Yet another Talk on Multilevel Monte Carlo
Different I Promise!

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Joint work over 8 years with a large number of collaborators, including

G Detommaso, **I Graham**, **E Müller**, M Parkinson & **T Shardlow** (all Bath);
J Charrier (Marseille); A Cliffe †; T Dodwell (Exeter); M Giles (Oxford);
A Teckentrup (Edinburgh); E Ullmann (TUM)

SAMBa Integrative Think Tank 6
BRLSI, Bath, June 5th 2017

Motivation

INPUT $\longrightarrow$ **MODEL** $\longrightarrow$ **OUTPUT**

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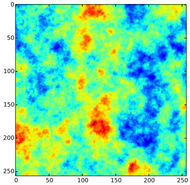

Rock permeability

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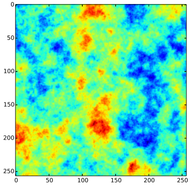

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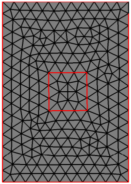

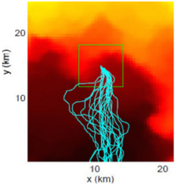

FE analysis of leaking waste

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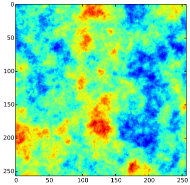

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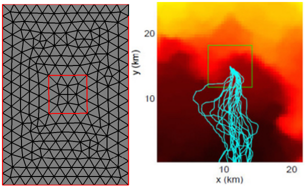

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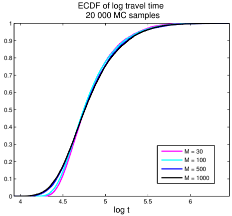

Radionuclides reaching drinkwater?

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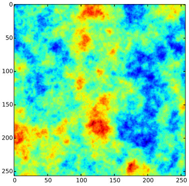

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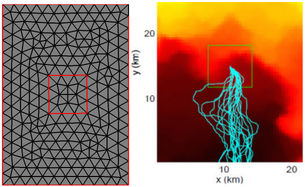

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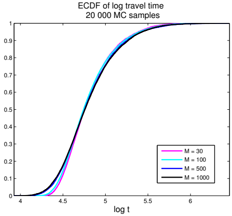

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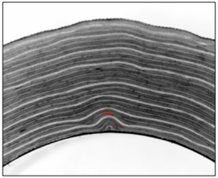

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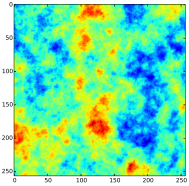

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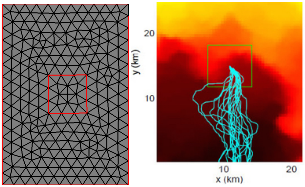

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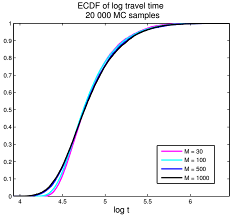

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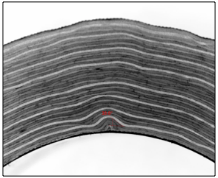

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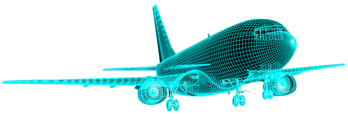

FE analysis of aircraft wing

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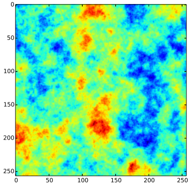

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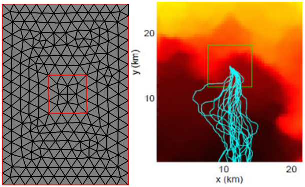

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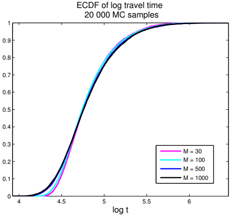

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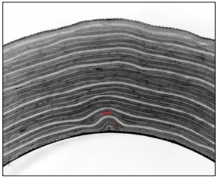

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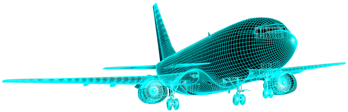

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Wing failing?

