The solution of high dimensional elliptic PDEs with random data

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Joint work with:

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High dimensional Problems: PDE with random data

- Many problems involve PDEs with spatially varying data which is subject to uncertainty.

  Example: groundwater flow in rock underground.

- Uncertainty enters the PDE through its coefficients. (random fields). The quantity of interest: is a random number or field derived from the PDE solution.

  Examples: (i) pressure in medium, (ii) effective permeability, (iii) breakthrough time of a pollution plume .

- Typical Computational Goal: expected value of quantity of interest.

This is the **Forward problem of uncertainty quantification**

Some ingredients

PDE Problem:

$$-\nabla.k\nabla p = f \quad \text{with} \quad k(\mathbf{x},\omega) = \exp(Z(\mathbf{x},\omega)), \quad \text{lognormal}$$

Random field $Z(\mathbf{x},\omega)$ Gaussian at each $\mathbf{x}$
specified mean ($= 0$ here) and (rough) covariance.

no uniform ellipticity, Low regularity,
high contrast, high stochastic dimension,

Computational goal: Functionals of p, e.g.

$$\mathbb{E}(p(\mathbf{x},\omega)) = \int_\Omega p(\mathbf{x},\omega)d\mathbb{P}(\omega) \quad \text{high dimensional}$$

Classical method: Monte-Carlo

- random sampling of Z (how to do it?)
- Finite element method for p
- convergence $\mathcal{O}(1/\sqrt{N})$ (N = # samples) + FE Error.

Outline of talk

Part I: Algorithm: circulant embedding with Quasi-Monte Carlo

IGG, Kuo, Nuyens, Scheichl, Sloan JCP 2011

Part II: Rigorous error estimates

IGG, Kuo, Nicholls, Scheichl, Schwab, Sloan

Numer Math 2014

IGG, Scheichl, Ullmann

Stochastic PDE: Analysis and Computation 2014

IGG, Kuo, Nuyens, Scheichl, Sloan in preparation 2016

Gaussian Random Fields (more generally)

PDE Problem:

$$-\nabla . k \nabla p = f \quad \text{+ Boundary conditions} \qquad k \;=\; \exp(Z)$$

Covariance function: (centred) stationary field:

$$\mathbb{E}[Z(\boldsymbol{x},\cdot)Z(\boldsymbol{y},\cdot)] = \rho(\boldsymbol{x}-\boldsymbol{y}), \quad \rho \quad \text{positive definite}$$

Examples:

$$\rho(\boldsymbol{x}-\boldsymbol{y}) = \sigma^2 \exp\Big(-\|\boldsymbol{x}-\boldsymbol{y}\|/\lambda\Big) \quad \text{“exponential”.}$$

$$\rho(\boldsymbol{x}-\boldsymbol{y}) = \sigma^2 \exp\Big(-\|\boldsymbol{x}-\boldsymbol{y}\|^2/\lambda\Big) \quad \text{“Gaussian”.}$$

σ^2 = variance , λ = lengthscale

The Matérn family: $\rho = \rho_\beta, \quad \beta \in [1/2, \infty)$.
Limiting cases: exponential ($\beta = 1/2$), Gaussian ($\beta = \infty$).

Gaussian Random Fields (more generally)

Loss of uniform ellipticity and boundedness: for all $\epsilon > 0$:

$$\min[\mathbb{P}(k(\boldsymbol{x},\cdot) < \epsilon),\ \mathbb{P}(k(\boldsymbol{x},\cdot)) > \epsilon^{-1})] \ > \ 0$$

Mild smoothness condition on $\rho(\mathbf{0})$:
Karhunen-Loeve (KL) Expansion: (a.s. convergence)

$$Z(\boldsymbol{x},\omega) \ = \ \sum_{j=1}^{\infty} \sqrt{\mu_j}\xi_j(\boldsymbol{x})Y_j(\omega) \qquad Y_j \ \sim \ N(0,1)$$

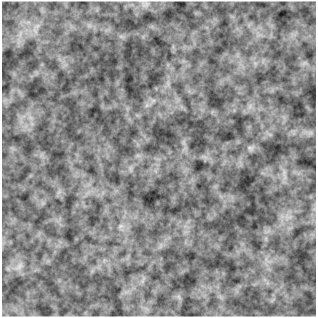
(ξ_j, μ_j) eigenpairs of covariance operator with kernel $\rho(\boldsymbol{x}-\boldsymbol{y})$.

