Multilevel Monte Carlo methods for uncertainty quantification in subsurface flow

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Joint work with:

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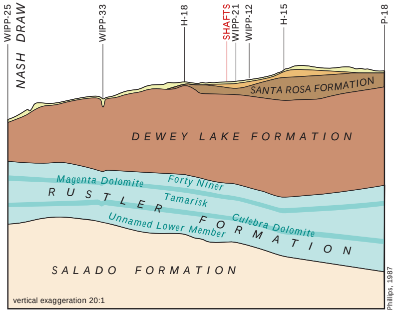
Outline

- Motivation and model problem: uncertainty quantification in radioactive waste disposal
- Standard Monte Carlo
- **Multilevel Monte Carlo**
- **Multilevel Markov chain Monte Carlo**

Application: WIPP test case

US Dept Energy Radioactive Waste Isolation Pilot Plant (WIPP) in New Mexico



Cross-section at WIPP

Cross section through the rock at the WIPP site

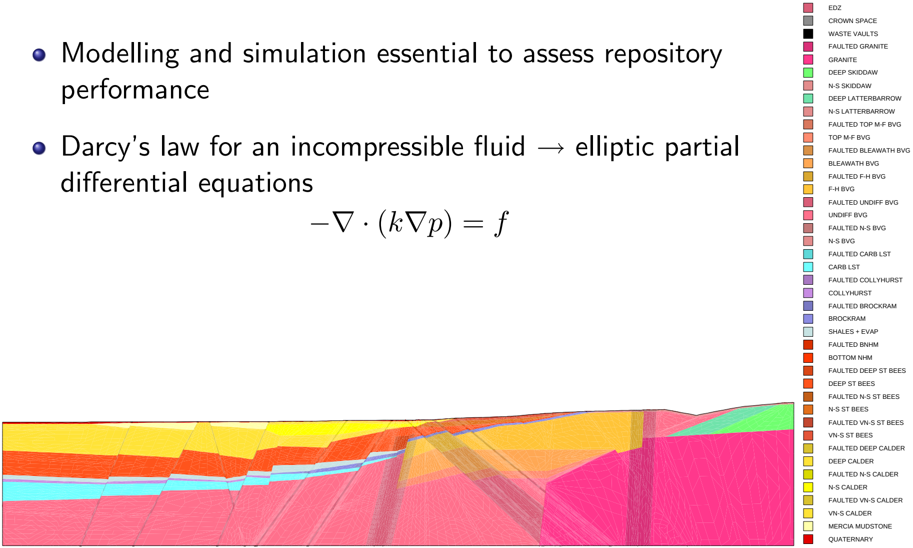
- Crucial to assess the risk of radionuclides reentering the human environment
- Culebra Dolomite layer acts as principal pathway for transport of radionuclides

  (2D to reasonable approximation)

Uncertainty in Groundwater Flow

- Modelling and simulation essential to assess repository performance
- Darcy's law for an incompressible fluid → elliptic partial differential equations

$$-\nabla \cdot (k \nabla p) = f$$



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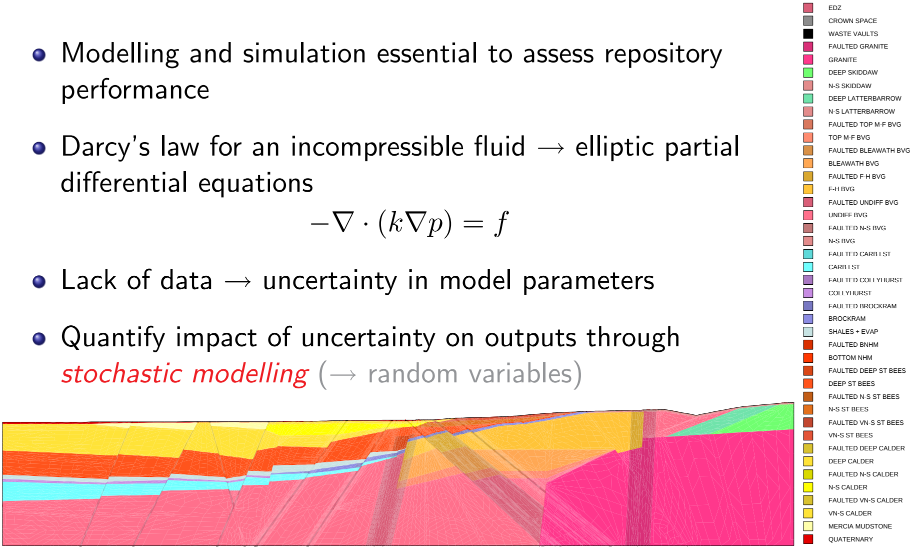
- Lack of data → uncertainty in model parameters
- Quantify impact of uncertainty on outputs through *stochastic modelling* (→ random variables)