Uncertainty Quantification / Stochastic Simulation

$$Z(\omega) \in X \xrightarrow{\text{Model}} u(\omega) \in V \xrightarrow{\text{Output}} Q(\omega) \in \mathbb{R}(\text{or } \mathbb{R}^J) \xrightarrow{\text{Statistics}} \mathbb{E}[Q]$$

noise process | state of process | quantity of interest

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SDE: $Z = Z_t$, e.g. the driving Brownian (or Levy) process W_t;
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Q (non)linear functional of u_t (at end time T or along whole path)

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UQ: $Z = Z(x)$ (or $Z(x,t)$), spatial (or spatiotemporal) random field;
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Even though $Q(\omega)$ may only be a **single random variable**. Its distribution is often defined only implicitly via the distributions of the **latent** fields $u \in V$ and $Z \in X$ which may be **infinite or high dimensional**!

Practical Implementation: Discretisation / Approximation

$$Z_\ell(\omega) \in X_\ell \xrightarrow{\text{Model}(\ell)} u_\ell(\omega) \in V_\ell \xrightarrow{\text{Output}} Q_\ell(\omega) \in \mathbb{R}(\text{or } \mathbb{R}^J) \xrightarrow{\text{Quadrature}} \widehat{Q}_\ell$$

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SDE: Discretisation with step size h_ℓ

$Z_\ell = (\Delta W_{\ell,j})_{j=1}^{M_\ell}$ vector of Brownian increments;

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This provides us with a natural **model hierarchy** (parametrised by ℓ). Assume, there exist $\alpha > 0$ and $\gamma > 0$ such that

(A1) $|\mathbb{E}[Q - Q_\ell]| = \mathcal{O}(2^{-\alpha\ell})$ and **(A2)** $\mathbb{E}[\text{Cost}_\ell] = \mathcal{O}(2^{\gamma\ell})$

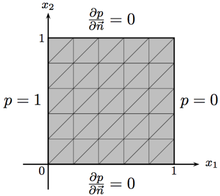
where Cost_ℓ is the cost to compute one realisation of Q_ℓ.

Running Example ("Fruit fly" of UQ)

- Single-phase subsurface flow on unit square D:

$$-\nabla \cdot \left(e^{Z(\omega)} \nabla u(\omega) \right) = 0$$

subject to Neumann BC $\nabla u \cdot \nu = 0$ (top & bottom)
& Dirichlet BC $u = 1$ (left) and $u = 0$ (right)



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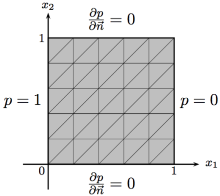

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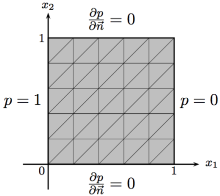

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- Gaussian $Z(\omega)$ w. **exponential** covariance (i.e. $e^{Z(\omega)}$ lognormal)
- Parametrised by $Z_\ell(\omega) \in X_\ell := \mathbb{R}^{s_\ell}$ with $Z_{\ell,j} \sim \mathcal{N}(0, 1)$ i.i.d.
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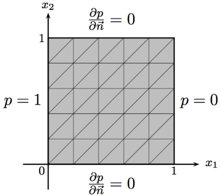

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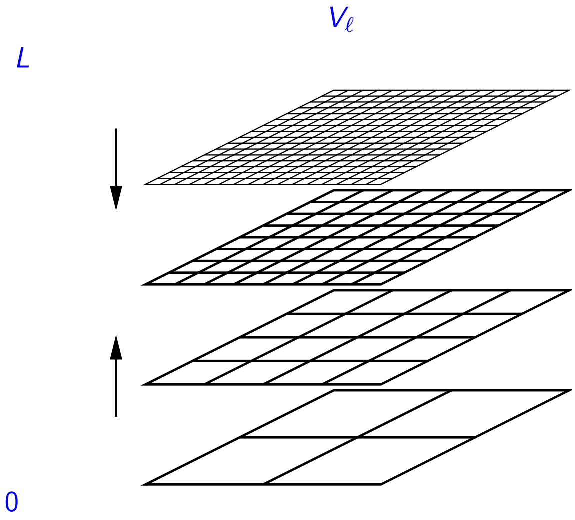
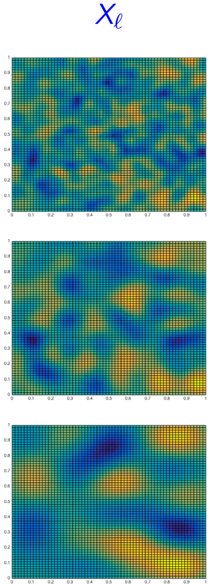
  (e.g. via truncated KL-expansion of Z or via circulant embedding & FFT)
- FE discretisation: $u_\ell \in V_\ell \subset V$
  (e.g. continuous p.w. linears w.r.t. $\mathcal{T}_\ell$ with mesh size $h_\ell = 2^{-\ell+1/2}$):