Kolmogorov's theorem: With probability 1,
$k(\boldsymbol{x},\omega) \in C^t(D)$, with $t \in [0,\beta)$

In fact, for all $q \in (1,\infty)$,

- $k \in L^q(\Omega, C^t(D))$,
- and $\|p\|_{L^q(\Omega,H_0^1(D))} \le \|a_{\min}^{-1}\|_{L^q(\Omega)}\|f\|_{H^{-1}}$ (Dirichlet problem).

Non-smooth fields : a typical realization (exponential)



λ - "frequency": Finite element accuracy requires $h \approx \lambda/10$

σ^2 - "amplitude":

$$\frac{\max_x k(\boldsymbol{x}, \omega)}{\min_x k(\boldsymbol{x}, \omega)} \sim \exp(\sigma)$$ high contrast

Mixed FEM ($f = 0$ mixed BCs)

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

Mixed formulation $(q, p) \in H(\mathrm{div}, D) \times L_2(D)$:

$$\begin{aligned} \int_D k^{-1}\mathbf{q}.\mathbf{v} - \int_D p\nabla.\mathbf{v} &= - \int_{\partial D_2} g\mathbf{v}.n \;, \\ - \int_D w\nabla.\mathbf{q} &= 0 \qquad \text{for all} \quad (\mathbf{v}, w). \end{aligned}$$

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Mixed formulation $(\mathbf{q}, p) \in H(\mathrm{div}, D) \times L_2(D)$:

$$\begin{aligned} m(\mathbf{q}, \mathbf{v}) + b(p, \mathbf{v}) &= G(\mathbf{v}), \\ b(w, \mathbf{q}) &= 0 \qquad \text{for all} \quad (\mathbf{v}, w). \end{aligned}$$

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

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

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$h =$ finite element grid size.

PC = Piecewise constants

Space RT_0:
$\mathbf{q}_h = a + b\mathbf{x}$ but divergence free $\implies b = 0$.

Mixed FEM $(f = 0$ mixed BCs)

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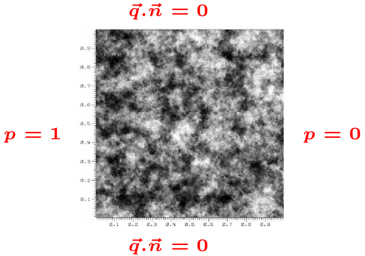
Space RT_0:
$\mathbf{q}_h = a + b\mathbf{x}$ but divergence free $\implies b = 0$.

Quadrature rule: sample $k(\boldsymbol{x}, \omega)$ one point per element
Enough for accuracy: IGG, Scheichl, Ullmann, 2014

Quantities of Interest - computational cell $D = (0,1)^2$



- Pressure head $p(\boldsymbol{x}, \omega)$, e.g. $\boldsymbol{x} = (1/2, 1/2)$.
- Effective permeability

$$k_{\text{eff}}(\omega) = \frac{\int_D q_1(\boldsymbol{x}, \omega) \mathrm{d}\boldsymbol{x}}{-\int_D \partial p / \partial x_1(\boldsymbol{x}, \omega) \mathrm{d}\boldsymbol{x}} = \int_{\Gamma_{\text{out}}} q_1(\boldsymbol{x}, \omega) \, \mathrm{d}\boldsymbol{x}$$

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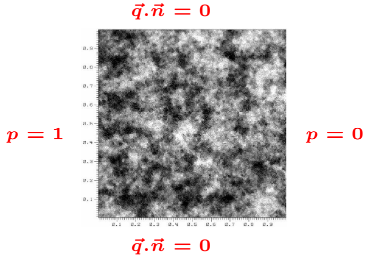

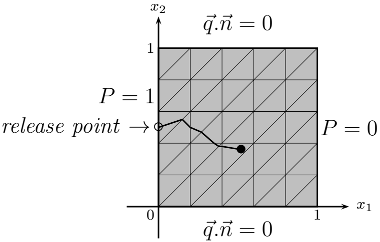

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- Breakthrough time $T_{\text{out}}(\omega)$ from q.
  (Time to reach outflow boundary)

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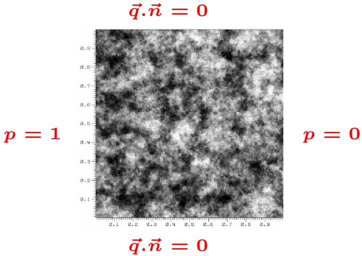

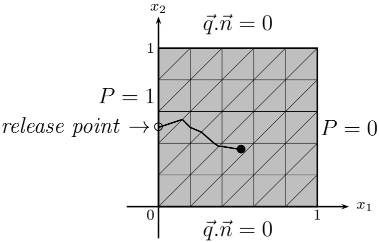

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- Breakthrough time $T_{\text{out}}(\omega)$ from q.

