PDE with random coefficients as a problem in high-dimensional integration

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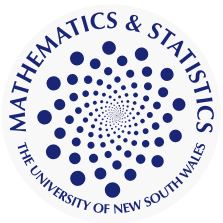
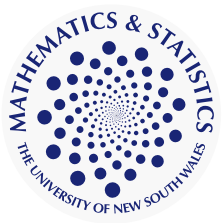


Theory

– Quasi-Monte Carlo methods

Application

– PDE with random coefficients



Motivating example

Uncertainty in groundwater flow

eg. risk analysis of radioactive waste disposal or CO_2 sequestration

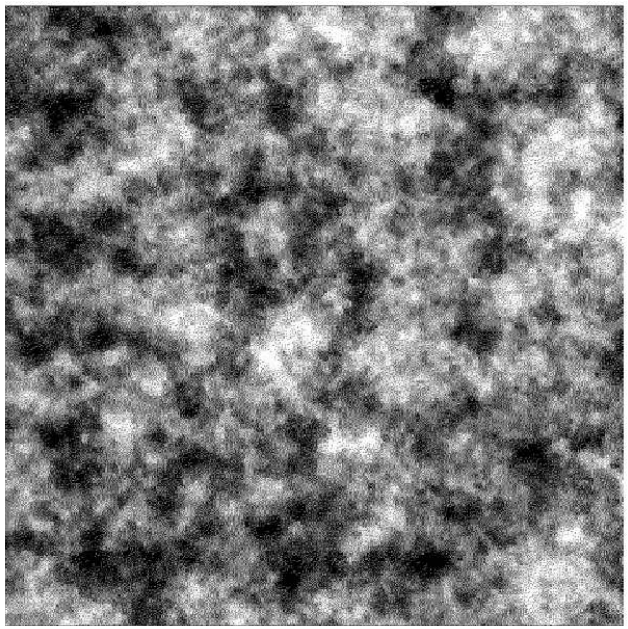
Darcy's law

mass conservation law

$$\vec{q} = -a\,\vec{\nabla} p$$
$$\nabla \cdot \vec{q} = 0$$

in $D \subset \mathbb{R}^d$, $d = 1, 2, 3$

$$\Longrightarrow \quad \nabla \cdot (a\,\vec{\nabla} p) = 0$$



together with boundary conditions

[Cliffe, *et. al.* (2000)]

Uncertainty in $a(\boldsymbol{x}, \omega)$ leads to uncertainty in $q(\boldsymbol{x}, \omega)$ and $p(\boldsymbol{x}, \omega)$

Expected values of quantities of interest

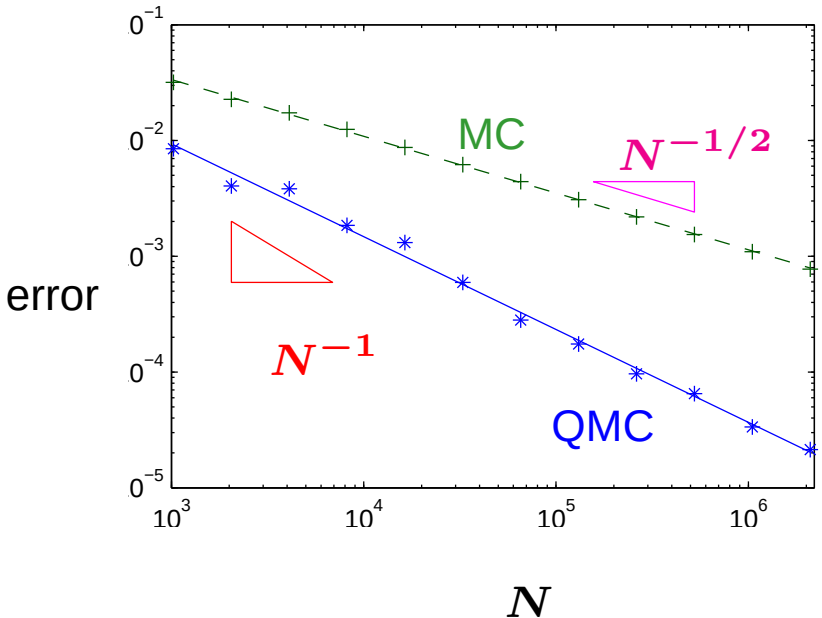
To compute the expected value of some quantity of interest:

1. Generate a number of realizations of the random field
   (Some approximation may be required)
2. For each realization, solve the PDE using e.g. FEM / FVM / mFEM
3. Take the average of all solutions from different realizations

This describes Monte Carlo simulation.

Or, because the **expected value** is a (high dimensional) **integral**

use **quasi-Monte Carlo methods**



Monte Carlo (MC)

Approximate the s-dimensional integral

$$I_s(F) := \int_{[0,1]^s} F(\boldsymbol{y})\, d\boldsymbol{y}$$

by

$$Q_{N,s}^{\mathrm{MC}}(F) = \frac{1}{N} \sum_{k=1}^{N} F(\boldsymbol{t}_k),$$

with $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_N$ chosen randomly and independently from a uniform distribution on $[0,1]^s$.

Error: For $F \in L^2([0,1]^s)$,

where

$$\boxed{\text{error}^{\mathrm{MC}} = \frac{\sigma(F)}{\sqrt{N}},}$$

$$\sigma^2(F) = I_s((F - I_s(F))^2) = I_s(F^2) - (I_s(F))^2.$$

Quasi-Monte Carlo (QMC)

$$Q_{N,s}(F) = \frac{1}{N} \sum_{k=1}^{N} F(\boldsymbol{t}_k) \ ,$$

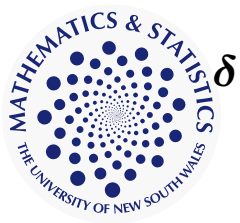
with $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_N$ deterministic (and cleverly chosen).

What do we wish for? For F sufficiently smooth we might hope for

$$\text{error}^{\mathbf{QMC}} \leq \frac{C}{N}$$

with C independent of s.

In practice we can get $\text{error}^{\mathbf{QMC}} \leq \frac{C_\delta}{N^{1-\delta}}$ for arbitrary $\delta > 0$, with $C_\delta \to \infty$ as $\delta \to 0$, for suitably smooth F.

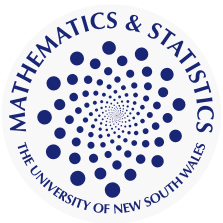


How to choose the QMC points?