$$\int_D \nabla v_\ell \cdot \left(e^{Z_\ell(\omega)} \nabla u_\ell(\omega)\right) = 0 \quad \forall v_\ell \in V_\ell \quad \Leftrightarrow \quad A_\ell(\omega) U_\ell(\omega) = b$$

$M_\ell \times M_\ell$ random lin. sys.

Running Example – Model Hierarchy





Here $\alpha \approx 1$ (smooth functionals) and $\gamma \approx 2$ (with AMG)

Monte Carlo

- The **standard Monte Carlo** estimator for $\mathbb{E}[Q]$ is

$$\hat{Q}_L^{\mathrm{MC}} := \frac{1}{N}\sum_{i=1}^{N} Q_L^{(i)}, \quad Q_L^{(i)} \text{ i.i.d. samples with } \mathsf{Model}(L)$$

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- Convergence of plain vanilla MC **(mean square error)**:

$$\underbrace{\mathbb{E}\Big[\big(\hat{Q}_L^{\mathrm{MC}} - \mathbb{E}[Q]\big)^2\Big]}_{=:\,\mathrm{MSE}} = \underbrace{\frac{\mathbb{V}[Q_L]}{N}}_{\textbf{sampling error}} + \underbrace{\Big(\mathbb{E}[Q_L - Q]\Big)^2}_{\textbf{model error ("bias")}}$$

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- Recall $|\mathbb{E}[Q_\ell - Q]| = \mathcal{O}(2^{-\alpha\ell})$ and $\mathbb{E}\left[\mathrm{Cost}_\ell\right] = \mathcal{O}(2^{\gamma\ell})$.
- To get $\mathrm{MSE} = \mathcal{O}(\varepsilon^2)$, we need $L \sim \log_2(\varepsilon^{-1})\alpha^{-1}$ & $N \sim \varepsilon^{-2}$

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Complexity Theorem for (plain vanilla) Monte Carlo

$\mathrm{Cost}(\hat{Q}_L^{\mathrm{MC}}) = \mathcal{O}(NM_L) = \mathcal{O}\left(\varepsilon^{-2-\gamma/\alpha}\right)$ to obtain $\mathrm{MSE} = \mathcal{O}(\varepsilon^2)$.

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For **fruit fly**: $\mathrm{Cost}(\hat{Q}_L^{\mathrm{MC}}) \approx \mathcal{O}(\varepsilon^{-4})$ **Prohibitively expensive!**

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

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Multilevel Monte Carlo [Heinrich, '98], [Giles, '07]

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Complexity Theorem [Giles, '07], [Cliffe, Giles, RS, Teckentrup, '11]

Assume approximation error $\mathcal{O}(2^{-\alpha\ell})$, Cost/sample $\mathcal{O}(2^{\gamma\ell})$ **and**

$$\mathbb{V}[Q_\ell - Q_{\ell-1}] = \mathcal{O}(2^{-\beta\ell}) \qquad \text{(strong error/variance reduction)}$$

Then there exist L, $\{N_\ell\}_{\ell=0}^{L}$ to obtain $\text{MSE} = \mathcal{O}(\varepsilon^2)$ with

$$\text{Cost}(\widehat{Q}_L^{MLMC}) = \mathcal{O}\left(\varepsilon^{-2-\max\left(0,\frac{\gamma-\beta}{\alpha}\right)}\right) + \text{possible log-factor}$$

using **dependent** or **independent** estimators $\hat{Q}_0^{\text{MC}}$, and $\left(\hat{Y}_\ell^{\text{MC}}\right)_{\ell=1}^{L}$.

