A multigrid multilevel Monte Carlo method for transport in the Darcy-Stokes flow

Prashant Kumar

Joint work with

P. Luo, C. Rodrigo, F. J. Gaspar, C. W. Oosterlee

Workshop Day: Multilevel and Multigrid Methods, 30 May, 2018

TU Delft

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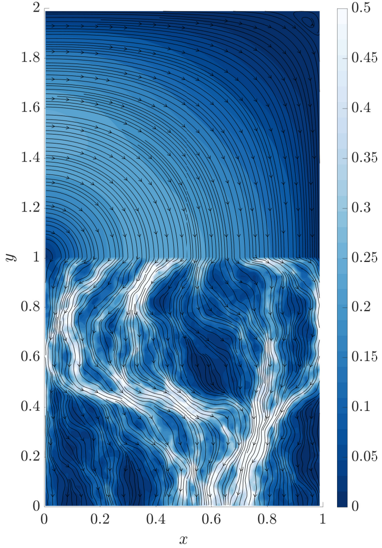
Introduction

Darcy-Stokes flow



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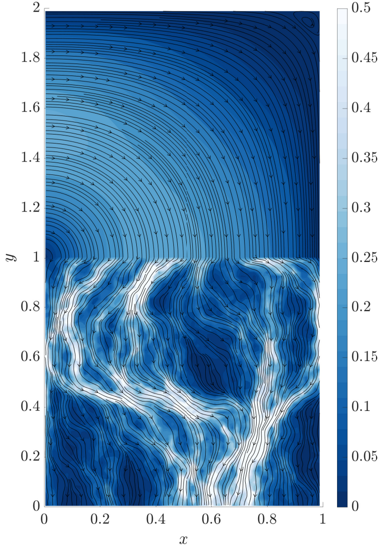
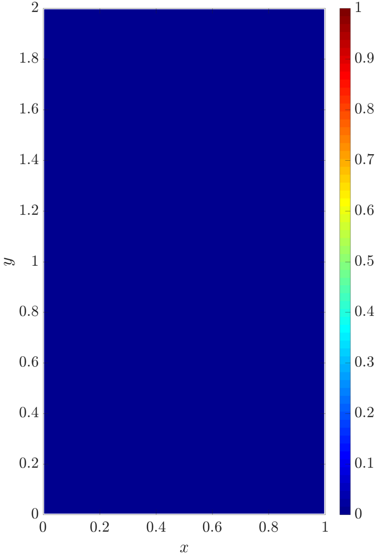


Convection dominated transport



Outline

Three parts:

1. Solver optimized w.r.t random inputs
   - Monolithic multigrid for Darcy-Stokes flow
   - Benchmarking
   - ADI time-stepping for transport

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   - MLMC estimator and error analysis
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3. Performance of the Multigrid MLMC method

Governing equations

Stokes flow

$$-\nabla \cdot \boldsymbol{\sigma}^s = \mathbf{f}^s$$

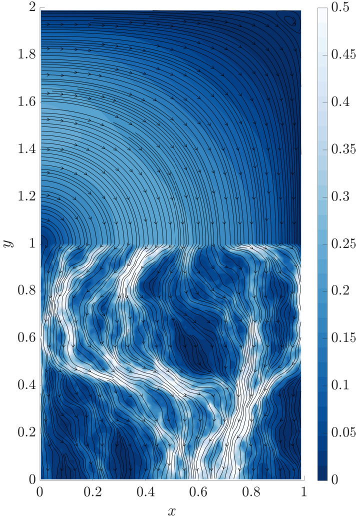
$$\nabla \cdot \mathbf{u}^s = \mathbf{0}$$

Darcy flow

$$\eta K^{-1}\mathbf{u}^d + \nabla p^d = \mathbf{0}$$

$$\nabla \cdot \mathbf{u}^d = f^d$$

K: log-normal random field



Discretization: FV on a staggered mesh

Interface conditions

1. Mass conservation
$$\mathbf{u}^s \cdot \mathbf{n} = \mathbf{u}^d \cdot \mathbf{n}$$
2. Normal stress balance
$$-\mathbf{n} \cdot \boldsymbol{\sigma}^s \cdot \mathbf{n} = p^d$$
3. Beaver-Joseph-Saffman condition
$$\mathbf{u}^s \cdot \boldsymbol{\tau} + \left(\frac{\sqrt{K}}{\alpha_{BJ}} \right) \boldsymbol{\tau} \cdot \boldsymbol{\sigma}^s \cdot \mathbf{n} = \mathbf{0}$$

   No slip condition
$$\mathbf{u}^s \cdot \boldsymbol{\tau} = \mathbf{0}$$

$\mathbf{n}, \boldsymbol{\tau}$ are normal and tangential vectors to the interface

Stochastic model for permeability

Parametrized Matérn covariance model

$$C_\Phi(r) = \sigma_c^2 \frac{2^{1-\nu_c}}{\Gamma(\nu_c)} \left(2\sqrt{\nu_c}\frac{r}{\lambda_c}\right)^{\nu_c} K_{\nu_c}\left(2\sqrt{\nu_c}\frac{r}{\lambda_c}\right), \qquad r = ||\mathbf{x} - \mathbf{y}||$$

$$\Phi = (\nu_c, \lambda_c, \sigma_c^2) = \textbf{(smoothness, correlation length, variance)}$$