How to choose $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_N$? There are two main methods:

- **Low discrepancy points** Sobol (1950s), Faure, Niederreiter (1980s), and more recently, Dick, Pillichshammer, ...
- **Lattice rules** Korobov, Hlawka, Hua & Wang (1950s), and more recently Sloan, Kachoyan, Lyness, Woźniakowski, L'Ecuyer, Hickernell, Joe, Kuo, Dick, Larcher, Wang, Waterhouse, ...

For this talk consider only "lattice rules".



Lattice rule definition

Lattice Rule (of rank 1)

$$Q_{N,s}F = \frac{1}{N}\sum_{k=1}^{N} F\left(\left\{k\frac{\boldsymbol{z}}{N}\right\}\right),$$

$$\boldsymbol{z} \in \{1,\ldots,N-1\}^s$$

Shifted lattice rule

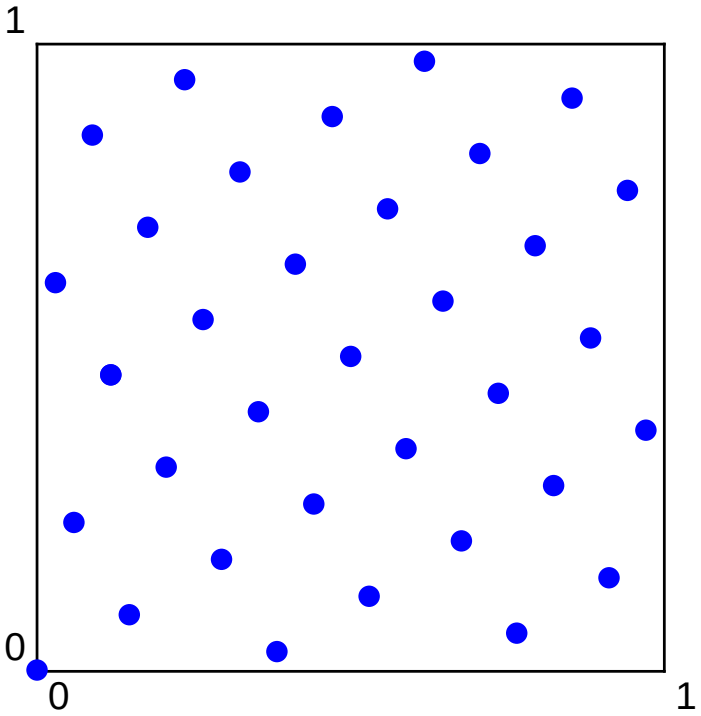
$$Q_{N,s}F = \frac{1}{N}\sum_{k=1}^{N} F\left(\left\{k\frac{\boldsymbol{z}}{N} + \boldsymbol{\Delta}\right\}\right),$$

$\boldsymbol{\Delta}$ (the "shift") $\in [0,1]^s$

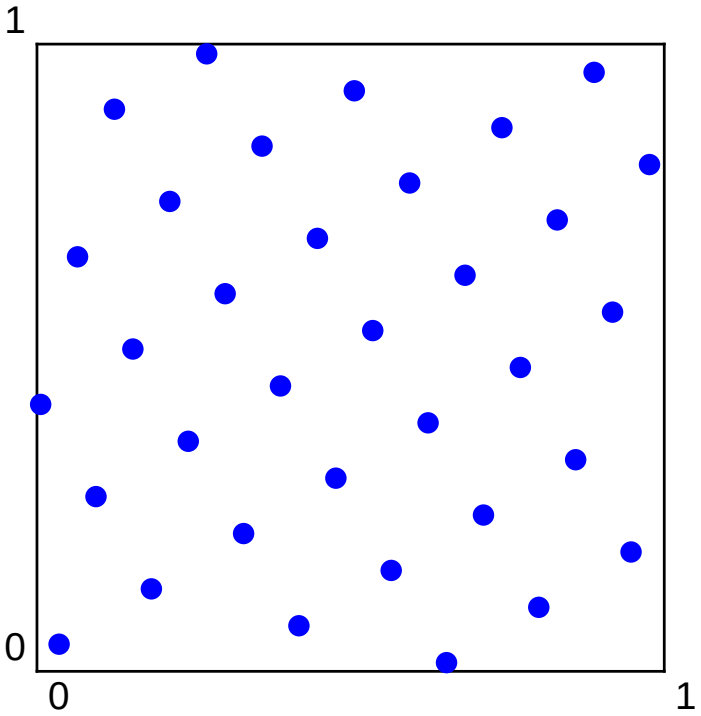
Ref: IHS & S. Joe, "Lattice Methods for Multiple Integration", Oxford '94.

Example of lattice & shifted lattice rules

$\boldsymbol{N} = 34, \boldsymbol{z} = (1, 21)$



$\boldsymbol{N} = 34, \boldsymbol{z} = (1, 21), \Delta = (0.8, 0.1)$



Randomly shifted lattice rules

In practice we like randomly shifted lattice rules:

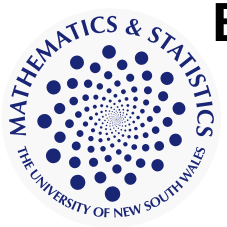
$$Q_{N,s}F = \frac{1}{q}\sum_{i=1}^{q}\left(\frac{1}{N}\sum_{k=1}^{N} F\left(\left\{k\frac{\boldsymbol{z}}{N} + \boldsymbol{\Delta}_i\right\}\right),\right)$$

where $\boldsymbol{\Delta}_i$ for $i = 1, \ldots, q$ are random vectors chosen independently from a uniform distribution on $[0,1]^s$.

As with MC, this gives an unbiased estimate of the integral, and allows a practical estimate of the error.

Now there is only one thing to choose: namely the integer vector $\boldsymbol{z}$.

But how to choose $\boldsymbol{z}$?



