Computational Methods in Uncertainty Quantification

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HGS MathComp Compact Course
IWR, Universität Heidelberg, June 11-17 2015

PART 1

Course Structure

- This compact course will consist of five 90 minute lectures and three exercise classes (see below for a schedule).
- There will also be two related talks on Monday and Tuesday.
- Due to the large class size we changed to bigger rooms whenever this was possible (room number in brackets below).
- I will start C.T., i.e. at 9.15 and 14:15.

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	9:15-10:45	11:00-12:00	14:15-16:00
Thu 11	Lecture (520)	Office Hour (424)	–
Fri 12	Lecture (532)	Office Hour (424)	Exercise Class (532)
Mon 15	Lecture (532)	Exercise Class (532)	*Heinkenschloss* (432)
Tue 16	Lecture (520)	Office Hour (424)	*Wellmann* (432)
Wed 17	Lecture (432)	Office Hour (424)	Exercise Class (432)

Please bring a laptop to the exercise classes (with Matlab or Octave on it).

Acknowledgements and Resources

Large parts of this course are based on a course at the **TU Chemnitz** "Mathematische Methoden der Unsicherheitsquantifizierung" by Prof. Oliver Ernst `www.tu-chemnitz.de/mathematik/numa/lehre/uq-2014`

The latter parts of the course are based on my research papers that are available at `people.bath.ac.uk/masrs/publications.html`

See also M. Giles' very useful webpage `people.maths.ox.ac.uk/gilesm/`

Other useful resources are:

- G. Lord, C. Powell and T. Shardlow. *An Introduction to Computational Stochastic PDEs.* Cambridge University Press, 2014.
- R. C. Smith. *Uncertainty Quantification: Theory, Implementation and Applications.* Computational Science and Engineering. SIAM, 2014.
- M. B. Giles. Multilevel Monte Carlo methods, *Acta Numerica*, 2016.
- D. Xiu. *Numerical Methods for Stochastic Computations: A Spectral Method Approach.* Princeton University Press, Princeton, NJ, 2010.

Part 1 – What are the Challenges in UQ?

- What is uncertainty quantification (UQ) about?

- What is uncertainty?
- How can uncertainty be described?
- How can the effects of uncertainty be treated and quantified?
- A case study – radioactive waste disposal.
- Methods for solving the resulting mathematical problems.
- What are the challenges?

What is Uncertainty Quantification (UQ)?

What is 'uncertain'?

uncertain: *not able to be relied on; not known or definite.*

Oxford Collegiate Dictionary

uncertain: *not exactly known or decided; not definite or fixed; not known beyond doubt; not constant*

Merriam Webster Online Dictionary

uncertain: *not able to be accurately known or predicted; not precisely determined, established, or decided; liable to variation; changeable*

Collins Online Dictionary

What is Uncertainty Quantification (UQ)?

A poetic description

There are known knowns;
there are things we know we know.

We also know there are known unknowns;
that is to say, we know there are some things we do not know.

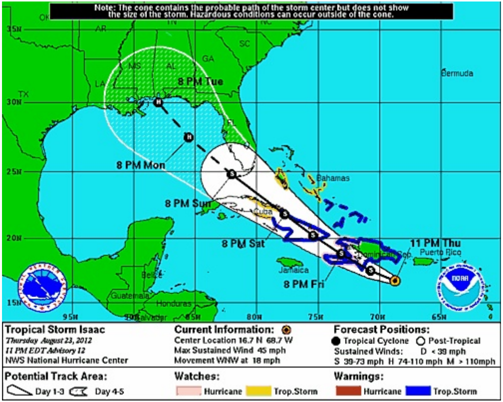
But there are also unknown unknowns the ones we dont know we dont know. *U. S. Secretary of Defence, Donald Rumsfeld*
DoD News Briefing; Feb. 12, 2002

Many aspects of modern life involve uncertainty:

- **Social systems:** military, finance, insurance industry, elections
- **Environmental systems:** weather, climate, seismic, subsurface geophysics
- **Engineering systems:** automobiles, aircraft, bridges, structures
- **Biological systems:** health and medicine, pharmaceuticals, gene expression, cancer research
- **Physical systems:** quantum physics, radioactive decay

What is Uncertainty Quantification (UQ)?

Uncertainty in Modern Life

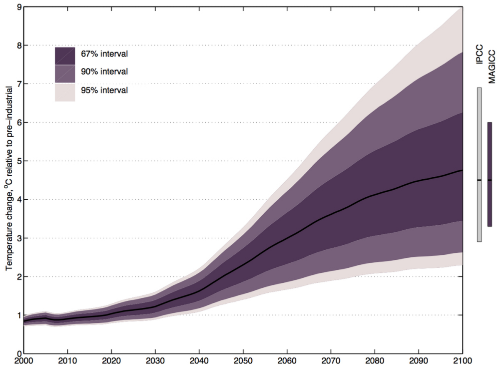


Source: National Hurricane Center, USA

Predicted storm path with uncertainty cones.

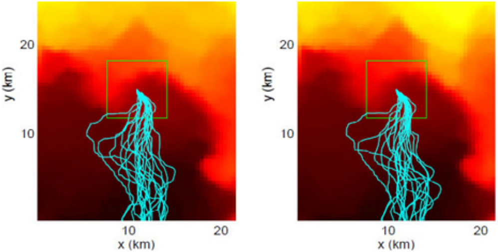
What is Uncertainty Quantification (UQ)?

Uncertainty in Modern Life



Source: Brodman & Karoly, 2013

Global-mean temperature change for a business-as-usual emission scenario, relative to pre-industrial. Black line: median, shaded regions 67% (dark), 90% (medium) and 95% (light) confidence intervals.



Source: K. A. Cliffe, 2012

Sample paths of groundwater-borne contaminant particles emanating from an underground radioactive waste disposal site.

What is Uncertainty Quantification (UQ)?

Examples

Radioactive decay

- Radium-226: half-life of 1602 years
- Decays into Radon gas (Radon-222) by emitting alpha particles.
- Over a period of 1602 years, half the radium atoms in a given sample will decay.
- But we cannot say which half!

This kind of uncertainty seems to be 'built in' to the physical world.

What is Uncertainty Quantification (UQ)?

Examples

Rolling dice

- Cube, 6 faces, numbered 1–6
- One or more thrown onto a table.
- For "fair dice", expect to see the numbers 1–6 appear equally often, provided the dice are thrown sufficiently many times.

How does this differ from radioactive decay?

Is this uncertainty also built in to the physical world, or are we just not able to calculate what will happen when the dice are thrown?