  (Time to reach outflow boundary)

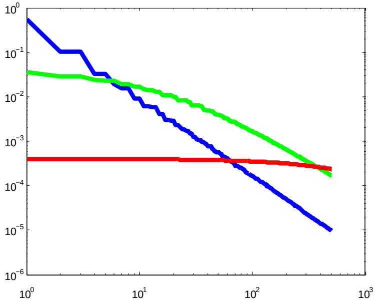
- General format: find $\mathbb{E}[\mathcal{G}(p, \mathbf{q})]$ - some functional $\mathcal{G}(p, \mathbf{q})$.

Sampling by K-L truncation : the effect of lengthscale

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

exponential covariance in 1D

$\log\log$ plot of μ_j for $1 \le j \le 500$:



Plateau before decay starts

$\boldsymbol{\lambda = 1}$

$\boldsymbol{\lambda = 0.1}$

$\boldsymbol{\lambda = 0.01}$

An extreme eigenvalue solver challenge!

Avoiding KL truncation: discretize first in space

Approximation of $\mathbb{E}[\mathcal{G}(p)]$ by $\mathbb{E}[\mathcal{G}(p_h)]$ (focus on pressure)

FEM + quadrature requires random vector
$\boldsymbol{Z} := \{Z(\boldsymbol{x}_i)\}$ at M quadrature points

Covariance Matrix: $R_{i,j} = \rho(\boldsymbol{x}_i - \boldsymbol{x}_j)$ $\quad M \times M$

Seek matrix decomposition:

$$R = BB^\top \qquad (*)$$

where B is $M \times s$, $s \geq M$.

Then (finite "discrete KL" expansion)

$$\mathbf{Z}(\omega) = BY(\omega), \quad \text{where} \quad \mathbf{Y} \sim N(0,1)^s \quad \text{i.i.d.}$$

Because

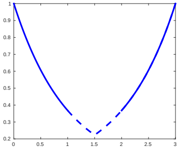
$$\mathbb{E}[\mathbf{Z}\mathbf{Z}^\top] = \mathbb{E}[B\mathbf{Y}\mathbf{Y}^\top B^\top] = BB^\top = R$$

$M \sim h^{-d}$ and so s very large so (*) expensive(?), **but....**

Sampling via Circulant Embedding

For uniform grids (not restrictive) and stationary fields: R is block Toeplitz

Embed R into C - **block circulant** $s \times s$ (Typically $s \sim (2^d)M$)



$$C = \begin{bmatrix} R & A \\ A^T & B \end{bmatrix}$$

(Cheap) Factorization: $C = F\Lambda F^H$ (by FFT)

implies Real Factorization: $C = BB^T$ (provided $\mathrm{diag}(\Lambda) \geq \mathbf{0}$)

$$\mathbb{E}[\mathcal{G}(p)] \approx \int_{\mathbb{R}^s} F(\mathbf{y}) \prod_{j=1}^{s} \phi(y_j) \mathrm{d}\boldsymbol{y}, \qquad F(\mathbf{y}) = \mathcal{G}(p_h(\cdot, \mathbf{y}))$$

$$= \int_{[0,1]^s} F(\Phi_s^{-1}(\mathbf{v}))\mathrm{d}\mathbf{v} =: I_s(F) .$$

$\phi(y) = \exp(-y^2/2)/\sqrt{2\pi}$, Φ_s^{-1} = inv. cum. normal

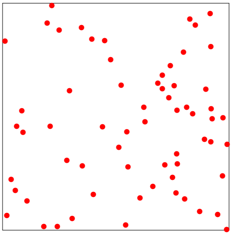
FEM (h) + high dimensional integration (?)

