Seminar: Efficient Monte Carlo Methods for Uncertainty Quantification

Elisabeth Ullmann

Lehrstuhl für Numerische Mathematik (M2)

TU München

Prerequisites

Bachelor:

MA1304 Introduction to Numerical Linear Algebra

MA1401 Introduction to Probability Theory

Master:

MA3303 Numerical Methods for PDEs

Language: English

Supervison Team

- Prof. Dr. Elisabeth Ullmann

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Seminar setup

- Each participant prepares a **60 min** presentation (projector or blackboard, we recommend projector) followed by 30 min discussion and feedback
- **One consultation meeting** with your supervisor at least **2 weeks** before the presentation is required (more meetings possible upon request; recommended for Master's students)
- Attendance of **every** session and active participation in the discussion is expected
- **Before** the presentation: each participant submits executable computer code (in a suitable language, e.g. MATLAB) and a **handout** (2–4 pages) summarising the basic ideas and experiments performed

More information

- Schedule, Material, etc:

  `http://www-m2.ma.tum.de/bin/view/Allgemeines/UQSEM`

- Tips for preparing and delivering your presentation

- Simple slides for LaTeX

- Equipment for presentation (blackboard, projector, laptop)

What is Uncertainty Quantification?

Mathematical models and **computer simulations** are widely used in engineering and science applications.

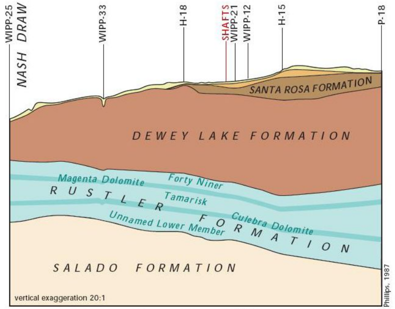
However, in many cases, the **parameters** in the model **are affected by uncertainty**, either because they are not perfectly known or because they are intrinsically variable.

Goal: Develop and analyse **efficient algorithms** to include and treat uncertainty in a mathematical model.

Uncertainty Propagation, **Uncertainty Quantification (UQ)**

Motivation: Groundwater flow

(e.g. risk analysis for radioactive waste disposal)



Cross-section at WIPP

Typical Quantities of Interest:

flux at repository,

effective conductivity,

particle position at time t_0,

travel time (to boundary), ...

Simple flow model – Elliptic PDE

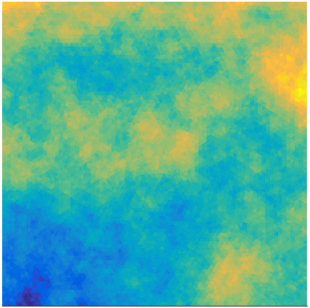
Steady-state fluid flow in a porous medium:

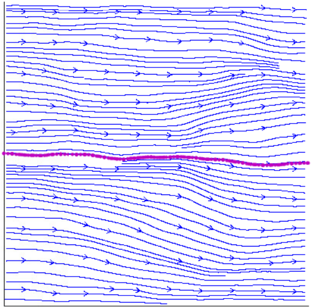
$$\begin{aligned} -\nabla \cdot (a \nabla u) &= f \qquad \text{in } D, \\ u &= 0 \qquad \text{on } \partial D. \end{aligned}$$

Solution variable: $u = u(\boldsymbol{x})$ (pressure)

$a = a(\boldsymbol{x})$	conductivity coefficient
$f = f(\boldsymbol{x})$	source or sink terms
$D \subset \mathbb{R}^d$	spatial/computational domain

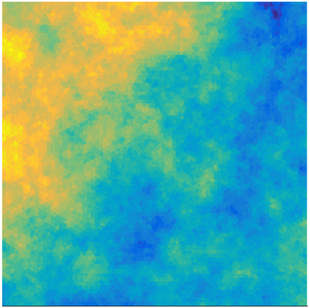
Uncertainty in conductivity

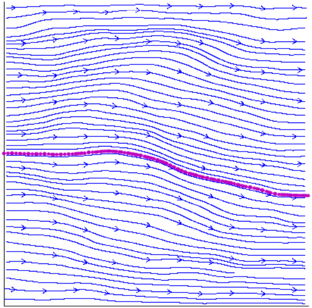




Uncertainty Propagation, **Uncertainty Quantification (UQ)**

Uncertainty in conductivity





Uncertainty Propagation, **Uncertainty Quantification (UQ)**

Goal: Compute Solution Statistics

(e.g. expected value or probability of an event)

Quantities of Interest: $Q = Q(\omega) = \mathscr{F}(u(\omega))$

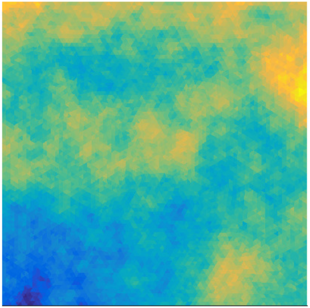
Physical discretisation: Q_h on FE grid $\mathscr{T}_h$

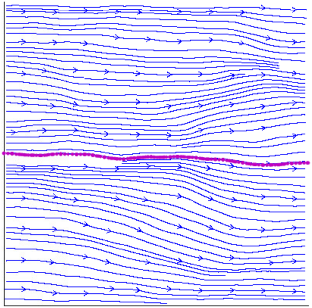
Monte Carlo Estimator for $\mathbb{E}[Q]$

$$\mathbb{E}[Q] \approx \widehat{Q}_h^{MC} := \frac{1}{N_h} \sum_{i=1}^{N_h} Q_h(\omega_i)$$

Sampling is expensive!

