

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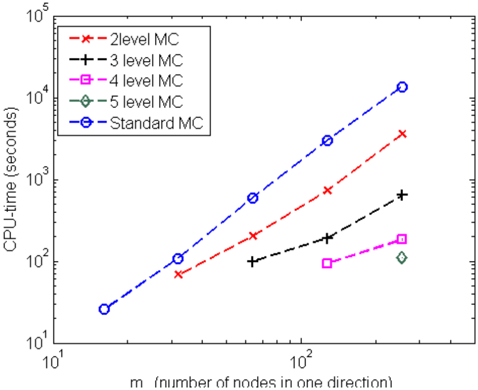
Proof. $\hat{Q}_L^{\mathrm{ML}}$ is unbiased estimator of $\mathbb{E}[Q_L]$ and the $\widehat{Y}_\ell^{\mathrm{MC}}$ are independent. Hence

$$\mathbb{E}\big[\big(\hat{Q}_L^{\mathrm{ML}} - \mathbb{E}[Q]\big)^2\big] = \sum\nolimits_\ell \mathbb{V}[Y_\ell]/N_\ell + \big(\mathbb{E}[Q_L - Q]\big)^2$$

Then minimise cost for fixed MSE (simple constrained minimisation problem).

Numerical Example

$D = (0,1)^2$, $\sigma^2 = 1$, $\lambda = 0.1$, $s = 500$, $Q = k_{\text{eff}}$, $\text{TOL} = 10^{-3}$



`Matlab` implementation on 3GHz Intel Core 2 Duo E8400 proc, 3.2GByte RAM

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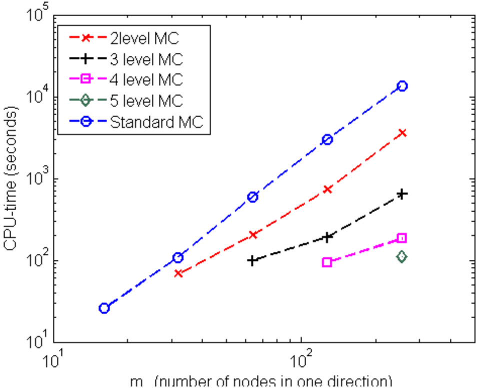

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In subsurface model problem assumptions can be verified theoretically.
[Charrier, RS, Teckentrup, 2011], [Teckentrup, RS, Giles, Ullmann, 2012], . . .

Reducing #Samples (Multilevel Quasi–Monte Carlo)

[Graham, Kuo, Nuyens, RS, Sloan '11]. . . [Kuo, RS, Schwab, Sloan, Ullmann '15]

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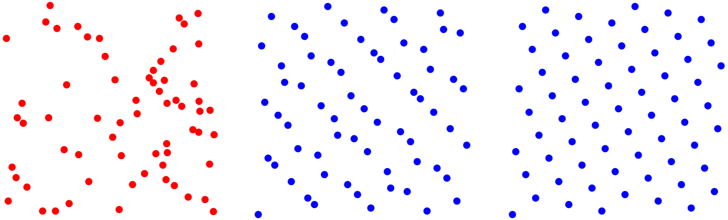

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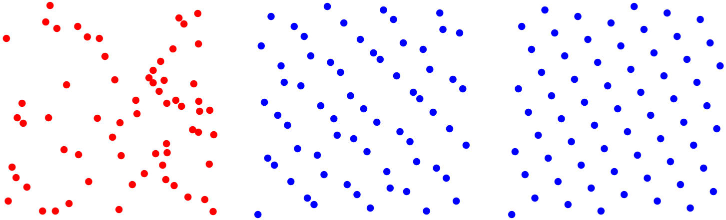

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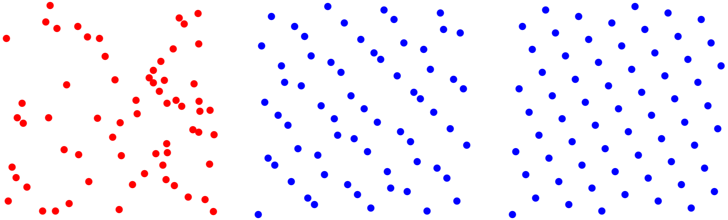

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- **In practice** #samples (and thus cost) always **significantly smaller**

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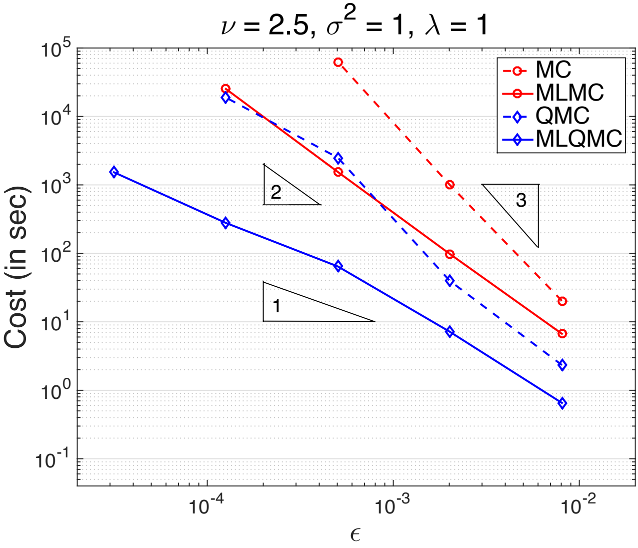
$D = (0,1)^2$; $Q = k_{\text{eff}}$; randomised lattice rule w. $\gamma_j = 1/j^2$



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- Several other extensions: CDFs, PDFs, failure probabilities, rare events, exit times, Levy noise, ...

Numerical Example (MLMCMC)

$D = (0,1)^2$; $Q = k_{\text{eff}}$; exponential covariance w. $\lambda = 0.5$, $\sigma^2 = 1$; conditioned on 16 "measurements"