Integration over $[0,1]^s$ (very large s): QMC methods

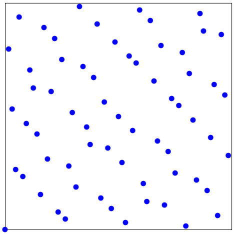
$$\int_{[0,1]^s} f(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} \;\approx\; \frac{1}{N}\sum_{k=1}^{N} f(\boldsymbol{z}^{(k)})$$

Monte Carlo method
$\boldsymbol{z}^{(k)}$ **random uniform**
$\mathcal{O}(N^{-1/2})$ convergence
order of variables irrelevant

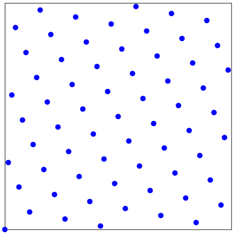
Quasi-Monte Carlo method
$\boldsymbol{z}^{(k)}$ deterministic
close to $\mathcal{O}(N^{-1})$ convergence
order of variables very important



64 random points



64 Sobol′ points



64 lattice points

Numerical Results

Covariance

$$r(\boldsymbol{x},\boldsymbol{y}) = \sigma^2 \exp\Big(-\|\boldsymbol{x}-\boldsymbol{y}\|_1/\lambda \Big) .$$

($\|\cdot\|_2$ similar).

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

FEM: Uniform grid $h = 1/m$ on $(0,1)^2$, $M \sim m^2$.

Sampling: circulant embedding via FFT (dimension $s \geq 4M$)

High dimensional integration: QMC with N Sobol' points

Algorithm profile

Time (sec) for $N = 1000$, CASE 1:

percentages in red, orders in blue

m	s	Setup	InvN	FFT	AMG	TOT
33	4.1 (+3)	0.00	1.0 17	0.22 4	4.5 76	5.9
65	1.7 (+4)	0.01	3.9 17	1.2 5	16.5 75	22
129	6.6 (+4)	0.06	15 16	5.1 6	67 73	92
257	2.6 (+5)	0.15	62 16	31 8	290 73	400
513	1.0 (+6)	0.6	258 15	145 8	1280 73	1750
	m^2	m^2	m^2	$m^2 \log m$	$\sim m^2$	$\sim m^2$

InvN = Inversion of cumulative normal

AMG = Algebraic Multigrid = Fast system solver

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	m^2	m^2	m^2	$m^2 \log m$	$\sim m^2$	$\sim m^2$

InvN = Inversion of cumulative normal

AMG = Algebraic Multigrid = Fast system solver

One MFE solve with $513^2 = 2.6(+5)$ DOF takes ≈ 1.3 sec

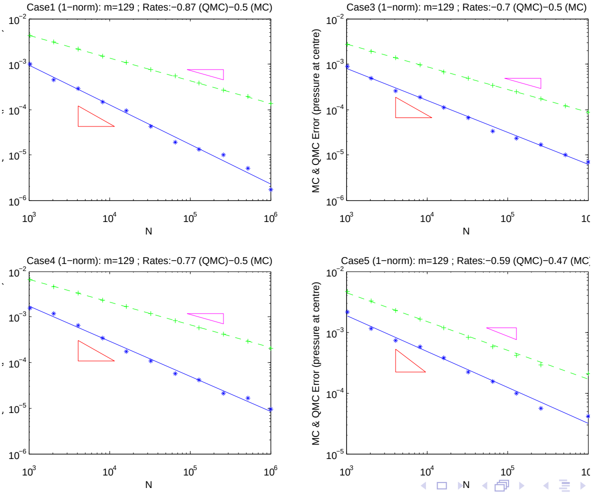
Standard deviation of mean pressure

16 random shifts used to estimate standard deviation.

Theorem: $\mathbb{E}[p_h(1/2,1/2)] = \mathbb{E}[p(1/2,1/2)]$ for all h.

No discretization error : good test for QMC

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

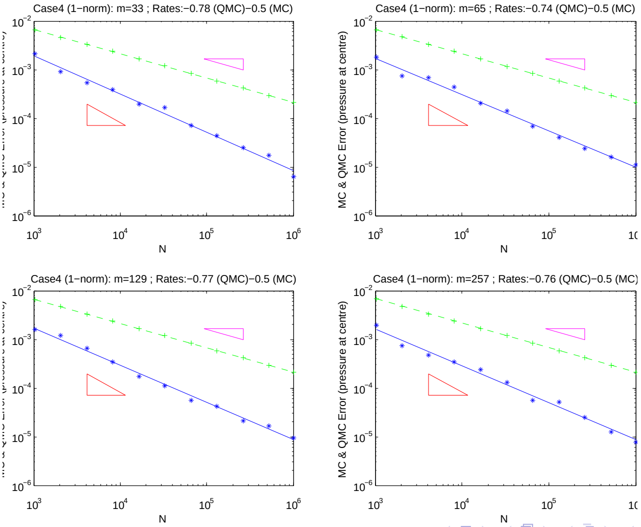


Dimension independence of QMC (and MC)

Standard deviation of mean pressure, Case 4:

as $m(= 1/h)$ (and hence s) 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 $< 10^{-3}$ ($< 2 \times 10^{3}$)
N needed to obtain (Q)MC error $< 0.5 \times 10^{-3}$ (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 (lengthscale) needs smaller h but also smaller N.
Bigger σ^2 (variance) doesn't affect h but needs larger N

* extrapolated projections.