Weighted function spaces – the anchored case

IDEA: the variables are *not* equally important

Assume that F belongs to a ***weighted* Sobolev space**, with sqd. norm

$$\|F\|^2_{s,\boldsymbol{\gamma}} = \sum_{\mathfrak{u}\subseteq\{1,\ldots,s\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{[0,1]^{|\mathfrak{u}|}} \left| \frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}; 0) \right|^2 \mathrm{d}\boldsymbol{y}_{\mathfrak{u}}$$

2^s subsets

"weights"

"anchor" at 0

Mixed first derivatives are square integrable

Small weight $\gamma_{\mathfrak{u}}$ means that F depends weakly on the variables $\boldsymbol{y}_{\mathfrak{u}}$

- **"product" weights** – the "standard setting" as in Sloan and Woźniakowski (1998)

$$\gamma_{\mathfrak{u}} = \prod_{j\in\mathfrak{u}} \gamma_j, \quad \gamma_1 \geq \gamma_2 \geq \gamma_3 \geq \cdots > 0$$

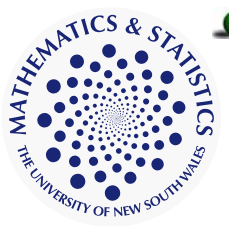
- **"order dependent" weights** – Sloan, Wang, Woźniakowski (2004)

$$\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|}, \quad \Gamma_0 = 1, \Gamma_1, \Gamma_2, \Gamma_3, \ldots > 0$$

- **"POD" weights ("product and order dependent" weights)**

$$\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|} \prod_{j\in\mathfrak{u}} \gamma_j$$

– Kuo, Schwab, Sloan (SINUM '12): *PDE with random coefficient*



Examples (for product weights)

- $s = 1:\quad \|F\|_{1,\gamma}^2 = |F(0)|^2 + \frac{1}{\gamma_1}\int_0^1 \left|\frac{dF}{dy}\right|^2 \mathrm{d}y$
- $s = 2:$

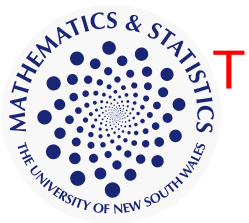
$$\|F\|_{2,\gamma}^2 = |F(0,0)|^2$$

$$+\frac{1}{\gamma_1}\int_0^1 \left|\frac{\partial F}{\partial y_1}(y_1,0)\right|^2 \mathrm{d}y_1 + \frac{1}{\gamma_2}\int_0^1 \left|\frac{\partial F}{\partial y_2}(0,y_2)\right|^2 \mathrm{d}y_2$$

$$+\frac{1}{\gamma_1\gamma_2}\int_0^1\int_0^1 \left|\frac{\partial^2 F}{\partial y_1 \partial y_2}\right|^2 \mathrm{d}y_1\mathrm{d}y_2$$

Note that if $F(y_1,y_2) = g(y_1)h(y_2)$ then $\|F\|_{2,\gamma} = \|g\|_{1,\gamma}\|h\|_{1,\gamma}$.

This makes the product case the easiest.



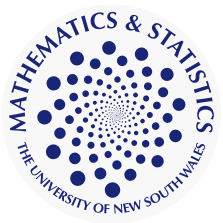
Worst case error

The **worst case error** (wce) of a QMC rule with points $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_N$ is defined by:

$$e_{N,s,\boldsymbol{\gamma}} := \sup_{\|F\|_{s,\boldsymbol{\gamma}} \le 1} \left| \int_{[0,1]^s} F(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} - \frac{1}{N} \sum_{k=1}^{N} F(\boldsymbol{t}_k) \right|$$

$$\Longrightarrow \quad \textbf{(error for given } F\textbf{)} \le e_{N,s,\boldsymbol{\gamma}} \times \|F\|_{s,\boldsymbol{\gamma}}$$

- An explicit formula exists for the wce – wce's can be computed!



An early existence result

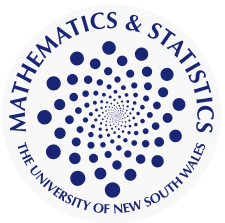
THEOREM IHS & H Woźniakowski, '98 *Assume product weights,*

$\gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j$. *Then if (and only if)* $\sum_{j=1}^{\infty} \gamma_j < \infty$ *there exist points*

$\boldsymbol{t}_1, \ldots, \boldsymbol{t}_N \in [0,1]^s$ *such that*

$$e_{N,s,\boldsymbol{\gamma}} \le \frac{D_\gamma}{\sqrt{N}},$$

with D_γ *independent of* s.



Remarks

1. The bound holds e.g. for $\gamma_j = 1/j^2$. It does **not** hold for the classical weights $\gamma_j = 1$.

2. D_γ is known explicitly: for example, we can take

$$D_\gamma = \exp\left(\frac{1}{4}\sum_{j=1}^{\infty}\gamma_j\right).$$

3. The condition $\sum_{j=1}^{\infty}\gamma_j < \infty$ is necessary as well as sufficient. For every choice of points we can construct a lower bound on the worst-case error, which grows unboundedly with s if the condition fails.

4. The convergence rate is only the Monte Carlo rate; and

   the proof that $\exists$ a good QMC rule is not constructive!

A better existence result

THEOREM Sloan and Woźniakowski ('01): *If*

$$\sum_{j=1}^{\infty} \gamma_j^{1/2} < \infty,$$

and if N is prime, then for each s $\exists$ a SHIFTED LATTICE RULE $Q^{\text{lattice}}_{N,s,\boldsymbol{z},\Delta}$ such that

$$e_{N,s,\gamma} \le \frac{C_{\gamma,\delta}}{N^{1-\delta}} \qquad \forall \delta > 0.$$

Recall – a shifted lattice rule (with N prime) is a QMC rule of special form

$$Q^{\text{lattice}}_{N,s,\boldsymbol{z},\Delta}(F) = \frac{1}{N} \sum_{k=1}^{N} F\left(\left\{\frac{k\boldsymbol{z}}{N} + \Delta\right\}\right),$$

$$\boldsymbol{z} \in \{1, 2, \ldots, N-1\}^s, \ \Delta \in [0,1)^s$$

Proof is by averaging in a different way over Δ and z.

Shift-averaged wce

Now turn to construction.

It is convenient to work with the "root-mean square shift-averaged" worst case error: for a given choice of points $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_N$,

$$e^{\mathrm{rms}}_{N,s,\boldsymbol{\gamma}} := \sqrt{\int_{[0,1]^s} \cdots \int_{[0,1]^s} e_{N,s,\boldsymbol{\gamma}}(\boldsymbol{\Delta}_1, \ldots, \boldsymbol{\Delta}_q)^2 \mathrm{d}\boldsymbol{\Delta}_1 \ldots \mathrm{d}\boldsymbol{\Delta}_q}$$

We do this because the shift-averaged wce is simpler than the wce for a shift $\boldsymbol{\Delta}$.

$\Longrightarrow$ for given F, **RMS error** $\le e^{\mathrm{rms}}_{N,s,\boldsymbol{\gamma}} \times \|F\|_{s,\boldsymbol{\gamma}}$.