Typical model

- Typical simplified model for k is a log–normal random field, $k = \exp[g]$, where g is a scalar, isotropic Gaussian field.
- To sample from k, use Karhunen-Loève 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. $N(0,1)$.

Stochastic modelling

- Many reasons for stochastic modelling in earth sciences:
  - **lack of data** (e.g. data assimilation for weather prediction)
  - **unresolvable scales** (e.g. atmospheric dispersion modelling)
- **Input:** best knowledge about system, statistics of input parameters, measured data with error statistics, etc...
- **Output:** statistics of quantities of interest or of entire state space

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$$\mathbf{Z}_J(\omega) \in \mathbb{R}^J \xrightarrow{\text{Model}(M)} \mathbf{X}_M(\omega) \in \mathbb{R}^M \xrightarrow{\text{Output}} Q_{M,J}(\omega) \in \mathbb{R}$$

random input | state vector | quantity of interest

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- e.g. $\mathbf{Z}_J$ multivariate Gaussian; $\mathbf{X}_M$ numerical solution of PDE; $Q_{M,J}$ a (non)linear functional of $\mathbf{X}_M$
- $Q(\omega)$ inaccessible random variable s.t. $\mathbb{E}[Q_{M,J}] \xrightarrow{M,J\to\infty} \mathbb{E}[Q]$

Standard Monte Carlo

Usually interested in finding the expected value (or higher order moments) of output functional Q.

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The standard **Monte Carlo estimator** for this is

$$\mathbb{E}[Q] \approx \mathbb{E}[Q_{M,J}] \approx \frac{1}{N}\sum_{i=1}^{N} Q_{M,J}^{(i)} := \hat{Q}^{\mathrm{MC}},$$

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The **mean square error** can be shown to equal

$$\begin{aligned}\mathbb{E}\Big[\big(\hat{Q}_h^{\mathrm{MC}} - \mathbb{E}[Q]\big)^2\Big] \;&=\; \mathbb{V}[\hat{Q}_h^{\mathrm{MC}}] \;+\; \big(\mathbb{E}[\hat{Q}_h^{\mathrm{MC}}] - \mathbb{E}[Q]\big)^2 \\ &=\; \underbrace{\frac{\mathbb{V}[Q_{M,J}]}{N}}_{\text{sampling error}} \;+\; \underbrace{\Big(\mathbb{E}[Q_{M,J} - Q]\Big)^2}_{\text{model error ("bias")}}\end{aligned}$$

$\Rightarrow$ **very large N and M!**

Complexity of Standard Monte Carlo

Assuming that

(A1) $\left|\mathbb{E}[Q_{M,J} - Q]\right| = \mathcal{O}(M^{-\alpha})$ (model error)

(A2) $\text{Cost}(Q_{M,J}^{(i)}) = \mathcal{O}(M^{\gamma})$ (PDE solver)

there exist M and N such that the **total cost** to obtain a **mean square error**

$$\mathbb{E}\left[(\hat{Q}^{\mathrm{MC}} - \mathbb{E}[Q])^2\right] \;=\; \mathcal{O}(\varepsilon^2)$$

is

$$\text{Cost}(\hat{Q}^{\mathrm{MC}}) \;=\; \mathcal{O}(\varepsilon^{-2-\gamma/\alpha})$$

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- Typically $\alpha = 1/2$, $\gamma = 1$: for $\varepsilon = 10^{-3}$ we have Cost $= \mathcal{O}(10^{12})$!

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

The multilevel method works on a **sequence of levels**, s.t. $M_\ell = sM_{\ell-1}$ and $J_\ell = sJ_{\ell-1}$, $\ell = 0, 1, \ldots, L$, and set $Q_\ell = Q_{M_\ell, J_\ell}$.