Strong superiority of QMC in all cases.

Breakthrough time T_{out}

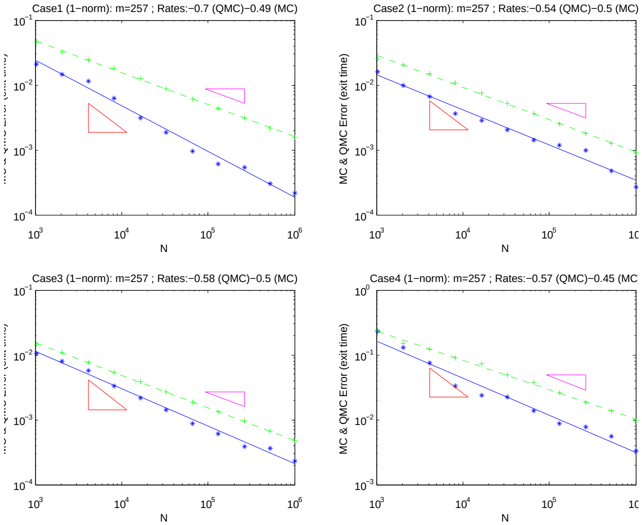
Here discretization error is more significant.

For **Cases 2 and 4** for discr. error $< 5 * (10^{-3})$ need $h = 1/65$

For statistical error $< 2.5 * 10^{-3}$ (95% confidence) need:

Case 2	$\sigma^2 = 1, \ \lambda = 0.3$	$N_{MC} = 5.2(+5)$	$N_{QMC} = 1.2(+5)$ speedup $\approx$ 4
Case 4	$\sigma^2 = 3, \ \lambda = 1$	$N_{MC} = 6.5(+7)$	$N_{QMC} = 4.3(+6)$ speedup $\approx$ 15

Breakthrough time, Cases 1-4



MC in green QMC in blue

QMC still superior but rate $1/N$ is now missing.

Recent progress on theory (brief)

Primal form (Dirichlet problem)

$$-\nabla.k(\boldsymbol{x},\omega)\nabla p = f \quad \text{on} \quad D, \qquad p = 0 \quad \text{on} \quad \partial D\ .$$

- lognormal case: $k(\boldsymbol{x},\omega) = \exp(Z(\boldsymbol{x},\omega))$
- piecewise linear FEM with quadrature: p_h
- Linear functional $\mathcal{G}(p)$ $\mathcal{G}(p_h)$
- Quantity of interest: $\mathbb{E}[\mathcal{G}(p)]$ $I_s(F)$

  where $F(\mathbf{y}) = \mathcal{G}(p_h(\cdot,\mathbf{y}))$
- Randomly shifted lattice rules $Q_{s,N}(\boldsymbol{\Delta}, F)$
  (with N points, defined next slide)

RMS Error $e_{h,N}^2 \ := \ \mathbb{E}^{\Delta}\left[|I_s(F) - Q_{s,N}(\boldsymbol{\Delta},F)|^2\right]$

Some QMC Theory (Lattice rules)

$$I_s(F) \quad := \quad \int_{\mathbb{R}^s} F(\boldsymbol{y}) \prod \phi(y_j) \mathrm{d}\boldsymbol{y} \;=\; \int_{[0,1]^s} F(\Phi_s^{-1}(\boldsymbol{z})) \mathrm{d}\boldsymbol{z}$$

$$Q_{s,N}(\boldsymbol{\Delta}; F) \quad := \quad \frac{1}{N} \sum_{i=1}^{N} F\left(\Phi_s^{-1}\left(\mathrm{frac}\left(\frac{i\,\boldsymbol{z}}{N} + \boldsymbol{\Delta}\right)\right)\right)$$

generating vector: $\boldsymbol{z} \in \mathbb{N}^s, \quad 1 \le z_j \le N-1$

random shift $\boldsymbol{\Delta} \in [0,1]^s$ uniformly distributed.