What is Uncertainty Quantification (UQ)?

Examples

Screening/testing for disease

- Incidence of disease among general population: 0.01 %
- Test has true positive rate (*sensitivity*) of 99.9 %.
- Same test has true negative rate (*specificity*) of 99.99 %.
- What is the chance that someone who tests positive actually has the disease?

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Answer (using relative/conditional probabilities, Bayes' formula):

$$\mathbf{P}(\text{diseas}|\text{pos}) = \frac{\mathbf{P}(\text{pos}|\text{diseas}) \cdot \mathbf{P}(\text{diseas})}{\mathbf{P}(\text{pos}|\text{diseas}) \cdot \mathbf{P}(\text{diseas}) + \mathbf{P}(\text{pos}|\text{no diseas}) \cdot \mathbf{P}(\text{no diseas})}$$

$$= \frac{0.999 \cdot 0.0001}{0.999 \cdot 0.0001 + (1 - 0.9999) \cdot (1 - 0.0001)} \approx 0.4998$$

What is Uncertainty Quantification (UQ)?

Examples

Alternative answer (using natural frequencies):

- Think of random sample 10,000 people.
- Of these, on average 1 will have the disease, 9,999 will not.
- Person who has the disease will almost certainly test positive.
- on average 1 of the 9,999 healthy people will test (falsely) pos.
- Thus, (roughly) only one out of every two positive patients actually has the disease.

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In [GIGERENZER, 1996] medical practitioners were given the following information regarding mammography screenings for breast cancer:

incidence: 1 %; sensitivity: 80 %; specificity: 90 %.

When asked to quantify probability of a patient actually having breast cancer given a positive screening result (7.5%), 95 out of 100 physicians estimated this probability to lie above 75%.

What is Uncertainty Quantification (UQ)?

Examples

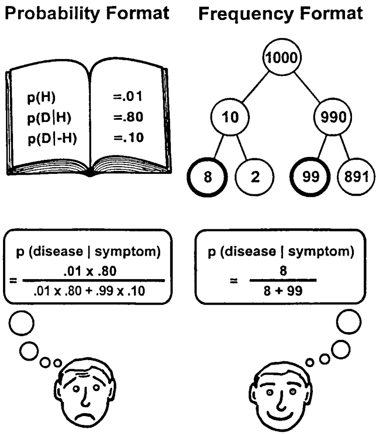


FIGURE 1. Bayesian computations are simpler when information is represented in a frequency format (right) than when it is represented in a probability format (left). p(H) = prior probability of hypothesis. H (breast cancer), p(D|H) = probability of data D (positive test) given H, and p(D|−H) = probability of D given −H (no breast cancer).

We see how crucial it is for its transparent communication how uncertainty is described.

Source: Gigerenzer, 1996

What is Uncertainty Quantification (UQ)?
Examples

Modeling biological systems

- From one view, biology is just very complicated physics and chemistry.
- But even the simplest biological systems are far too complicated to be understood from basic principles at the moment.
- Models are constructed that attempt to capture the essential features of what is happening, but often there are competing models and they may all fail in some way or other to predict the observed phenomena.
- In short, we dont really know what the model is!

How does this situation differ from the previous two?

What is Uncertainty Quantification (UQ)?

Examples

Climate change

The weight of evidence makes it clear that climate change is a real and present danger. The Exeter conference was told that whatever policies are adopted from this point on, the Earths temperature will rise by 0.6F within the next 30 years. Yet those who think climate change just means Indian summers in Manchester should be told that the chances of the Gulf stream - the Atlantic thermohaline circulation that keeps Britain warm - shutting down are now thought to be greater than 50%.

The Guardian, 2005

Most of the observed increase in globally-averaged temperatures since the mid-20th century is very likely due to the observed increase in anthropogenic GHG concentrations. It is likely there has been significant anthropogenic warming over the past 50 years averaged over each continent (except Antarctica).

IPCC Fourth Assessment Summary for Policymakers.

What is Uncertainty Quantification (UQ)?

Examples

Unknown unknowns

- Obviously can't give a current example.
- Good example is the state of Physics at end of 19th century.

  There is nothing new to be discovered in physics now. All that remains is more and more precise measurement.

  Lord Kelvin, 1900

- Quantum mechanics and relativity theory were unknown unknowns.

It is easy to underestimate uncertainty.

What is Uncertainty Quantification (UQ)?

Political Implications

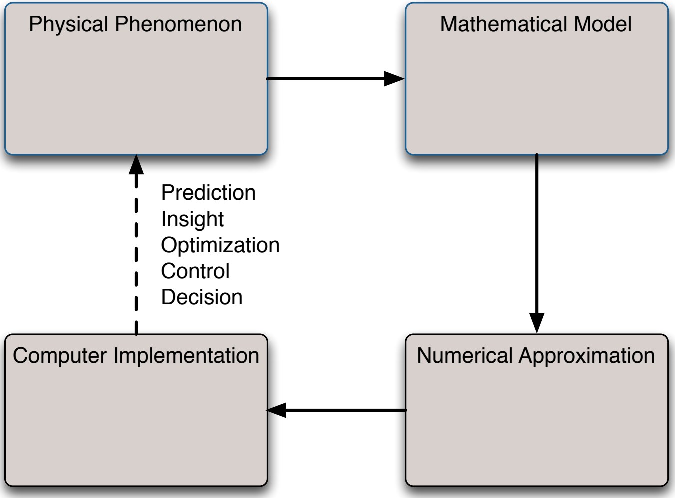
Questions:[1]

1. How do we account for all the uncertainties in the complex models and analyses that inform decision makers?
2. How can those uncertainties be communicated simply but quantitatively to decision makers?
3. How should decision makers use those uncertainties when combining scientific evidence with more socio-economic considerations?
4. How can decisions be communicated so that the proper acknowledgment of uncertainty is transparent?

[1] posed on entry at the 2006 UK EPSRC Ideas Factory on the topic *Scientific Uncertainty and Decision Making for Regulatory and Risk Assessment Purposes*.

What is Uncertainty Quantification (UQ)?