Shift-averaged wce – the anchored case

The shift-averaged worst-case error for the case of the anchored norm and product weights is given by

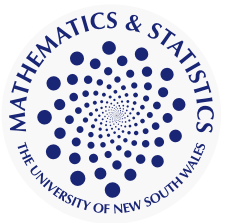
$$e^{\mathrm{rms}}_{N,s,\gamma}(\boldsymbol{z})^2 = -\prod_{j=1}^{s}(1+\gamma_j/3) + \frac{1}{N}\sum_{i=1}^{N}\prod_{j=1}^{s}\left[1+\gamma_j\left(B_2(\{iz_j/N\})+\frac{1}{3}\right)\right]$$

where $B_2(x) = x^2 - x + \frac{1}{6}$.

Component-by-component construction

- We want a $\boldsymbol{z}$ that makes the *shift-averaged worst case error* as small as possible. $\sim$ Exhaustive search is in practice impossible - too many choices! $\sim$
- **CBC algorithm** [Korobov (1960s), Sloan, Kuo, Joe (2002);. . .]
  1. Set $z_1 = 1$.
  2. With z_1 fixed, choose z_2 to minimize the $s = 2$ worst case error.
  3. With z_1, z_2 fixed, choose z_3 to minimize the $s = 3$ worst case error.
  4. etc.
  - Cost for product wts. is only $\mathcal{O}(s\, N \log N)$ using FFTs. [Nuyens, Cools (2006)]
  - Optimal rate of convergence $\mathcal{O}(N^{-1+\delta})$ in weighted Sobolev space, with the implied constant independent of s under an appropriate condition on the weights. [Kuo (2003); Dick (2004)]

    $\sim$ Averaging argument: $\exists$ one choice as good as average! $\sim$



The optimal convergence property of CBC

THEOREM (for product weights) Frances Kuo, J. Complexity, (2003)

Assume product weights, $\gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j$. *Let* N *be prime, and let* $z_1, z_2, \ldots, z_s$ *be chosen by the CBC algorithm. Assume also*

$$\sum_{j=1}^{\infty} \gamma_j^{1/2} < \infty.$$

Then $\forall \delta > 0$

$$e_{\boldsymbol{\gamma}}^{\mathrm{rms}}(\boldsymbol{t}_1, \ldots, \boldsymbol{t}_N) \leq \frac{C_{\boldsymbol{\gamma},\delta}}{N^{1-\delta}}.$$

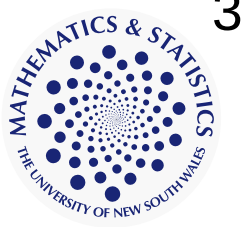
Thus the optimal rate is achieved by the CBC algorithm with product weights.

Proof: Averaging argument again: ∃ one choice as good as average!

Now to applications: the present state of play

... *in the application of QMC to PDEs with random coefficients:*

0. Graham, Kuo, Nuyens, Scheichl, Sloan (J. Comput. Physics, 2011)
   - application of QMC to the lognormal case
   - use circulant embedding to avoid truncation of KL expansion
   - detailed numerical experiments, but no error analysis
1. Kuo, Schwab, Sloan (SINUM, to appear)
   - application of QMC to the uniform case
   - no numerical results, but we gave a complete error analysis
   - matches the best N term result by Cohen, De Vore, Schwab (2010)
   - for the first time we know precisely how to choose the weights
2. Kuo, Schwab, Sloan (submitted)
   - a multi-level version of the analysis for the uniform case
3. Graham, Kuo, Nichols, Scheichl, Schwab, Sloan (in progress)
   - application of QMC to the lognormal case
   - detailed numerical experiments as well as complete error analysis



A model problem – the uniform case

$$-\nabla \cdot (a(\boldsymbol{x},\boldsymbol{y})\,\nabla u(\boldsymbol{x},\boldsymbol{y})) \;=\; f(\boldsymbol{x}) \quad \text{in} \quad D\,,$$

$$u(\boldsymbol{x},\boldsymbol{y}) \;=\; 0 \quad \text{on} \quad \partial D, \quad \boldsymbol{y} \in U := [-\tfrac{1}{2},\tfrac{1}{2}]^{\mathbb{N}},$$

with D a bounded Lipschitz domain in $\mathbb{R}^d$, and

$$a(\boldsymbol{x},\boldsymbol{y}) \;=\; \bar{a} + \sum_{j=1}^{\infty} y_j\,\psi_j(\boldsymbol{x}), \qquad \boldsymbol{x} \in D, \quad \boldsymbol{y} \in U\,.$$

Here $y_1, y_2, \ldots$ are independent random variables uniformly distributed on $[-\frac{1}{2},\frac{1}{2}]$; with ψ_j such that $\sum_j \|\psi_j\|_\infty < \infty$, and with $\bar{a}$ large enough and $\sum_j \|\psi_j\|_\infty$ small enough to ensure

$$a_{\max} \geq a(\boldsymbol{x},\boldsymbol{y}) \geq a_{\min} > 0,$$

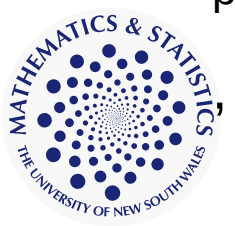
making the PDE **strongly elliptic** for every $\boldsymbol{y}$.

Why this problem?

Recently Cohen, De Vore and Schwab, in "Convergence rates of best N-term Galerkin approximations for a class of elliptic sPDEs", Foundations of Computational Mathematics (2010), established sharp error bounds for exactly this problem. They used a stochastic Galerkin method, combined with (non-constructive) 'best N-term approximation'.

We aim to design QMC rules that achieve the same result.

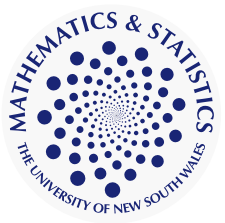
This problem is one in which the dimensionality (i.e. the number of parameters y_j) is infinite.



Method: FEM plus QMC

Finite element method to solve PDE for a fixed $\boldsymbol{y}$.

Quasi-Monte Carlo method to integrate over $\boldsymbol{y}$.



Other approaches

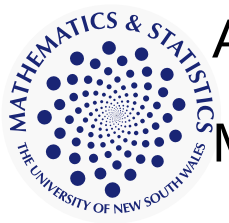
Wiener, Babuska, Schwab, Tempone, Nobile, Karniadakis, Xiu, Scheichl, Ghanem, . . .

There are many other approaches, including

- polynomial chaos,
- generalized polynomial chaos,
- stochastic Galerkin,
- stochastic collocation
- Monte Carlo

All methods for PDE with random coefficients face serious challenges when the dimensionality is high.

And when all else fails, people who need answers generally turn to Monte Carlo methods. We aim to beat Monte Carlo.



What do we want to calculate?