Weighted Sobolev norm: $\|F\|_{s,\gamma}^2 := \sum_{\mathfrak{u} \subseteq \{1:s\}} \frac{1}{\gamma_{\mathfrak{u}}} J_{\mathfrak{u}}(F)^2$

where $J_{\mathfrak{u}}(F)^2 =$

$$\int_{\mathbb{R}^{|\mathfrak{u}|}} \left(\int_{\mathbb{R}^{s-|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}; \boldsymbol{y}_{\{1:s\}\setminus\mathfrak{u}}) \prod_{j \in \{1:s\}\setminus\mathfrak{u}} \phi(y_j)\, \mathrm{d}\boldsymbol{y}_{\{1:s\}\setminus\mathfrak{u}} \right)^2 \prod_{j\in\mathfrak{u}} \psi_j^2(y_j)\, \mathrm{d}\boldsymbol{y}_{\mathfrak{u}}$$

$\gamma_{\mathfrak{u}}$ - controls relative importance of the derivatives

$\psi_j(y_j) = \exp(-\alpha_j |y_j|)$ - controls behaviour as $|\mathbf{y}| \to \infty$

QMC Theory...

Theorem (Kuo and Nuyens FoCM 2015) Suppose $\|F\|_{s,\boldsymbol{\gamma}} < \infty$. Then a generating vector $\boldsymbol{z} \in \mathbb{N}^s$ can be constructed (efficiently) so that

$$\sqrt{\mathbb{E}^{\boldsymbol{\Delta}}\left[|I_s(F) - Q_{s,N}(\boldsymbol{\Delta}, F)|^2\right]} \leq 2\left(\frac{1}{N}\right)^{1/2\lambda} C_s(\boldsymbol{\gamma}, \boldsymbol{\alpha}, \lambda)\|F\|_{s,\boldsymbol{\gamma}} \quad (*)$$

for all $\lambda \in (1/2, 1]$. **So the next steps are ...**

- Estimate the derivatives $\partial^{|\mathfrak{u}|} p_h / \partial \mathbf{y}_{\mathfrak{u}}$, then derivatives of F.....
- Then the norm $\|F\|_{s,\boldsymbol{\gamma}}$.
- Choose $\gamma_{\mathfrak{u}}$ and α_j to minimise the RHS of (*).
- RHS becomes $C(\lambda)\left(\frac{1}{N}\right)^{1/(2\lambda)}$, $C(\lambda)$ independent of s

provided.... eigenvalues of the circulant satisfy:

$$\sum_{j=1}^{s} \left(\frac{\lambda_j}{s}\right)^{\lambda/(1+\lambda)} \leq C \quad \text{for all} \quad s.$$

Based on a heuristic for the Matérn family ....

Rates for the Matérn class

- Dimension independent rate $\mathcal{O}\left(\frac{1}{N^{-(1-\delta)}}\right)$ δ arbitrarily small, if $\nu > 2$.
- Dimension independent rate at least $\mathcal{O}\left(\frac{1}{N}\right)^{1/2}$ if $\nu > 1$

Heuristic assumes eigenvalues of the circulant approach eigenvalues of the corresponding periodic covariance integral operator.

Conclusion:

For Matérn parameter ν large enough, combined FE and QMC error:

$$\sqrt{\mathbb{E}^{\boldsymbol{\Delta}}\left[\left|\mathbb{E}[\mathcal{G}(p)] - Q_{s,N}(\boldsymbol{\Delta}, \mathcal{G}(p_h))\right|^2\right]} \;\leq\; C[h^2 + N^{-(1-\delta)}].$$

with δ arbitrarily close to 0 independent of dimension s.

Summary

- QMC improved on MC in all cases tested
- Speed up factors between 4 and 200.
- Can solve relatively hard problems of some interest in applications. Readily extends to 3D
- Rigorous analysis shows convergence up to $\mathcal{O}(h^2) + \mathcal{O}(1/N)$ independent of dimension.
- Theory contains some assumptions which have to be verified empirically.
- Constructing Sobol' sequences and lattice rules: http://web.maths.unsw.edu.au/~fkuo
- Lots of recent work: Multilevel and higher order methods (Giles, Scheichl, Kuo, Schwab, Sloan, Dick, ...many others...)
- The exponential covariance leaves open questions!

Dimension independence of QMC (and MC)

Standard deviation of mean pressure, Case 4:
as $m(=1/h)$ (and hence s) increases
MC in green   QMC in blue