UQ and the scientific computing paradigm



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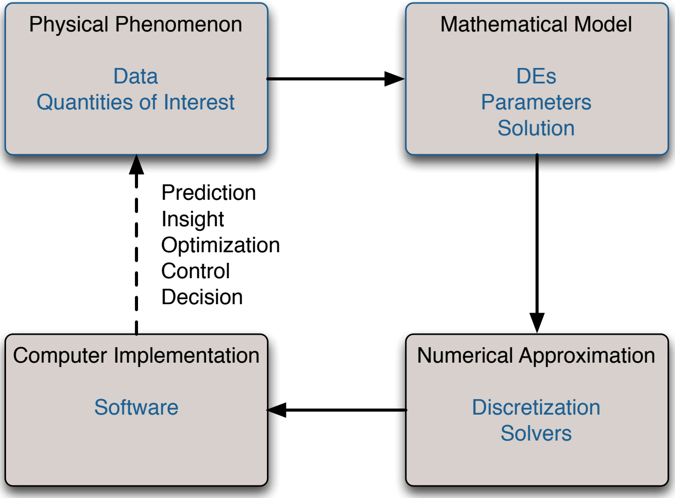
UQ and the scientific computing paradigm



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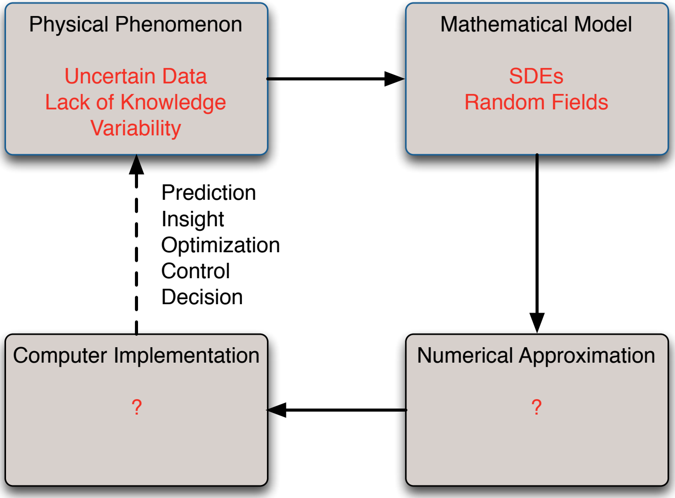

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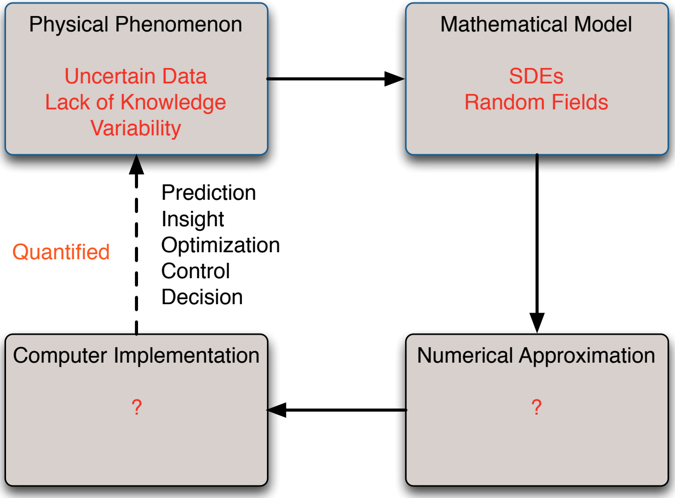

What is Uncertainty Quantification (UQ)?

Validation and Verification (V & V)

What confidence can be assigned to a computer prediction of complex phenomena?

Validation: Determination of whether a mathematical model adequately represents physical/engineering phenomenon under study.

"Are we solving the right problem?"

Is this even possible? (cf. Carl Popper)

Verification: Determination of whether an algorithm and/or computer code correctly implements given mathematical model.

"Are we solving the problem correctly?"

- code verification (software engineering)
- solution verification (a posteriori error estimation)

What is Uncertainty Quantification (UQ)?

Aleatoric and Epistemic Uncertainty

Aleatoric Uncertainty: Uncertainty due to true intrinsic variability; cannot be reduced by additional experimentation, improvement of measuring devices, better model, etc.

Examples:

- rolling a die
- wind stress on a structure
- production variations

Epistemic Uncertainty: Uncertainty due to lack of knowledge or incomplete information.

Examples:

- turbulence modeling assumptions
- surrogate chemical kinetics
- probability distribution of a random quantity

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Note: This distinction is not always meaningful or even possible.

What is Uncertainty Quantification (UQ)?
The “Fruit Fly” of UQ

The most popular **model problem** in the UQ community is the steady-state diffusion problem with uncertain coefficient function:

$$-\nabla\cdot(a\nabla u) = f \qquad \text{on domain} \quad D \subset \mathbb{R}^d.$$

(an elliptic partial differential equation)

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$$-\nabla\cdot(a\nabla u) = f \qquad \text{on domain} \quad D \subset \mathbb{R}^d.$$

(an elliptic partial differential equation)

Typically, rather than the PDE solution u (pressure, temperature, concentration, ...) we are interested in a functional Q of the solution. Such a functional is known as a quantity of interest (QoI).

Examples:

$$Q(u) = u(\mathbf{x}_0), \qquad Q(u) = \frac{1}{|D_0|}\int_{D_0} u(\mathbf{x})\,\mathrm{d}\mathbf{x}.$$

In what way might uncertainty in the coefficient a be addressed?

What is Uncertainty Quantification (UQ)?
Worst case analysis

Introduce an ϵ-ball around a given function a_0 (in a suitable norm).

Examples:

$$S := \begin{cases} \{a \in C^0(D) : \|a - a_0\|_\infty \le \epsilon\}, \\ \{a \in C^1(D) : \|\nabla(a - a_0)\|_\infty \le \epsilon\}, \\ \{a \; constantin \; D : |a - a_0| \le \epsilon\}. \end{cases}$$

Worst case analysis: determine uncertainty interval

$$I = [\inf_{a \in S} Q(u(a)), \sup_{a \in S} Q(u(a))].$$

The uncertainty range of Q is then the length of I.

This is a generalisation of interval analysis.

What is Uncertainty Quantification (UQ)?

Probabilistic model

But: In general, some coefficients $a \in S$ are more likely than others.

Probabilistic approach:

- Introduce probability measure on S.
- $Q(u(\cdot))$ as a (measurable) mapping from S to the output set $\{Q(u(a)) : a \in S\}$ induces a probability measure for the QoI. ("uncertainty propagation")
- **Big issue:** choice of distribution, too much subjective information?
- Some classical guidelines: Laplace's principle of insufficient reason, maximum entropy, etc.
- Choosing distribution based on data is point of departure for Bayesian inference (genuine "uncertainty quantification").

What is Uncertainty Quantification (UQ)?

Other models

- Evidence theory (generalisation of probabilistic model)
- Fuzzy sets (deterministic approach introduced by [Zadeh, 1965])
- Possibility theory
- Scenario analysis
- ...