The problem is to compute the expected value of

$$F(\boldsymbol{y}) := G(u(\cdot, \boldsymbol{y}))$$

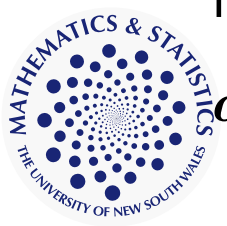
for some linear functional G of the solution u of the PDE.

The expected value is an infinite-dimensional **integral**, where the meaning is:

$$I[F] := \int_{\left[-\frac{1}{2},\frac{1}{2}\right]^{\mathbb{N}}} F(\boldsymbol{y}) \mathrm{d}\boldsymbol{y}$$

$$:= \lim_{s\to\infty} \int_{\left[-\frac{1}{2},\frac{1}{2}\right]^{s}} F(y_1, \ldots, y_s, 0, 0, \ldots) \mathrm{d}y_1 \ldots \mathrm{d}y_s.$$

Note that replacing $y_{s+1}, y_{s+2}, \ldots$ by 0 is equivalent to replacing $a(\boldsymbol{x}, \boldsymbol{y})$ by $a_s(\boldsymbol{x}, \boldsymbol{y}) := \bar{a}(\boldsymbol{x}) + \sum_{j=1}^{s} y_j \, \psi_j(\boldsymbol{x})$.



The smoother the better

The faster the decay of $\|\psi_j\|_\infty$, the smoother (with respect to $\boldsymbol{x}$) is the random field $a(\boldsymbol{x}, \boldsymbol{y})$, and the easier it is to get fast convergence.

We suppose that there exists p satisfying $0 < p \leq 1$ such that

$$\sum_{j \geq 1} \|\psi_j\|_\infty^p \ < \ \infty \ . \tag{1}$$

The smaller is p the faster the convergence of $\sum_j y_j \psi_j(\boldsymbol{x})$, and the fewer points we should need in our QMC rule.

Example: If $\psi_j(\boldsymbol{x}) = j^{-\frac{3}{2}-\delta} \times$ uniformly bounded functions of $\boldsymbol{x}$, with $\delta > 0$, then $\|\psi_j\|_\infty \leq c j^{-\frac{3}{2}-\delta}$, and we may take $p = 2/3$.

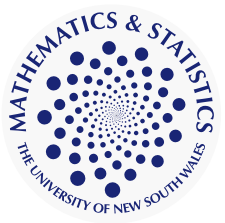
This is exactly the smoothness required by Cohen et al. to achieve $O(N^{-1})$ convergence, so $p = 2/3$ is special.

The approximation

Recall: the problem is to compute the expected value (i.e. the integral) of a linear functional of u,

$$F(\boldsymbol{y}) := G(u(\cdot, \boldsymbol{y})).$$

We will approximate $I(F)$ by $Q_{N,s}(F_h)$, where $F_h = G(u_h(\cdot, \boldsymbol{y}))$ is the functional G applied to the finite element solution u_h.



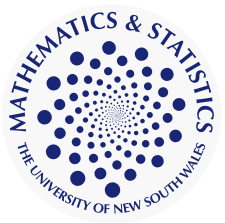
What is the error?

$$I(G(u)) - Q_{N,s}(G(u_h))$$

$$= (I - I_s)(G(u)) + (I_s(G(u)) - Q_{N,s}(G(u))) + Q_{N,s}(G(u - u_h)) \ .$$

The overall error is a sum of

- a *dimension truncation error* (which is inevitable when a finite-dimensional QMC method is used for an infinite dimensional integral),
- a *quadrature error*, and
- a *FE discretization error*



The quadrature error

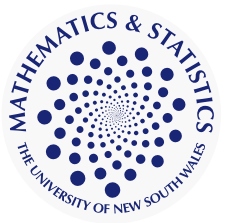
Here we use a QMC intergation rule, and focus on the quadrature error,

$$|I_s(F) - Q_{N,s}(F)|,$$

with $F(\boldsymbol{y}) = G(u(\cdot, \boldsymbol{y}))$.

First, look at the error $|I_s(F) - Q_{N,s,\boldsymbol{\Delta}}(F)|$ where $Q_{N,s,\boldsymbol{\Delta}}$ is the shifted lattice rule with shift $\boldsymbol{\Delta}$,

$$Q_{N,s,\boldsymbol{\Delta}}(F) = \frac{1}{N}\sum_{k=1}^{N} F\left(\left\{\frac{k\boldsymbol{z}}{N}+\boldsymbol{\Delta}\right\} - \left(\tfrac{1}{2},\ldots,\tfrac{1}{2}\right)\right)$$



From worst case error to error bound

Recall: the **worst case error** for the rule $Q_{N,s,\boldsymbol{\Delta}}$ in the space $H_{s,\boldsymbol{\gamma}}$ is:

$$e_{N,s,\boldsymbol{\gamma},\boldsymbol{\Delta}} := \sup_{\|F\|_{s,\boldsymbol{\gamma}} \le 1} |I_s(F) - Q_{N,s,\boldsymbol{\Delta}}(F)| .$$

$$\Longrightarrow \quad |I_s(F) - Q_{N,s,\boldsymbol{\Delta}}(F)| \le e_{N,s,\boldsymbol{\gamma},\boldsymbol{\Delta}} \times \|F\|_{s,\boldsymbol{\gamma}}$$

And if we now take the root mean square average over shifts,

$$\sqrt{\mathbb{E}[(I_s(F) - Q_{N,s,.}(F))^2]} \le e^{\mathbf{rms}}_{N,s,\boldsymbol{\gamma}} \times \|F\|_{s,\boldsymbol{\gamma}},$$

where $e^{\mathbf{rms}}_{N,s,\boldsymbol{\gamma}}$ is the shift-averaged worst-case error,

$$e^{\mathbf{rms}}_{N,s,\boldsymbol{\gamma}} := \sqrt{\mathbb{E}[e(Q_{N,s,.}; H_{s,\boldsymbol{\gamma}})]^2}.$$

(Here the expectation $\mathbb{E}$ is just the **integral** over all shifts $\boldsymbol{\Delta}$.)

