Quasi-Monte Carlo methods for computing flow in random porous media

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Flow in porous medium

On domain $D \subset \mathbb{R}^2$ (or $\mathbb{R}^3$)

$$\begin{aligned} \vec{q} + k\vec{\nabla} p &= 0, \\ \vec{\nabla}.\vec{q} &= 0 \end{aligned} \qquad \begin{aligned} \vec{q}.\vec{n} = 0 \quad &\text{on} \quad \partial D_1 \\ p = g \quad &\text{on} \quad \partial D_2 \end{aligned}$$

with **lognormal permeability**:

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

$Z(\vec{\boldsymbol{x}}, \omega)$ **a Gaussian random field** (**zero mean**) and

given covariance $r(\vec{\boldsymbol{x}}, \vec{\boldsymbol{y}}) = \mathbb{E}(Z(\vec{\boldsymbol{x}}, \cdot) Z(\vec{\boldsymbol{y}}, \cdot))$, $\boldsymbol{x}, \boldsymbol{y} \in D$.

e.g. $r(\vec{\boldsymbol{x}}, \vec{\boldsymbol{y}}) = \boldsymbol{\sigma^2} \exp\left(- \|\vec{\boldsymbol{x}} - \vec{\boldsymbol{y}}\| / \lambda \right)$.

$\boldsymbol{\sigma^2}$ = **variance** , λ = **lengthscale** (**or more general**)

FEM approximation

$$\begin{aligned} \vec{q} + k\vec{\nabla}p &= 0, & \vec{q}.\vec{n} = 0 \quad &\text{on} \quad \partial D_1 \\ \vec{\nabla}.\vec{q} &= 0 & p = g \quad &\text{on} \quad \partial D_2 \end{aligned}$$

Mixed FEM approximation $(\vec{q}_h, p_h) \in RT_0 \times PC$ on a mesh $\mathcal{T}_h$:

$$\begin{aligned} m(\vec{q}_h, \vec{v}_h) + b(p_h, \vec{v}_h) &= G(\vec{v}_h)\,, \\ b(w_h, \vec{q}_h) &= 0 \qquad \text{for all} \quad (\vec{v}_h, w_h) \end{aligned}$$

Note : $m(\vec{v}, \vec{q}) = \int_D \exp(Z(\cdot, \omega))\vec{v}.\vec{q}$

Low regularity $k \in C^\alpha(D)$, $\alpha < 1/2$, **almost surely**, so

$$\|\vec{q} - \vec{q}_h\|_{H(div,D)} = \mathcal{O}(h^\alpha)$$

Remains true if $Z(\cdot, \omega)$ sampled at nodes of the FE grid

Cliffe, IGG, Scheichl, Stals, 2000

Work Flow

- Compute **realization** of $Z(\vec{\boldsymbol{x}}, \omega)$ on FE grid
- Solve the **FEM equations** (large, ill-conditioned)
- **postprocess** $\vec{q}_h(\vec{\boldsymbol{x}}, \omega)$, $p_h(\vec{\boldsymbol{x}}, \omega)$ to approximate quantities of interest $\mathcal{G}(Z)$

e.g. **pressure head at a point**, **effective permeability** k_{eff}**, breakthrough time** T_{out}

Our method: (Deterministic) choice of realizations via sparse QMC points in high dimensional parameter space...

"stochastic sampling" or **"stochastic collocation"** - cf. **M. Gunzburger's lectures**

Avoiding KL truncation: discretize first in space

$\mathbb{E}(\mathcal{G}(Z)) \approx \mathbb{E}(\mathcal{G}^{\mathrm{FEM}}(Z))$ **requires only** $\boldsymbol{Z} = \{Z(\vec{\boldsymbol{x}}^{(i)})\}$

Covariance Matrix: $R_{i,j} = r(\vec{\boldsymbol{x}}^{(i)}, \vec{\boldsymbol{x}}^{(j)})$ $M \times M$

Factorization: $R = BB^T$ **May be expensive!**

Realizations: $\boldsymbol{Z} = B\mathbf{Y}$. **independent Gaussians**

Sampling on uniform grids:

Embed R into $\mathbf{C}$ - block circulant $\mathbf{d} \times \mathbf{d}$

(Cheap) Factorization: $\mathbf{C} = \mathbf{B}\mathbf{B}^{\mathrm{T}}$ **(by FFT)**

In fact diagonalization gives ordering of variables

(Irregular domains also OK)

$$\mathbb{E}(\mathcal{G}(Z)) \approx \int_{\mathbb{R}^{\mathbf{d}}} \mathcal{G}^{\mathrm{FEM}}([B\boldsymbol{y}]_{\mathrm{part}}) \frac{\exp(-\frac{1}{2}\boldsymbol{y}^{\mathrm{T}}\boldsymbol{y})}{(2\pi)^{d/2}} \mathrm{d}\boldsymbol{y}$$

Transform to $[0,1]^d$ and apply QMC. **Note:** $d = \mathcal{O}(M)$!!