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Linearity of expectation gives us

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

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

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

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

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

The **mean square error** of the this estimator is

$$\mathbb{E}\Big[\big(\hat{Q}_L^{\mathrm{ML}} - \mathbb{E}[Q]\big)^2\Big] = \underbrace{\mathbb{V}[\hat{Q}_L^{\mathrm{ML}}]}_{\text{sampling error}} + \underbrace{\big(\mathbb{E}[\hat{Q}_L^{\mathrm{ML}}] - \mathbb{E}[Q]\big)^2}_{\text{model error}}$$

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$$= \frac{\mathbb{V}[Q_0]}{N_0} + \sum_{\ell=1}^{L} \frac{\mathbb{V}[Q_\ell - Q_{\ell-1}]}{N_\ell} + \big(\mathbb{E}[Q_L - Q]\big)^2$$

- N_0 still needs to be large, **but** samples are much cheaper to obtain on coarser level
- N_ℓ $(\ell > 0)$ much smaller, **since** $\mathbb{V}[Q_\ell - Q_{\ell-1}] \to 0$ as $M_\ell \to \infty$

Complexity of Multilevel Monte Carlo

Assume **(A1)** (model error $\mathcal{O}(M_\ell^{-\alpha})$), **(A2)** (cost/sample $\mathcal{O}(M_\ell^{\gamma})$) and

(A3) $\mathbb{V}[Q_\ell - Q_{\ell-1}] = \mathcal{O}(M_\ell^{-\beta})$

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**

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

is

$$\mathrm{Cost}(\hat{Q}_L^{\mathrm{ML}}) \; = \; \begin{cases} \mathcal{O}(\varepsilon^{-2}) & \text{if} \;\; \beta > \gamma \\ \mathcal{O}(\varepsilon^{-2} \, \log(\varepsilon)^2) & \text{if} \;\; \beta = \gamma \\ \mathcal{O}(\varepsilon^{-2 - (\gamma - \beta)/\alpha}) & \text{if} \;\; \beta < \gamma \end{cases}$$

- $\{N_\ell\}$ chosen to minimise cost for a fixed variance

Convergence analysis of MLMC

Can prove that for typical 2D model problems in subsurface flow, **(A1)** and **(A3)** are satisfied with $\alpha = 1/2$, $\beta = 1$. With an optimal linear solver $(\gamma = 1)$, the computational costs are bounded by:

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

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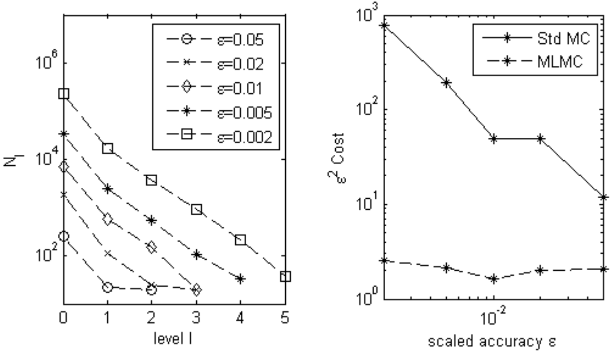
d	**MLMC**	**MC**
2	$\mathcal{O}(10^6)$	$\mathcal{O}(10^{12})$

0.1 % accuracy $\longrightarrow \varepsilon = 10^{-3}$

Numerical Example (multilevel MC)

$D = (0,1)^2$, $Q = \|p\|_{L^2(D)}$, $J_L = \infty$, $M_0 = 8^2$.

Typical **2D model problem**.



Left: Number of samples per level. *Right:* Total computational cost.

Can the multilevel idea be extended to Markov chain Monte Carlo?

Incorporating data - Bayesian approach

Recall:

$$\mathbf{Z}_J(\omega) \in \mathbb{R}^J \xrightarrow{\text{Model}(M)} \mathbf{X}_M(\omega) \in \mathbb{R}^M \xrightarrow{\text{Output}} Q_{M,J}(\omega) \in \mathbb{R}$$

random input — state vector — quantity of interest

- **"Prior"** in our model was multivariate Gaussian $\mathbf{Z}_J := [Z_1, \ldots, Z_J]$:

$$\mathcal{P}(\mathbf{Z}_J) \eqsim (2\pi)^{-J/2} \prod_{j=1}^J \exp\left(-\frac{Z_j^2}{2}\right)$$

- Usually **data** F_{obs} related to **outputs** (e.g. pressure) also available. To reduce uncertainty, incorporate F_{obs} $\rightarrow$ the **"posterior"**