Error bound

$$\sqrt{\mathbb{E}[(I(F) - Q_{N,s,.}(F))^2]} \leq e^{\mathrm{rms}}_{N,s,\gamma} \times \|F\|_{s,\boldsymbol{\gamma}}.$$

From before, with small modification to the norm,

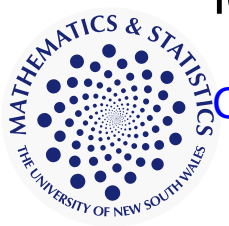
$$\|F\|_{s,\gamma} := \left(\sum_{\mathfrak{u} \subseteq \{1,\ldots,s\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{[-\frac{1}{2},\frac{1}{2}]^{|\mathfrak{u}|}} \left| \int_{[-\frac{1}{2},\frac{1}{2}]^{s-|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}} (\boldsymbol{y}_{\mathfrak{u}}, \boldsymbol{y}_{-\mathfrak{u}}) \mathrm{d}\boldsymbol{y}_{-\mathfrak{u}} \right|^2 \mathrm{d}\boldsymbol{y}_{\mathfrak{u}} \right)^{\frac{1}{2}}.$$

And for general weights $\gamma_{\mathfrak{u}}$, and $\boldsymbol{z}$ from CBC it can be shown that

$$e^{\mathrm{rms}}_{N,s,\gamma} \leq \frac{1}{N^{1/2\lambda}} \left(\sum_{\emptyset \neq \mathfrak{u} \subseteq \{1,\ldots,s\}} \gamma_{\mathfrak{u}}{}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}} \right)^{|\mathfrak{u}|} \right)^{1/2\lambda}$$

for all $\lambda \in (\frac{1}{2}, 1]$. (We would like $\lambda = 1/2$, but $\zeta(x) \to \infty$ as $x \to 1$.)

Choosing weights $\gamma_{\mathfrak{u}}$ is delicate: smaller weights reduces e^{rms} but increases $\|F\|_{s,\gamma}$.



We need to bound the norm

$$\|F\|_{s,\gamma} := \left(\sum_{u \subseteq \{1,\dots,s\}} \frac{1}{\gamma_u} \int_{[-\frac{1}{2},\frac{1}{2}]^{|u|}} \left| \int_{[-\frac{1}{2},\frac{1}{2}]^{s-|u|}} \frac{\partial^{|u|} F}{\partial \boldsymbol{y}_u}(\boldsymbol{y}_u, \boldsymbol{y}_{-u}) \mathrm{d}\boldsymbol{y}_{-u} \right|^2 \mathrm{d}\boldsymbol{y}_u \right)^{1/2},$$

We need to find a bound on the norm $\|F\|_{s,\boldsymbol{\gamma}}$.

This involves finding mixed first partial derivatives with respect to $\boldsymbol{y}$.

How? By differentiating the PDE.

The PDE in weak form

Let $V := H_0^1(D)$.

Then the weak (parametric) form of the PDE is: for $\boldsymbol{y} \in U$

$$\int_D a(\boldsymbol{x},\boldsymbol{y})\,\nabla u(\boldsymbol{x},\boldsymbol{y})\nabla v(\boldsymbol{x})\mathrm{d}\boldsymbol{x} = \int_D f(\boldsymbol{x})v(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \quad \forall v \in V\ ,$$

[**Stochastic Galerkin**: Integrate also with respect to $\boldsymbol{y}$. Choose $u(\boldsymbol{x},\boldsymbol{y}), v(\boldsymbol{x},\boldsymbol{y})$ from a tensor product of finite dimensional spaces.

Stochastic collocation: Collocate the above equation at $\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_M$]

Differentiating with respect to y_j, we get (with $\partial_y := \frac{\partial}{\partial y}$)

$$\int_D a(\boldsymbol{x},\boldsymbol{y})\,\nabla \partial_{y_j} u(\boldsymbol{x},\boldsymbol{y})\nabla v(\boldsymbol{x})\mathrm{d}\boldsymbol{x} + \int_D \psi_j(\boldsymbol{x})\,\nabla u(\boldsymbol{x},\boldsymbol{y})\nabla v(\boldsymbol{x})\mathrm{d}\boldsymbol{x} = 0,$$

$$\int_D a(\boldsymbol{x},\boldsymbol{y})\,|\nabla \partial_{y_j} u(\boldsymbol{x},\boldsymbol{y})|^2 \mathrm{d}\boldsymbol{x} \;=\; -\int_D \psi_j(\boldsymbol{x})\,\nabla u(\boldsymbol{x},\boldsymbol{y}) \nabla \partial_{y_j} u(\boldsymbol{x},\boldsymbol{y}) \mathrm{d}\boldsymbol{x}\;,$$

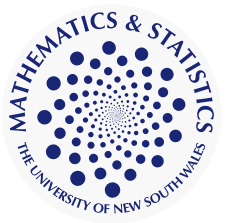
$$\Longrightarrow$$

$$a_{\min}\,\|\partial_{y_j} u(\boldsymbol{x},\boldsymbol{y})\|_V^2 \;\leq\; \|\psi_j\|_\infty\,\|u(\boldsymbol{x},\boldsymbol{y})\|_V \|\partial_{y_j} u(\boldsymbol{x},\boldsymbol{y})\|_V$$

$$\Longrightarrow$$

$$\|\partial_{y_j} u(\boldsymbol{x},\boldsymbol{y})\|_V \;\leq\; \frac{\|\psi_j\|_\infty}{a_{\min}} \|u(\boldsymbol{x},\boldsymbol{y})\|_V$$

$$\leq\; \frac{\|\psi_j\|_\infty}{a_{\min}} \frac{\|f\|_{H^{-1}}}{a_{\min}}\;.$$



Differentiating with respect to other y_k

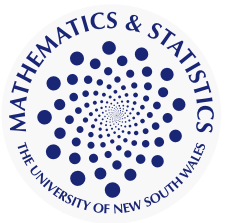
Keep differentiating, and getting similar estmates. Eventually,

$$\|u\|_{H_{s,\gamma}([-\frac{1}{2},\frac{1}{2}]^s,V)}$$

$$:= \left(\sum_{\mathfrak{u}\in\{1:s\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{[-\frac{1}{2},\frac{1}{2}]^{|\mathfrak{u}|}} \left\| \int_{[-\frac{1}{2},\frac{1}{2}]^{s-|\mathfrak{u}|}} \partial_{\boldsymbol{y}_{\mathfrak{u}}} u(\cdot;\boldsymbol{y}_{\mathfrak{u}},\boldsymbol{y}_{-\mathfrak{u}}) \mathrm{d}\boldsymbol{y}_{-\mathfrak{u}} \right\|_V^2 \mathrm{d}\boldsymbol{y}_{\mathfrak{u}} \right)^{\frac{1}{2}}$$

$$\le \left(\sum_{|\mathfrak{u}|<\infty} \frac{(|\mathfrak{u}|!)^2}{\gamma_{\mathfrak{u}}} \prod_{j\in\mathfrak{u}} \left(\frac{\|\psi_j\|_\infty}{a_{\min}} \right)^2 \right)^{\frac{1}{2}} \frac{\|f\|_{H^{-1}(D)}}{a_{\min}} .$$

But is this sum bounded as $s \to \infty$? It is if we choose the weights $\gamma_{\mathfrak{u}}$ large enough!