Fast computations with Mixed FEM (Scheichl 2000)

Saddle-point problem:

$$\begin{bmatrix} M(\mathbf{Z}) & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{Q} \\ \mathbf{P} \end{bmatrix} = \begin{bmatrix} \mathbf{g} \\ \mathbf{0} \end{bmatrix} \qquad (*)$$

Construct divergence-free basis for $\mathbf{Q}$ leads to

$$-\nabla.\left(k^{-1}\nabla u\right) = 0 \quad \text{with standard } P_1 \text{ elements} \qquad (\dagger)$$

($\dagger$) coercive and five times smaller than (*).

$\mathbf{P}$, k_{eff} and T_{out} easily computed.

($\dagger$) solved by algebraic multigrid (an interesting topic itself).

Numerical Results

easier $\longrightarrow \longrightarrow \longrightarrow$ **more difficult**

Case 1	Case 2	Case 3	Case 4	Case 5
$\sigma^2 = 1$ $\lambda = 1$	$\sigma^2 = 1$ $\lambda = 0.3$	$\sigma^2 = 1$ $\lambda = 0.1$	$\sigma^2 = 3$ $\lambda = 1$	$\sigma^2 = 3$ $\lambda = 0.1$

Sobol' points

covariance $\exp(-\|\mathbf{x} - \mathbf{y}\|_1/\lambda)$

(2-norm case is similar).

uniform finte element grid $h = 1/m$ on $(0, 1)^2$

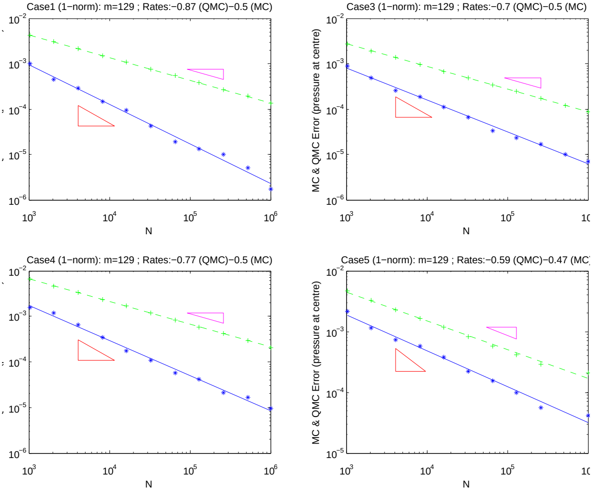
Number of samples $= N$

Standard error in mean pressure at $(1/2, 1/2)$

QMC with 16 random shifts.

No discretisation error present.

MC in green **QMC in blue**, Cases 1,3,4,5.

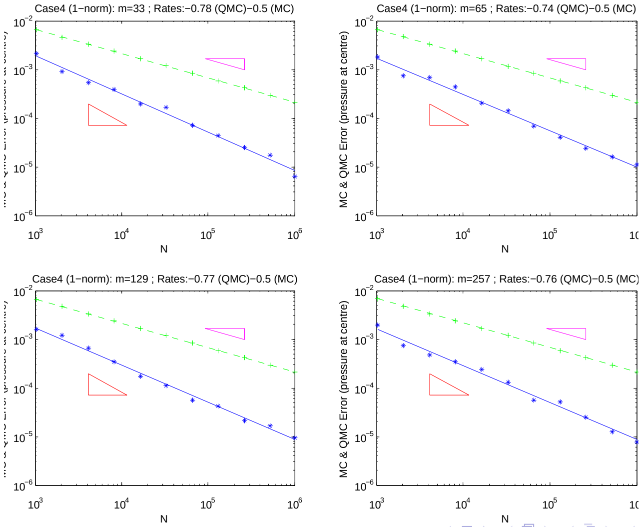


Dimension independence of QMC (and MC)

Standard deviation of mean pressure, Case 4:

as $M(= h^{-2})$ (and hence d) increases

MC in green **QMC in blue**



Effective permeability k_{eff}

discretization error is present.
We estimated (by **linear regression**):
h needed to obtain a **discretization error** $< 10^{-3}$ $(< \mathbf{2 \times 10^3})$
N needed to obtain (Q)MC error $< 0.5 \times 10^{-3}$ $(\mathbf{10^{-3}})$
(95% confidence)

σ^2	λ	$1/h$	N (QMC)	N (MC)	CPU (QMC)	CPU (MC)
1	1	17	1.2(+5)	1.9(+7)	3 min	8 h
1	0.3	129	3.3(+4)	3.9(+6)	55 min	110 h
1	0.1	513	1.2(+4)	5.9(+5)	6.5 h	330 h
3	1	33	4.3(+6)	3.6(+8) *	9 h	750 h *
3	0.1	**513**	**3.0(+4)**	**5.8(+5)**	**20 h**	**390 h**

Smaller λ needs smaller h but also smaller N.

* extrapolated projections.

Timings on a modest laptop!

Summary

- QMC improved on MC in all cases tested
- Speed up factors between 4 and 200.
- Can solve hard problems of interest in hydrogeology
- Readily extends to 3D
- Interesting open problems in rigorous error analysis
- Constructing Sobol' sequences:
  http://web.maths.unsw.edu.au/~fkuo/sobol/
  S. Joe and F. Y. Kuo, SIAM J. Sci. Comp, 30 (2008).