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- ...

For the remainder we will focus on the probabilistic approach.

Stochastic Modelling

Many reasons for stochastic modelling (not all strictly UQ):

- **lack of data** (e.g. data assimilation for weather prediction)
- **data uncertainty** (e.g. uncertainty quantification in subsurface flow)
- **parameter identification** (e.g. Bayesian inference in engineering)
- **unresolvable scales** (e.g. atmospheric dispersion modelling)
- **high dimensionality** (e.g. stochastic simulation in systems biology)

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Input: best knowledge about system (PDE), statistics of input parameters, measured ouput data with error statistics,...

Output: statistics of QoIs or of entire state space

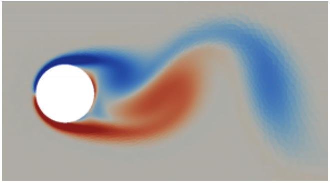
often very sparse (or no) output data $\rightarrow$ need a good physical model!

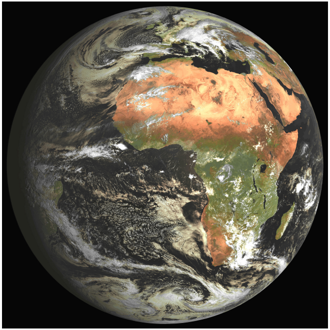
- Data assimilation in NWP: data misfit, rainfall at some location
- Radioactive waste disposal: flow at repository, 'breakthrough' time
- Oil reservoir simulation: production rate
- Atmospheric dispersion: amount of ash over Heathrow
- Aeronautical engineering: certification of carbon fibre composite wing

- **Navier–Stokes** (e.g. flow around wing, weather forecasting):

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla p + \mu\nabla^2\mathbf{v} + f \quad \text{in} \quad \Omega$$

$$\text{subject to IC} \quad v(x,0) = v_0(x) \quad + \quad \text{BCs}$$





Stochastic Modelling

Examples – PDEs with random coefficients

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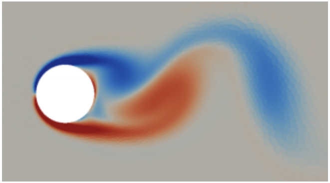

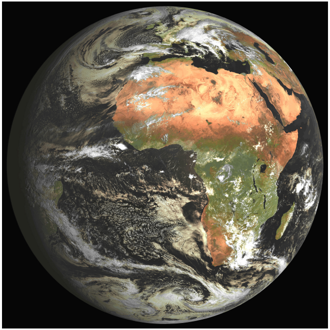

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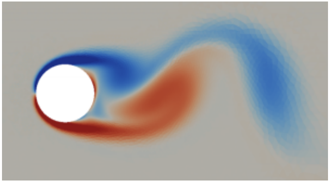
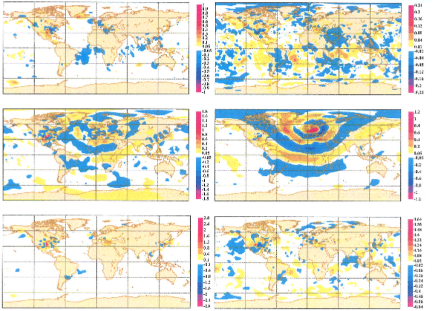




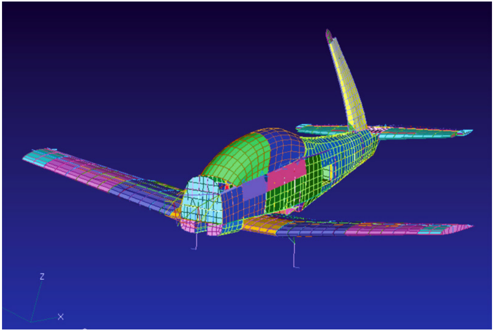
Stochastic Modelling

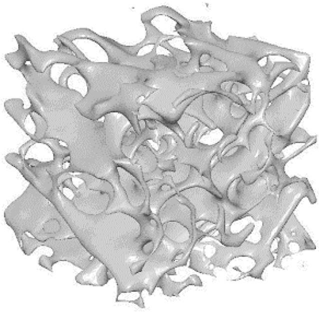
Examples – PDEs with random coefficients

- **Structural Mechanics** (e.g. composites, tires or bone):

$$\nabla \cdot \left(\overline{\overline{C}} : \frac{1}{2} \left[\nabla \mathbf{u} + \nabla \mathbf{u}^T \right] \right) + \mathbf{F} \;=\; 0 \quad \text{in} \quad \Omega$$

subject to BCs





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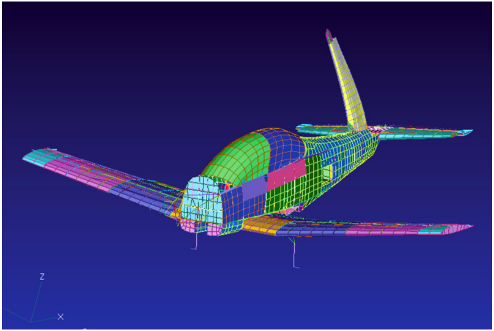

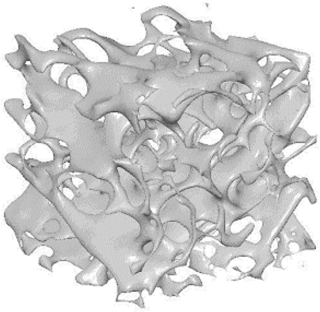

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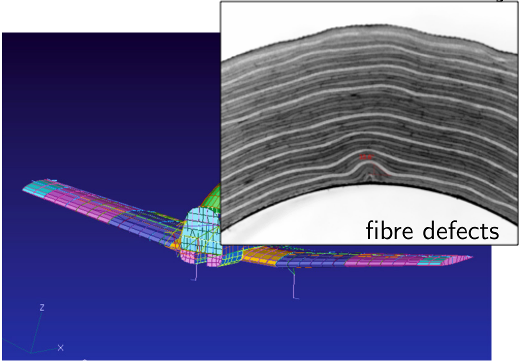
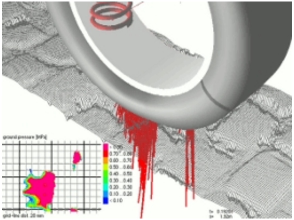


fibre defects

contact on rough surface



Stochastic Modelling

Examples – PDEs with random coefficients

- **Neutron Transport**:

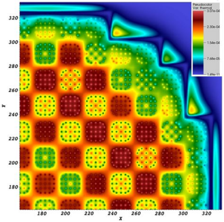
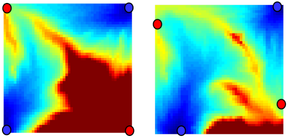


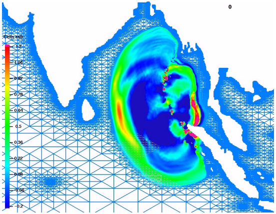
Figure 1 2D Slice of Thermal Flux Distribution near the Core Mid-plane

- **Oil Reservoir Simulation**:



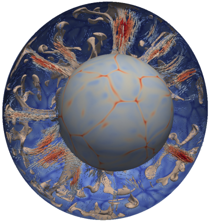
optimal well placement

- **Tsunami Simulation**:



[Behrens et al]

- **Mantel Convection**:



[Gmeiner et al]

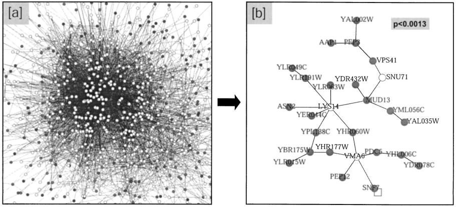
Atmospheric Dispersion (e.g. volcanic ash, radionuclides, ...)

Given large-scale atmospheric flow $\vec{v}(\vec{x},t)$, model turbulent dispersion of particles by a system of SDEs:

$$d\vec{U} = a(\vec{U},\vec{X},t)dt + b(\vec{X},t)d\vec{W}(t)$$
$$d\vec{X} = \big(\vec{v}(\vec{X},t) + \vec{U}(\vec{X},t)\big)dt$$

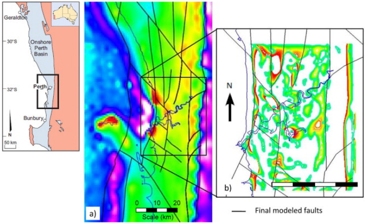
$\vec{U}(t)\ldots$ turbulent correction; $\vec{X}(t)\ldots$ particle position; $\vec{W}(t)\ldots$ Brownian motion

Gene Regulatory Networks
(direct stochastic simulation)



Source: Shannon et al, 2003

Geostatistics
(and other imaging applications)

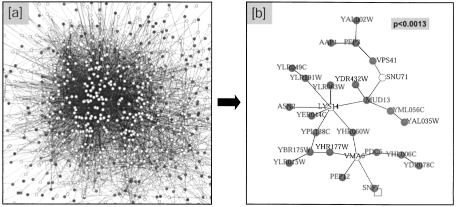


Source: Corbel, Wellmann, 2015

Stochastic Modelling

Examples – Stochastic Reaction Networks and Imaging

Gene Regulatory Networks
(direct stochastic simulation)



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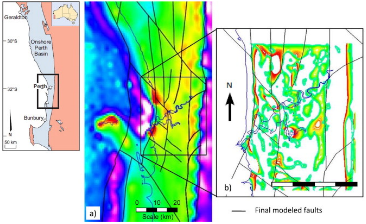
More on Monday!

Geostatistics
(and other imaging applications)



Source: Corbel, Wellmann, 2015

Talk by Florian Wellmann, Tuesday

A Case Study: Radioactive Waste Disposal

- An area where UQ has played a central role in the past 25 years is the assessment of strategies and sites for the long-term storage of radioactive waste.
- Uncertainties arise from technological complexity as well as the long time scales to be considered.
- Many leading industrial countries (USA, UK, Germany) have scrapped previous plans for national long-term disposal sites and are re-evaluating their strategies.
- Consider a basic UQ problem which occurs in site assessment.

A Case Study: Radioactive Waste Disposal

Background

- Radioactive waste is produced mainly by nuclear power plants (Other sources: medical, weapons, non-nuclear industries)
- Exposure to high radiation levels seriously harmful to humans and animals; long-term exposure to low-level radiation can cause cancer and other long-term health problems.
- Classification of waste "level":
  - *high (HLW)*: highly radioactive, produces heat, small amount
  - *intermediate (ILW)*: still very radioactive, no heat produced
  - *low (LLW)*: low radioactivity; packaging material, protective clothing, soil, concrete that has been exposed to radioactivity
- Quantities in storage (excl. LLW; source: `http://newmdb.iaea.org`)
  - Germany: 120,000 m^3 (2007)
  - France: 90,000 m^3 (2007)
  - UK: 350,000 m^3 (2007)
  - USA: 540,000 m^3 (2008)

A Case Study: Radioactive Waste Disposal

Management Options

Since this problem has received serious consideration ($\approx$ 1970s), several options have been discussed

- Surface storage: current universal solution, not long-term, risky.
- Disposal at sea: banned by international treaty (London Convention)
- Disposal in space: too dangerous, prohibitive cost (but permanent)
- Transmutation: not yet proven, would mitigate but not solve problem
- Deep geological disposal: favoured by nearly all countries with a radioactive waste disposal programme

A Case Study: Radioactive Waste Disposal

Deep Geological Disposal

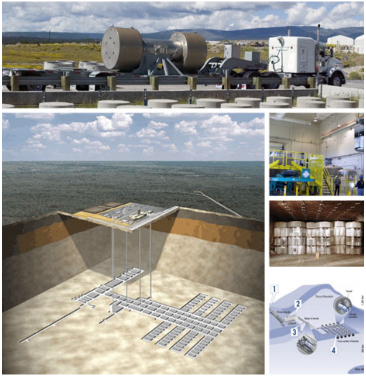
- Storage in containers in tunnels, several hundred meters deep, in stable geological formations.
- Issue: retrievable or not?
- No human intervention required after final closure of repository.
- Several barriers: chemical, physical, geological.
- Substantial engineering challenge (containment must be assured for at least 10,000 years).
- Main escape route for radionuclides: groundwater pathway.
- **Assessing safety** of potential sites of utmost importance
  long timescales $\rightarrow$ **modelling essential!**

- **Key aspect:** How to quantify uncertainties in the models?