Incorporating data - Bayesian approach

Bayes' Theorem: (RHS computable! Proportionality constant $1/\mathcal{P}(F_{\text{obs}})$ not!)

$$\underbrace{\pi^{M,J}(\mathbf{Z}_J)}_{\textbf{posterior}} := \mathcal{P}(\mathbf{Z}_J \,|\, F_{\text{obs}}) \eqsim \underbrace{\mathcal{L}_M(F_{\text{obs}} \,|\, \mathbf{Z}_J)}_{\textbf{likelihood}} \underbrace{\mathcal{P}(\mathbf{Z}_J)}_{\textbf{prior}}$$

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- **Likelihood model** (e.g. Gaussian):

$$\mathcal{L}_M(F_{\text{obs}} \,|\, \mathbf{Z}_J) \;\eqsim\; \exp\left(\frac{-\|F_{\text{obs}} - F_M(\mathbf{Z}_J)\|^2}{\sigma^2_{\text{fid},M}}\right)$$

$F_M(\mathbf{Z}_J)$ ... model response; $\sigma_{\text{fid},M}$ ... fidelity parameter (M-dep.)

ALGORITHM 1. (Standard Metropolis Hastings MCMC)

- Choose $\mathbf{Z}_J^0$.
- At state $\mathbf{Z}_J^n$ generate proposal $\mathbf{Z}'_J$ from distribution $q(\mathbf{Z}'_J \,|\, \mathbf{Z}_J^n)$ (for simplicity symmetric, e.g. random walk).
- Accept sample $\mathbf{Z}'_J$ with probability $\alpha^{M,J} = \min\left(1, \frac{\pi^{M,J}(\mathbf{Z}'_J)}{\pi^{M,J}(\mathbf{Z}_J^n)}\right)$,

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Samples $\mathbf{Z}_J^n$ used as usual for inference (even though not i.i.d.):

$$\mathbb{E}_{\pi^{M,J}}[Q] \;\approx\; \mathbb{E}_{\pi^{M,J}}[Q_{M,J}] \;\approx\; \frac{1}{N}\sum_{n=1}^{N} Q_{M,J}^{(n)} := \widehat{Q}^{\text{MetH}}$$

Pros:

- Produces a Markov chain $\{\mathbf{Z}_J^n\}_{n\in\mathbb{N}}$, with $\mathbf{Z}_J^n \sim \pi^{M,J}$ as $n \to \infty$.

Cons:

- Evaluating $\alpha^{M,J}$ expensive for large M.
- Acceptance rate $\alpha^{M,J}$ very low for large J $(< 10\%)$.

Multilevel Markov Chain Monte Carlo

Key ingredients in multilevel method:

- Models with less DOFs on coarser levels **much cheaper** to solve
- $\mathbb{V}[Q_\ell - Q_{\ell-1}] \to 0$ as $\ell \to \infty$ $\Rightarrow$ **fewer samples** on finer levels
- **Telescoping sum:** $\mathbb{E}[Q_L] = \mathbb{E}[Q_0] + \sum_{\ell=1}^{L} \mathbb{E}[Q_\ell] - \mathbb{E}[Q_{\ell-1}]$

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In MCMC setting target distribution depends on ℓ, so need to define multilevel estimator carefully!

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$$\widehat{Q}_L^{\text{MLMetH}} := \frac{1}{N_0}\sum_{n=1}^{N_0} Q_0(\mathbf{Z}_0^n) + \sum_{\ell=1}^{L} \frac{1}{N_\ell}\sum_{n=1}^{N_\ell} \left(Q_\ell(\mathbf{Z}_\ell^n) - Q_{\ell-1}(\mathbf{Z}_{\ell-1}^n)\right)$$

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Idea: Split $\mathbf{Z}_\ell^n = [\mathbf{z}_{\ell,\mathsf{C}}^n, \mathbf{z}_{\ell,\mathsf{F}}^n]$, where $\mathbf{z}_{\ell,\mathsf{C}}^n$ has length $J_{\ell-1}$.