Sampling = Solve a discretised PDE





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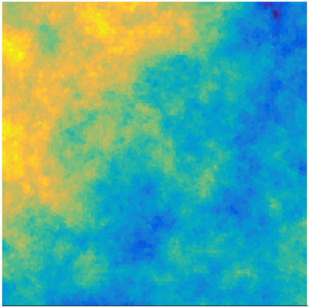

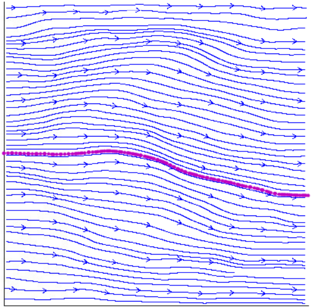

Topics

Combine well-known techniques from **Statistics** with PDE discretisations

- Variance reduction
- Reduced bases
- Bayesian inversion, Markov chains
- Failure probabilities/rare events

All these techniques are useful also in other applications (no PDEs required).

(B1) Simple Monte Carlo

Content:

- History of Monte Carlo (MC)
- Recap of basic probability theory, in particular: Law of Large Numbers, Central Limit Theorem
- Accuracy of MC (confidence intervals)
- Estimating probabilities, quantiles
- Failure of MC

Programming:

- MC quadrature (e.g. Buffon's needle)
- MC simulation (e.g. Traffic flow)

Literature: Owen Ch. 1–2, Dunn & Shultis Ch. 1–2

(B2) Random Number Generators (RNGs)

Content:

- Linear, Multiplicative congruential generators
- Tests, Characteristics of RNGs (seed, period, subsample)
- Practical Multiplicative congruential generators
- Skipping ahead, combining generators
- Optional: non-uniform generators (inverse CDF, acceptance-rejection)

Programming:

- Example 3.1 and Problem 7 in Dunn & Shultis Ch. 3

Literature: Dunn & Shultis Ch. 3, Owen Ch. 3

(B3) Variance Reduction

Content:

- Importance Sampling
- Systematic, Stratified Sampling
- Correlated Sampling, Antithetic Variates
- Control Variates
- Conditioning

Programming:

- Buffon's needle with Importance Sampling, Correlated Sampling, Antithetic Variates

Literature: Dunn & Shultis Ch. 5

(M1) Multilevel Monte Carlo (MLMC)

Topic 1:

- Basic idea of MLMC
- Programming: 1D Elliptic PDE
- Literature: Cliffe et al. (research paper)

Topic 2:

- Sampling by Circulant Embedding, MLMC with Coarse Grid Variates
- Programming: 2D random field and Elliptic PDE (finite differences)
- Literature: Lord/Powell/Shardlow §6.5, §7.2 (book), Park & Teckentrup (research paper)

(M2) Reduced bases and MLMC

Topic 1:

- Basic idea of reduced bases, variance reduction for MC
- Programming: RBmatlab, 1D Elliptic PDE
- Literature: Boyaval et al. (research paper)

Topic 2:

- Combine reduced bases and MLMC
- Programming: RBmatlab, 1D Elliptic PDE
- Literature: Vidal-Codina et al. (research paper)

(M3) Bayesian Inverse Problems

Topic 1:

- Bayesian Statistics, Markov chain Monte Carlo (MCMC)
- Programming: 1D linear regression, Gaussian mixture model (time permitting)

Topic 2:

- Bayesian Inverse Problems, MCMC
- Programming: 1D Elliptic PDE

Literature: Allmaras et al. (review paper), book chapters (Liu: MC Strategies in Scientific Computing, Robert: The Bayesian Choice)

(M4) Failure Probabilities

Topic 1:

- MLMC with Selective Refinement
- Programming: Normal distribution, 1D Elliptic PDE (time permitting)
- Literature: Elfverson et al. (research paper)

Topic 2:

- Subset simulation
- Programming: synthetic limit state function, 1D Elliptic PDE (time permitting)
- Literature: Au & Beck, Papaioannou et al. (research papers)

Supervision

Supervisor	**Topic**
Ullmann	Simple Monte Carlo
Ullmann	Random Number Generators
Ullmann	Variance Reduction
Parente/Ullmann	Multilevel Monte Carlo
Scarabosio	Reduced Bases
Latz	Bayesian Inverse Problems
Ullmann	Failure Probabilities

Tentative schedule

Date	Topic
01 June 2017	Simple Monte Carlo (1×)
08 June 2017	Random Number Generators (1×)
14 June 2017	Variance Reduction (1×)
29 June 2017	Multilevel Monte Carlo (2×)
06 July 2017	Reduced Bases (1×)
13 July 2017	Bayesian Inverse Problems (2×)
27 July 2017	Failure Probabilities (2×)

References

W.L. Dunn, J.K. Shultis: *Exploring Monte Carlo Methods*, Academic Press, 2011.

Art Owen: *Monte Carlo theory, methods and examples*.
http://statweb.stanford.edu/∼owen/mc/