A Case Study: Radioactive Waste Disposal

WIPP – Waste Isolation Pilot Plant

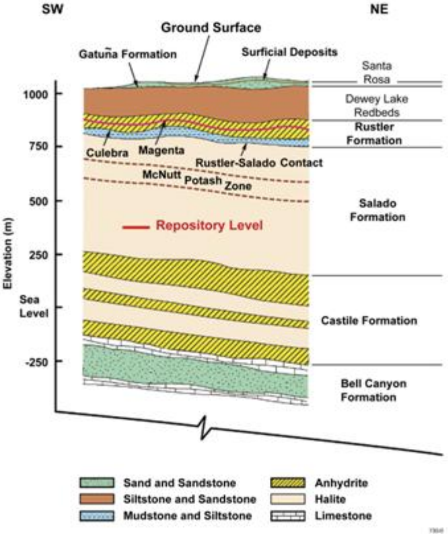
- US DOE repository for radioactive waste situated near Carlsbad, NM.
- Fully operational since 1999.
- Extensive site characterisation and performance assessment since 1976, also in course of compliance certification and recertification by US EPA (every 5 years).
- Lots of publicly available data.
- `http://www.wipp.energy.gov`



A Case Study: Radioactive Waste Disposal

WIPP Geology

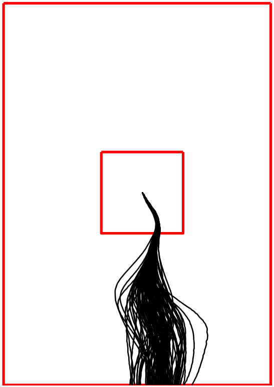
- Repository located at 655m depth in bedded evaporites (primarily halite, a salt).
- Most transmissive rock layer in the region is the Culebra Dolomite.
- In the event of an accidental breach, Culebra would be the principal pathway for transport of radionuclides away from the repository.



A Case Study: Radioactive Waste Disposal

WIPP UQ Scenario

- One scenario at WIPP is a release of radionuclides by means of a borehole drilled into the repository.
- Radionuclides are released into the Culebra Dolomite and then transported by groundwater.
- Travel time from release point in the repository to the boundary of the region is an important quantity.
- To a good approximation the flow is two-dimensional.



A Case Study: Radioactive Waste Disposal

Groundwater Flow Model – Darcy's Law

Stationary Darcy flow	$\mathbf{q} = -K\nabla p$	$\mathbf{q}$: Darcy flux
		K : hydraulic conductivity
		p : hydraulic head
mass conservation	$\nabla \cdot \mathbf{u} = 0$	$\mathbf{u}$: pore velocity
	$\mathbf{q} = \phi \mathbf{u}$	ϕ : porosity
transmissivity	$k = Kb$	b : aquifer thickness
particle transport	$\dot{\mathbf{x}}(t) = -\dfrac{k(\mathbf{x})}{b\phi}\nabla p(\mathbf{x})$	$\mathbf{x}$: particle position
	$\mathbf{x}(0) = \mathbf{x}_0$	$\mathbf{x}_0$: release location

Quantity of interest: $\log_{10}$ of particle travel time to reach boundary

A Case Study: Radioactive Waste Disposal

UQ Problem – PDE with Random Coefficient

Primal form of Darcy equations (our "fruit fly"):

$$-\nabla\cdot[k(\mathbf{x})\nabla p(\mathbf{x})] = 0, \quad \mathbf{x} \in D, \qquad p = p_0 \text{ along } \partial D.$$

Model k as a random field (RF) $k = k(\mathbf{x}, \omega)$, $\omega \in \Omega$, with respect to underlying probability space $(\Omega, \mathscr{A}, \mathbf{P})$.

Modeling Assumptions (standard in 2D hydrogeology):

- T has finite mean and covariance

$$\begin{aligned}\overline{k}(\mathbf{x}) &= \mathbf{E}\left[k(\mathbf{x},\cdot)\right], & \mathbf{x} \in D,\\ \mathbf{Cov}_k(\mathbf{x},\mathbf{y}) &= \mathbf{E}\left[\left(k(\mathbf{x},\cdot) - \overline{k}(\mathbf{x})\right)\left(k(\mathbf{y},\cdot) - \overline{k}(\mathbf{y})\right)\right], & \mathbf{x},\mathbf{y} \in D.\end{aligned}$$

- k is lognormal, i.e., $Z(\mathbf{x},\omega) := \log k(\mathbf{x},\omega)$ is a Gaussian RF.
- $\mathbf{Cov}_Z$ is stationary and isotropic, i.e., $\mathbf{Cov}_Z(\mathbf{x},\mathbf{y}) = c(\|\mathbf{x}-\mathbf{y}\|_2)$

A Case Study: Radioactive Waste Disposal

Matérn Family of Covariance Kernels

$$c(\mathbf{x},\mathbf{y}) = c_{\boldsymbol{\theta}}(r) = \frac{\sigma^2}{2^{\nu-1}\,\Gamma(\nu)} \left(\frac{2\sqrt{\nu}\,r}{\lambda}\right)^{\nu} K_{\nu}\left(\frac{2\sqrt{\nu}\,r}{\lambda}\right), \quad r = \|\mathbf{x}-\mathbf{y}\|_2$$

K_ν : modified Bessel function of order ν

Parameters $\boldsymbol{\theta} = (\sigma^2, \lambda, \nu)$

σ^2 : variance

λ : correlation length

ν : smoothness parameter

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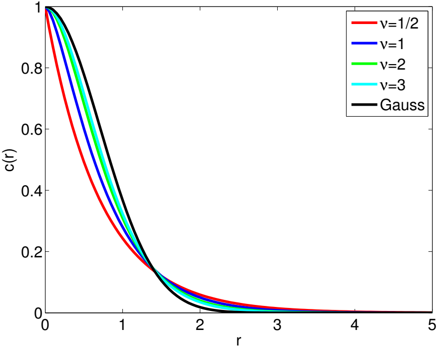
Special cases:

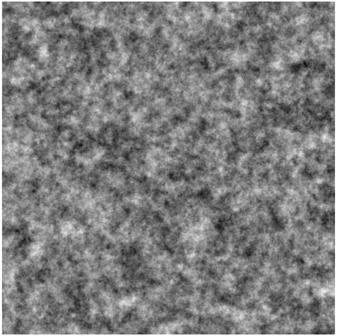
$\nu = \frac{1}{2}$:	$c(r) = \sigma^2 \exp(-\sqrt{2}r/\lambda)$	exponential covariance
$\nu = 1$:	$c(r) = \sigma^2 \left(\frac{2r}{\lambda}\right) K_1 \left(\frac{2r}{\lambda}\right)$	Bessel covariance
$\nu \to \infty$:	$c(r) = \sigma^2 \exp(-r^2/\lambda^2)$	Gaussian covariance

A Case Study: Radioactive Waste Disposal

Matérn Covariance Functions



$\sigma^2 = 1,\ \lambda = 1$



$\sigma^2 = 8,\ \lambda = 1/64,\ \nu = 1/2$

Smoothness: Realisations $Z(\cdot, \omega) \in C^\eta(D)$ (Hölder), for any $\eta < \nu$.