ALGORITHM 2 (Two-level Metropolis Hastings MCMC for $Q_\ell - Q_{\ell-1}$)

At states $\mathbf{Z}^n_{\ell-1}, \mathbf{Z}^n_\ell$ (of the **independent** level ℓ and level $\ell - 1$ Markov chains)

1. Generate new state $\mathbf{Z}^{n+1}_{\ell-1}$ using Algorithm 1.

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3. Accept $\mathbf{Z}'_\ell$ with probability

$$\alpha^\ell(\mathbf{Z}'_\ell \,|\, \mathbf{Z}^n_\ell) = \min\left(1, \frac{\pi^\ell(\mathbf{Z}'_\ell)\, \mathrm{q}^{\mathsf{ML}}(\mathbf{Z}^n_\ell \,|\, \mathbf{Z}'_\ell)}{\pi^\ell(\mathbf{Z}^n_\ell)\, \mathrm{q}^{\mathsf{ML}}(\mathbf{Z}'_\ell \,|\, \mathbf{Z}^n_\ell)}\right)$$

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   Follows quite easily & both terms have been computed previously.

Example: one step

Given $\mathbf{Z}^n_{\ell-1}$ and $\mathbf{Z}^n_\ell$, the possible $(n+1)^{th}$ states of the two chains are:

Level $\ell-1$ test	Level ℓ test	$\mathbf{Z}^{n+1}_{\ell-1}$	$\mathbf{Z}^{n+1}_{\ell}$
reject	accept	$\mathbf{Z}^n_{\ell-1}$	$[\mathbf{Z}^n_{\ell-1}, \mathbf{z}'_{\ell,\mathsf{F}}]$
accept	accept	$\mathbf{Z}'_{\ell-1}$	$[\mathbf{Z}'_{\ell-1}, \mathbf{z}'_{\ell,\mathsf{F}}]$
reject	reject	$\mathbf{Z}^n_{\ell-1}$	$[\mathbf{z}^n_{\ell,\mathsf{C}}, \mathbf{z}^n_{\ell,\mathsf{F}}]$
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Convergence analysis of MLMCMC

What can we prove?

- We have a genuine **Markov chain** on every level.
- Multilevel algorithm is **consistent** (no bias between levels).
- Multilevel algorithm **converges** for any initial state.
- **Same Complexity Theorem** as for Multilevel Monte Carlo.
  (completely abstract and applicable also in DA for NWP)
  - For typical 2D model problems in subsurface flow, we have $\alpha = 1/2$, $\beta = 1/2$. With an optimal linear solver $(\gamma = 1)$, the computational costs are bounded by:

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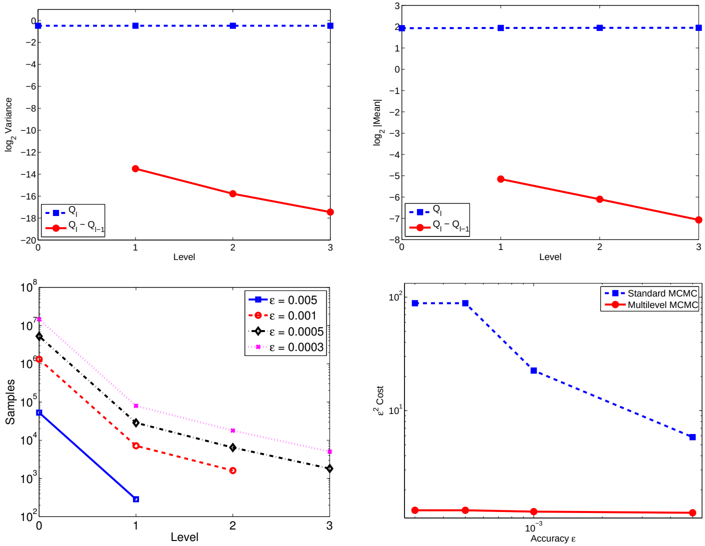
d	MLMCMC	MCMC
2	$\mathcal{O}(10^9)$	$\mathcal{O}(10^{12})$

0.1 % accuracy $\longrightarrow \varepsilon = 10^{-3}$

Numerical Example (multilevel MCMC)

$D = (0,1)^2$, $Q = k_{\text{eff}}$, $J_L = 169$, $M_0 = 16^2$.

Data (artificial): Pressure p at 9 random points in domain.



Conclusions

- Standard (Markov chain) Monte Carlo algorithms are often prohibitively expensive.
- Multilevel versions greatly reduce the cost.
- Multilevel algorithms are generally applicable.
- Full convergence analysis available.