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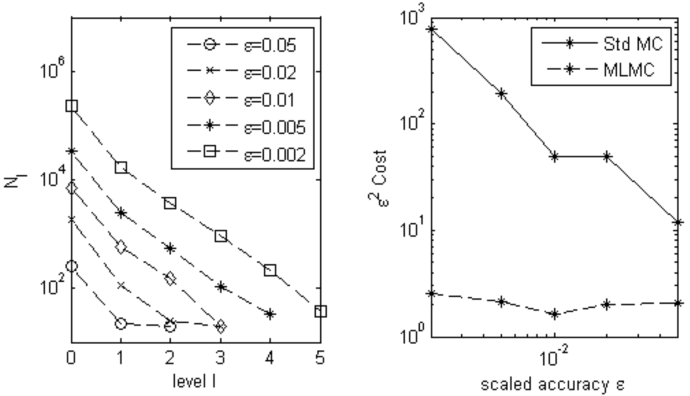
Optimality: Asymptotic cost of **one** deterministic solve (to tol$=\varepsilon$) **!**

Numerical Example (Multilevel MC)

Fruit fly with $Q = \|u\|_{L_2(D)}$ & circulant embedding with $s_\ell = \mathcal{O}(M_\ell)$



$$\sigma^2 = 1, \quad \lambda = 0.3, \quad h_0 = \frac{1}{8}$$

Observations, Extensions and Applications

- **Gains** even for small number of levels **(see below).**
- Substantial **practical gains** (not only asymptotic as $\varepsilon \to 0$)
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Strong (sample-wise) coupling is key: $\mathbb{V}[Q_\ell - Q_{\ell-1}] \ll \mathbb{V}[Q_\ell]$

Not always easy!!

Refs.: https://people.maths.ox.ac.uk/gilesm/mlmc_community.html

Not just theory & Not just for the Fruit Fly
(for simplicity consider only two levels)

Model 1		**Model 0**
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$$\textbf{Gain} \;=\; \frac{\mathrm{Cost}(\widehat{Q}_1^{\mathrm{MC}})}{\mathrm{Cost}(\widehat{Q}_1^{MLMC})} \;=\; \frac{1}{X + Y^2(1+X)}$$

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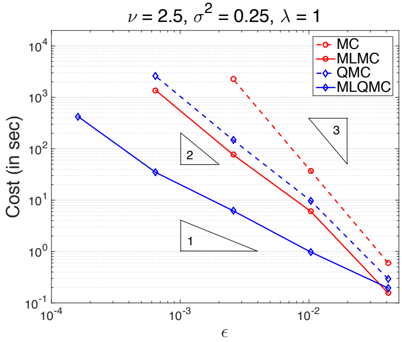
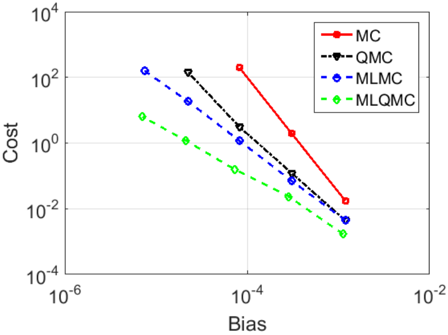
Examples / Gains	X	$Y = 0.5$	$Y = 0.1$	$Y = 0.05$
2D elliptic ($h_0 = 2h_1$)	1/4	1.8	3.8	4.0
3D elliptic ($h_0 = 2h_1$)	1/8	2.4	7.1	8.0
3D parab. ($h_0 = 2h_1$)	1/16	3.0	13.7	15.9
3D elliptic ($h_0 = 4h_1$)	1/64	3.7	38.8	62.4

Even higher gains with multiple levels!



Fruit fly (with Matern covariance)
[Kuo, RS, Schwab, Sloan, Ullmann, '17]



Neutron transport (Boltzmann)
[Graham, Parkinson, RS, '17(pre)]

Extension to Bayesian inference / Data assimilation

$$Z(\omega) \in X \xrightarrow{\text{Model}} u(\omega) \in V \xrightarrow{\text{Output}} Q(\omega) \in \mathbb{R}(\text{or } \mathbb{R}^J) \xrightarrow{\text{Statistics}} \mathbb{E}_\pi[Q]$$

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Similar gains possible! More difficult to achieve **both** consistency (collapsing sum) + variance reduction (strong coupling).