Since $c(\mathbf{x}, \mathbf{y})$ is symmetric, positive semidefinite, continuous, the covariance operator

$$C : L^2(D) \to L^2(D), \qquad (Cu)(\mathbf{x}) = \int_D u(\mathbf{y}) c(\mathbf{x}, \mathbf{y}) \, \mathrm{d}\mathbf{y}$$

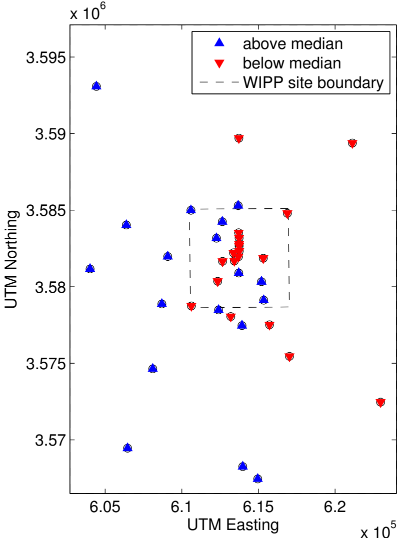
is selfadjoint, compact, nonnegative. Hence, its eigenvalues $\{\mu_m\}_{m \in \mathbb{N}}$ form a non-increasing sequence accumulating at most at 0.

Karhunen-Loève expansion (converges in $L^2_{\mathbb{P}}(\Omega; L^\infty(D))$):

$$Z(x, \omega) = \overline{Z}(\mathbf{x}) + \sum_{m=1}^{\infty} \sqrt{\mu_m} \, \phi_m(\mathbf{x}) \, Y_m(\omega)$$

where $\{\phi_m\}_{m \in \mathbb{N}}$ are normalised eigenfunctions and $Y_m \sim N(0, 1)$ i.i.d.

A Case Study: Radioactive Waste Disposal
WIPP Data



- transmissivity measurements at 38 test wells
- use head measurements to obtain boundary data via statistical interpolation (kriging)
- constant layer thickness $b = 8$m
- constant porosity $\phi = 0.16$
- SANDIA Nat. Labs reports [Caufman et al., 1990] [La Venue et al., 1990]

Calibrate statistical model to the transmissivity data:

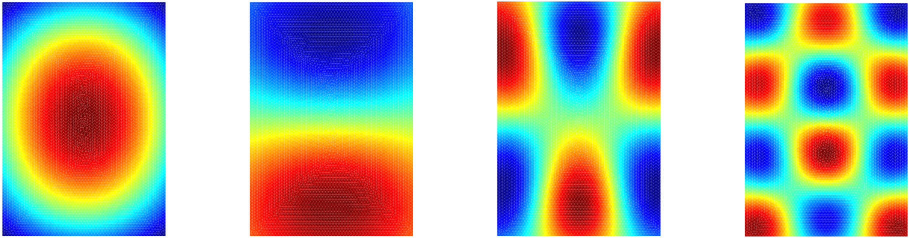
e.g. [Ernst et al., 2014]

1. Estimate parameters σ, λ and ν via restricted maximum likelihood estimation (REML).
2. Condition resulting covariance structure of $Z = \log k$ on transmissivity measurements. (Low-rank modification of covariance operator.)
3. Approximate Z by truncated Karhunen-Loève expansion, i.e use only the leading s terms.

A Case Study: Radioactive Waste Disposal

WIPP KL modes conditioned on 38 transmissivity observations

unconditioned, $m = 1, 2, 9, 16$



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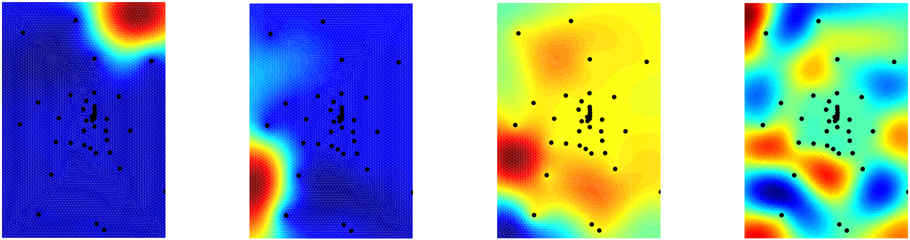

Computational Challenges

Simulating PDEs with Highly Heterogeneous Random Coefficients

$$-\nabla \cdot (k(\mathbf{x}, \omega) \nabla p(\mathbf{x}, \omega)) = f(\mathbf{x}, \omega), \quad \mathbf{x} \in D \subset \mathbb{R}^d, \ \omega \in \Omega \text{ (prob. space)}$$

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- **Sampling** from random field $\log k(\mathbf{x}, \omega)$ (correlated Gaussian):
  - truncated Karhunen-Loève expansion of $\log k$ (see above)
  - matrix factorisation, e.g. circulant embedding (FFT)
  - via pseudodifferential "precision" operator (PDE solves)

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  - Monte Carlo, Quasi-Monte Carlo
  - stochastic Galerkin/collocation (+ sparse grids)

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- **High-Dimensional Quadrature** – (the central problem!):
  - Monte Carlo, Quasi-Monte Carlo
  - stochastic Galerkin/collocation (+ sparse grids)
- **Solve** large number of **multiscale** deterministic PDEs:
  - Efficient discretisation & FE error analysis (mesh size h)
  - Multigrid Methods, AMG, DD Methods (robustness?)

Computational Challenges

Why is it computationally so challenging?

- Low regularity (global): $k \in C^\eta,\ \eta < \nu < 1 \implies$ **fine** mesh $h \ll 1$
- Large σ^2 & exponential $\implies$ **high** contrast $k_{\max}/k_{\min} > 10^6$
- Small $\lambda \implies$ **multiscale** + **high** stochast. dimension $s > 100$

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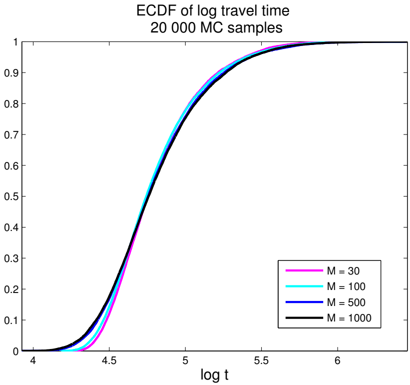

Source: Ernst et al, 2014 ($s = M$)