Now choose the weights

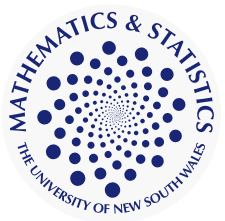
Now choose the weights to minmise the upper bound on worst-case error $\times$ norm, i.e. choose weights to minimise

$$\left(\sum_{\emptyset \neq \mathfrak{u} \subseteq \{1,\ldots,s\}} \gamma_{\mathfrak{u}}{}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\right)^{|\mathfrak{u}|}\right)^{1/2\lambda} \times \left(\sum_{|\mathfrak{u}|<\infty} \frac{(|\mathfrak{u}|!)^2}{\gamma_{\mathfrak{u}}} \prod_{j\in\mathfrak{u}} \left(\frac{\|\psi_j\|_\infty}{a_{\min}}\right)^2\right)^{\frac{1}{2}}.$$

The (elementary!) answer is:

$$\boxed{\gamma_{\mathfrak{u}} = (|\mathfrak{u}|!)^{\frac{2}{1+\lambda}} \prod_{j\in\mathfrak{u}} \alpha_j},$$

where $\alpha_j = \dfrac{\|\psi\|_\infty}{a_{\min}\sqrt{2\zeta(2\lambda)/(2\pi^2)^{\lambda}}}$



Main results for quad. error

Theorem Kuo, Schwab, S. SIAM J Nmer Anal, to appear

Assume that for some $p \leq 1$ we have $\sum_{j=1}^{\infty} \|\psi_j\|_{\infty}^{p} < \infty$,

eg $\|\psi_j\|_{\infty} = j^{-\frac{1}{p}-\epsilon}$, andf that the weights are as above.

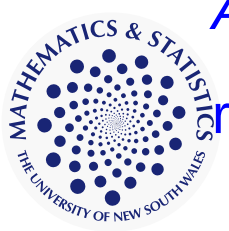
(a) Then $\|u\|_{H_\gamma(U,V)} < \infty.$

(b) And if we now assume $p \leq 2/3$ then for arbitrary $\epsilon > 0$ we have

$$\text{error}^{\text{QMC}} \leq C N^{-1+\epsilon}.$$

Thus we get the optimal $O(N^{-1+\epsilon})$ result for p=2/3, which is exactly as in the best N-term results of Cohen, De Vore and Schwab.

All our convergence results up to $O(N^{-1+\delta})$ match the best N-term results, under exactly the same conditions.

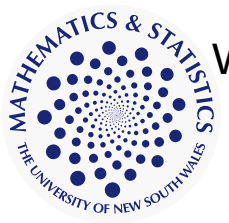


CBC for POD weights?

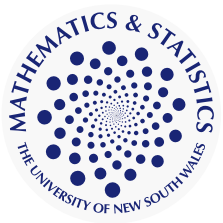
The weights in the Theorem are POD weights, i.e., weights of the "product and order-dependent" form

$$\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|} \prod_{j \in \mathfrak{u}} \alpha_j.$$

It turns out (Kuo, Scwhab, S, ANZIAM J, to appear) that fast CBC is possible for POD weights: only a small modification needed from the already existing CBC algorithm for 'order-dependent' weights $\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|}$ IHS, Wang and Woźniakowski 2004.



Thus we can construct cheaply a (randomly shifted) lattice rule that achieves the optimal result, for linear functionals of the solution to the model PDE – a simple PDE but one with an infinite number of terms to describe the random coefficient.



The lognormal permeability field

Write permeability as $a(\boldsymbol{x}, \omega)$

$\omega \in \Omega$, a probability space.

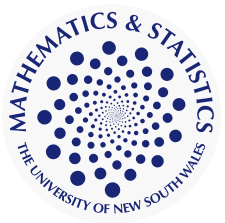
A common model is the lognormal field:

$$a(\boldsymbol{x}, \omega) = \exp(Z(\boldsymbol{x}, \omega))$$

where $Z(\boldsymbol{x}, \cdot)$ is a Gaussian random field with mean zero and covariance function $R(\boldsymbol{x}, \boldsymbol{z})$.

That is,

$$R(\boldsymbol{x}, \boldsymbol{z}) := \mathbb{E}[Z(\boldsymbol{x}, \cdot) Z(\boldsymbol{z}, \cdot)].$$



Examples of 2d covariance functions

$$R(\boldsymbol{x},\boldsymbol{y}) = \sigma^2 \exp\left(-\frac{|x_1-y_1|^2+|x_2-y_2|^2}{\lambda^2}\right),$$

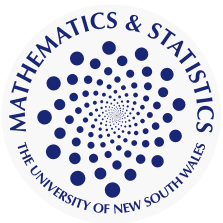
– very smooth

$$R(\boldsymbol{x},\boldsymbol{y}) = \sigma^2 \exp\left(-\frac{\sqrt{|x_1-y_1|^2+|x_2-y_2|^2}}{\lambda}\right),$$

– not smooth at $\boldsymbol{x}=\boldsymbol{y}$.

where σ^2 is the variance, and λ is the correlation length.

How to compute realisations of the input field? One way is:



Karhunen-Loève expansion

$$Z(\boldsymbol{x},\omega) = \sum_{j=1}^{\infty} \sqrt{\mu_j}\, y_j \phi_j(\boldsymbol{x}),$$

where (μ_j, ϕ_j) satisfy

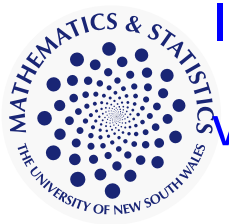
$$\int_D R(\boldsymbol{x},\boldsymbol{y})\phi_j(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \mu_j \phi_j(\boldsymbol{x}),$$

$$\int_D \phi_i(\boldsymbol{y})\phi_j(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \delta_{ij},$$

and the y_j are independent standard normal random numbers.

The sequence $(y_1, y_2, \cdots)$ corresponds to the point ω in the probability space.

In practice the sum is truncated after say s terms. Then the expected value is an s-dimensional integral.