Multilevel Markov Chain Monte Carlo – Idea
Dodwell, Ketelsen, RS, Teckentrup, JUQ 2015

Posterior distribution (Bayes):

$$\pi^\ell(\mathbf{Z}_\ell|\mathbf{y}^{\rm obs}) \eqsim \exp(-\|\mathbf{y}^{\rm obs} - F_\ell(\mathbf{Z}_\ell)\|^2_{\Sigma_{\mathbf{obs}}})\,\pi_{\rm prior}(\mathbf{Z}_\ell)$$

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$$\widehat{Q}^{\mathbf{MLMetH}}_{h,s} := \frac{1}{N_0}\sum_{n=1}^{N_0} \mathcal{Q}_0(\mathbf{Z}^n_{0,0}) + \sum_{\ell=1}^{L} \frac{1}{N_\ell} \sum_{n=1}^{N_\ell} \left(\mathcal{Q}_\ell(\mathbf{Z}^n_{\ell,\ell}) - \mathcal{Q}_{\ell-1}(\mathbf{Z}^n_{\ell,\ell-1})\right)$$

chains strongly coupled!

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Fruit fly (i.e. 2D lognormal diffusion on $D = (0,1)^2$ with linear FEs)

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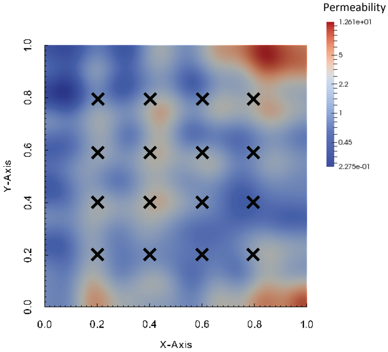
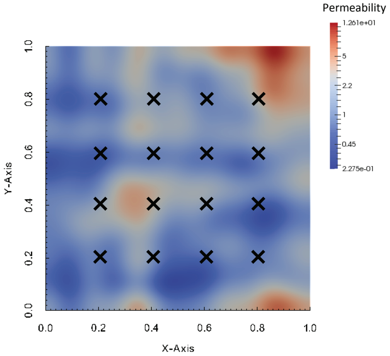
- **"Data"** $\mathbf{y}^{\text{obs}}$: Pressure at 16 points $x_j^* \in D$ and $\Sigma^{\text{obs}} = 10^{-4} I$.



Data

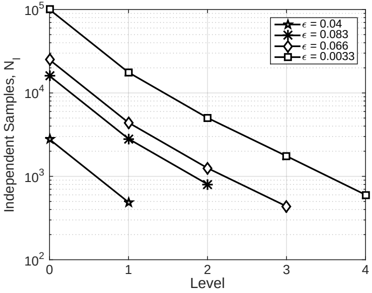


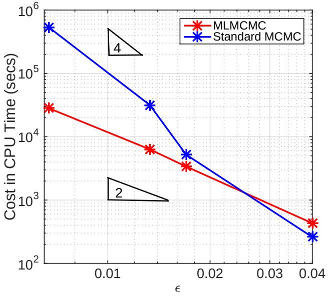
Posterior Sample

MLMCMC – Numerical Example

Fruit fly (i.e. 2D lognormal diffusion on $D = (0,1)^2$ with linear FEs)

- 5-level method w. #KL modes increasing from $s_0 = 50$ to $s_4 = 150$





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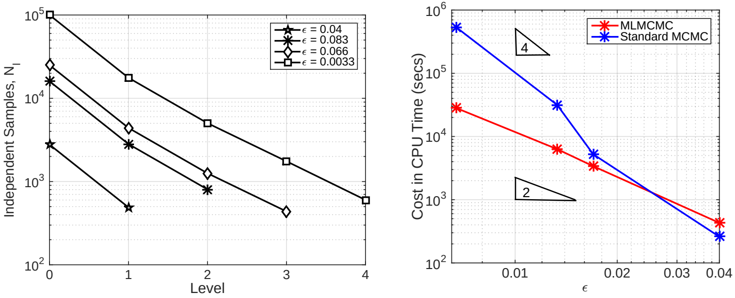

- #independent samples $= \dfrac{N_\ell}{t_\ell}$ (w. t_l … integrated autocorrelation time)

Level ℓ	0	1	2	3	4
a.c. time t_ℓ	136.23	3.66	2.93	1.46	1.23

Overall Summary

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- A vibrant research area with **many open questions**
- A **"no-brainer"** in practice (if you have a model hierarchy)
- Many **new application areas** await exploration
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