Computational Challenges

Standard Monte Carlo Quadrature

$$\mathbf{Y}(\omega) \in \mathbb{R}^s \quad \stackrel{\text{Model}(h)}{\longrightarrow} \quad \mathbf{P}(\omega) \in \mathbb{R}^{M_h} \quad \stackrel{\text{Output}}{\longrightarrow} \quad Q_{h,s}(\omega) \in \mathbb{R}$$

random input — state vector — quantity of interest

- **Here:** $\mathbf{Y}$ multivariate Gaussian for KL expansion; $\mathbf{P}$ numerical solution of PDE; $Q_{h,s}$ a (non)linear functional of $\mathbf{P}$

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- Real QoI $Q(\omega)$ inaccessible (exact PDE), but we can assume $\mathbb{E}[Q_{h,s}] \xrightarrow{h\to 0,\, s\to\infty} \mathbb{E}[Q]$ and $|\mathbb{E}[Q_{h,s} - Q]| = \mathcal{O}(h^\alpha) + \mathcal{O}(s^{-\alpha'})$
- **Standard Monte Carlo** estimator for $\mathbb{E}[Q]$:

More on Friday!

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

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

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- Cost per sample is $\mathcal{O}(M_h^\gamma)$ (optimal: $\gamma = 1$)

Computational Challenges

Standard Monte Carlo Quadrature

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

$$\underbrace{\mathbb{E}\Big[\big(\hat{Q}^{\mathrm{MC}} - \mathbb{E}[Q]\big)^2\Big]}_{=:\ \mathsf{MSE}} = \mathbb{V}[\hat{Q}^{\mathrm{MC}}] + \big(\mathbb{E}[\hat{Q}^{\mathrm{MC}}] - \mathbb{E}[Q]\big)^2$$

$$= \underbrace{\frac{\mathbb{V}[Q_{h,s}]}{N}}_{\textbf{sampling error}} + \underbrace{\Big(\mathbb{E}[Q_{h,s} - Q]\Big)^2}_{\textbf{model error (“bias”)}}$$

- Typical: $\alpha = 1 \;\Rightarrow\; \mathsf{MSE} = \mathcal{O}(N^{-1}) + \mathcal{O}(h^2) \le \mathsf{TOL}^2$, and so $h \sim \mathsf{TOL}$ and $N \sim \mathsf{TOL}^{-2}$.

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- Using optimal PDE solver: $\mathsf{Cost} = \mathcal{O}(Nh^{-d}) = \mathcal{O}(\mathsf{TOL}^{-(d+2)})$

  (e.g. for $\mathsf{TOL} = 10^{-3}$: $h \sim 10^{-3}$, $N \sim 10^6$ and $\mathsf{Cost} = \mathcal{O}(10^{12})$ in 2D!!)

Quickly becomes **prohibitively expensive !**

Computational Challenges

Numerical Experiment with standard Monte Carlo

$D = (0,1)^2$, unconditioned KL expansion, $Q = \| - k \frac{\partial p}{\partial x_1} \|_{L^1(D)}$
using mixed FEs and the AMG solver `amg1r5` [Ruge, Stüben, 1992]

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- Numerically observed FE-error: $\approx \mathcal{O}(h^{3/4}) \implies \alpha \approx 3/4$.
- Numerically observed cost/sample: $\approx \mathcal{O}(h^{-2}) \implies \gamma \approx 1$.

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- Numerically observed FE-error: $\approx \mathcal{O}(h^{3/4}) \implies \alpha \approx 3/4$.
- Numerically observed cost/sample: $\approx \mathcal{O}(h^{-2}) \implies \gamma \approx 1$.
- **Total cost** to get RMSE $\mathcal{O}(\mathrm{TOL})$: $\approx \mathcal{O}(\mathrm{TOL}^{-14/3})$
  to get error reduction by a factor 2 $\rightarrow$ cost grows by a factor 25!

Case 1: $\sigma^2 = 1$, $\lambda = 0.3$, $\nu = 0.5$

TOL	h^{-1}	N_h	Cost
0.01	129	1.4×10^4	21 min
0.002	1025	3.5×10^5	30 days

Case 2: $\sigma^2 = 3$, $\lambda = 0.1$, $\nu = 0.5$

TOL	h^{-1}	N_h	Cost
0.01	513	8.5×10^3	4 h
0.002	**Prohibitively large!!**		

(actual numbers & CPU times on a cluster of 2GHz Intel T7300 processors)

Computational Challenges

Alternatives – The Curse of Dimensionality

- **Stochastic Galerkin/collocation methods** More on Mon!
  - cost grows v. fast with dimension s & polynomial order q (faster than exponential) $\rightarrow$ #stochastic DOF $N_{SC} = \mathcal{O}\left(\frac{(s+q)!}{s!q!}\right)$
  - lower # with sparse grids (Smolyak) but still fast growth with s!

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  - convergence of plain vanilla Monte Carlo is **always dimension independent** (even for rough problems)!
  - **BUT** (as we have seen) order of convergence too slow: $\mathcal{O}(N^{-1/2})$!

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  - **BUT** (as we have seen) order of convergence too slow: $\mathcal{O}(N^{-1/2})$!
  - Quasi-MC also **dimension independent** and (almost) $\mathcal{O}(N^{-1})$! **But** requires also **(some) smoothness** ! More on Wed!

Computational Challenges

Nonlinear Parameter Dependence (e.g. lognormal coefficients)

- Monte Carlo methods **do not** rely on KL-type expansion
  (can use circulant embedding or sparse pseudodifferential operators)
- Stochastic Galerkin matrix is **block dense** due to nonlinear parameter dependence $\rightarrow$ even applying matrix is expensive!
  (can transform to convection-diffusion problem, but requires more smoothness and is not conservative [Elman, Ullmann, Ernst, 2010])
- best N-term theory by [Cohen, Schwab et al] does **not** apply!

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- best N-term theory by [Cohen, Schwab et al] does **not** apply!

Monte Carlo methods do not suffer from **Curse of Dimensionality**, they are **"non-intrusive"** and nonlinear parameter dependence is no problem,

but the plain vanilla version is **too slow!**

Computational Challenges

Nonlinear Parameter Dependence (e.g. lognormal coefficients)

- Monte Carlo methods **do not** rely on KL-type expansion
  (can use circulant embedding or sparse pseudodifferential operators)
- Stochastic Galerkin matrix is **block dense** due to nonlinear parameter dependence $\rightarrow$ even applying matrix is expensive!
  (can transform to convection-diffusion problem, but requires more smoothness and is not conservative [Elman, Ullmann, Ernst, 2010])
- best N-term theory by [Cohen, Schwab et al] does **not** apply!

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Alternatives?