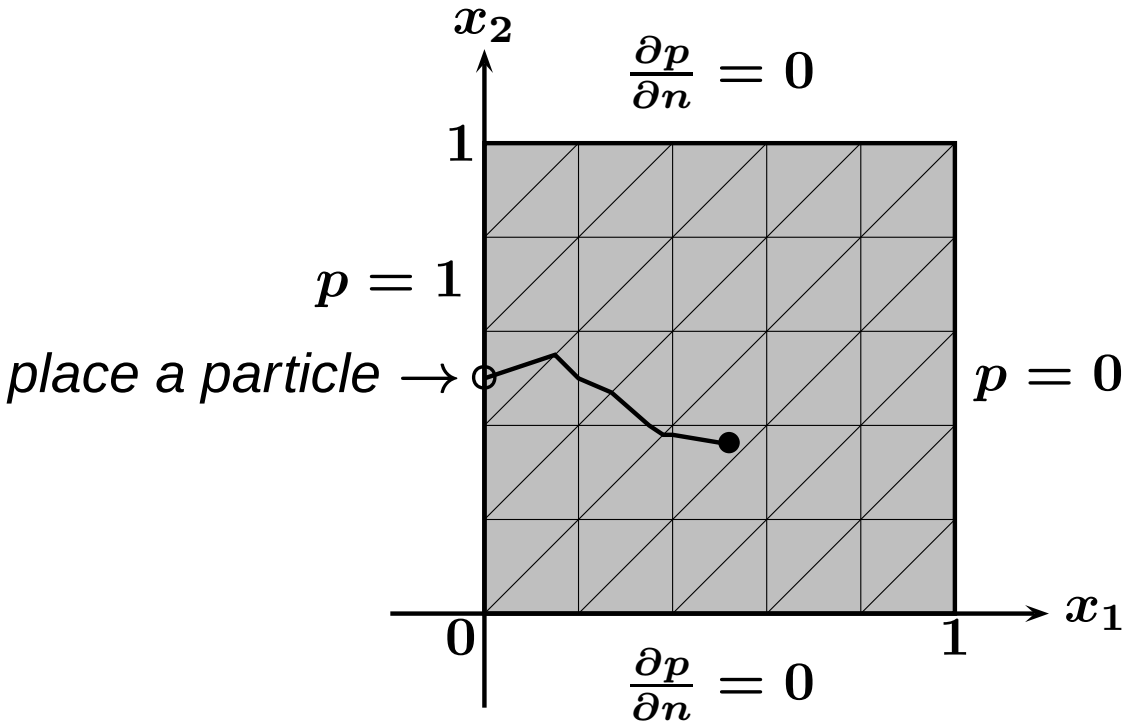


Particle paths

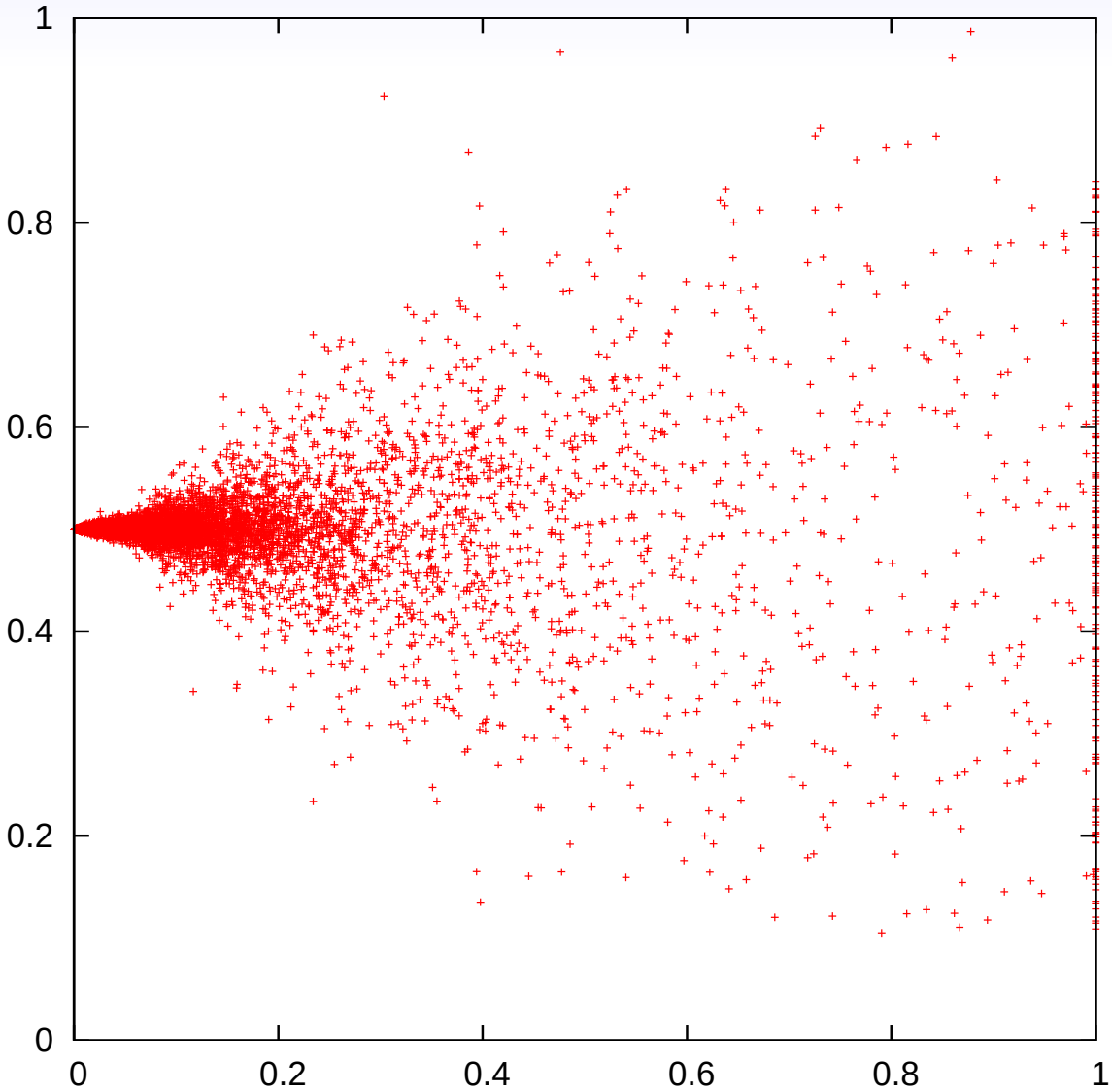
For a particular realisation of the permeability field, after we have found the pressure field p, to find the position $\boldsymbol{x}$ of a particle of the fluid solve

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \vec{q}(\boldsymbol{x}) = -a(\boldsymbol{x})\nabla p(\boldsymbol{x}),$$

subject to $\boldsymbol{x} = (0, 0.5)$ at $t = 0$.



Particle displacement after time $t = 0.1$



Note: Each time the permeability field is different!