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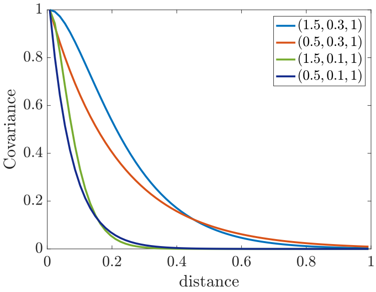

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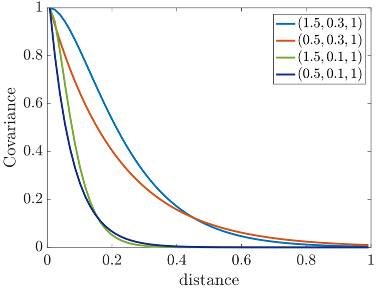
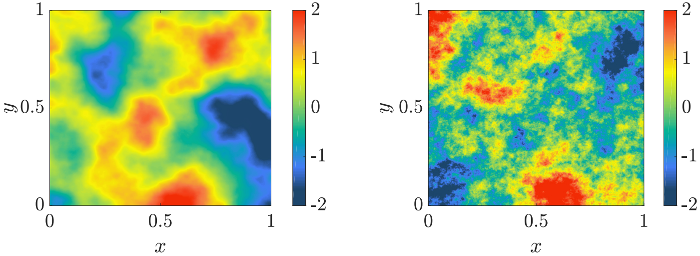


Sampling technique: Karhunen-Loéve expansion, **Circulant embedding**, etc

Isotropic random fields



$\Phi_1 = (1.5, 0.3, 1)$ $\Phi_2 = (0.5, 0.3, 1)$

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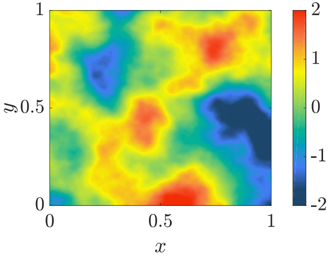

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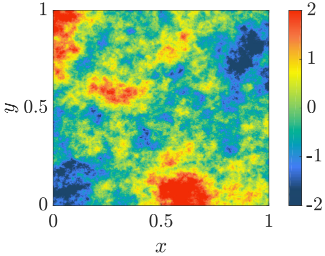

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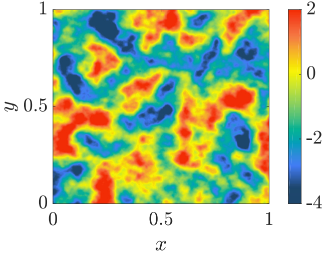

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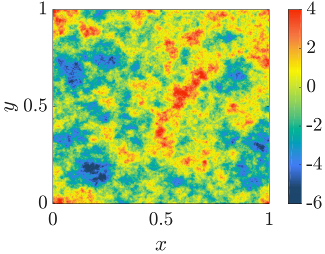
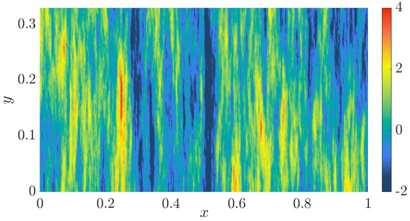
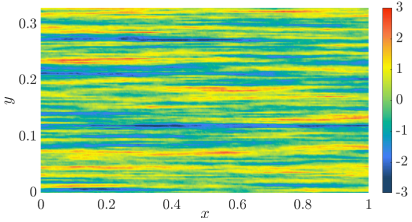


$\Phi_4 = (0.5, 0.1, 3)$

Anisotropic random fields



$\lambda_{cx} = 0.06, \lambda_{cy} = 0.33$



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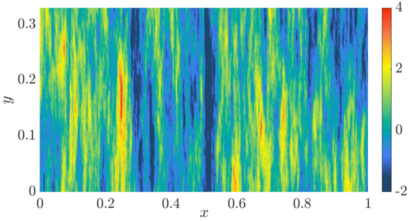

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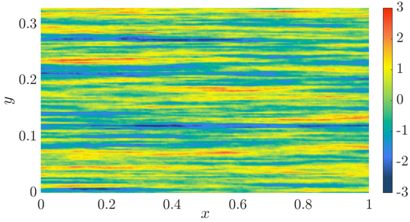

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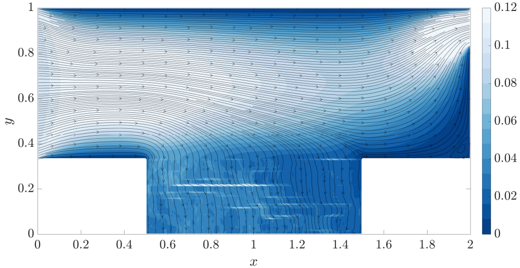


Cross-flow filtration problem

Stochastic transport model

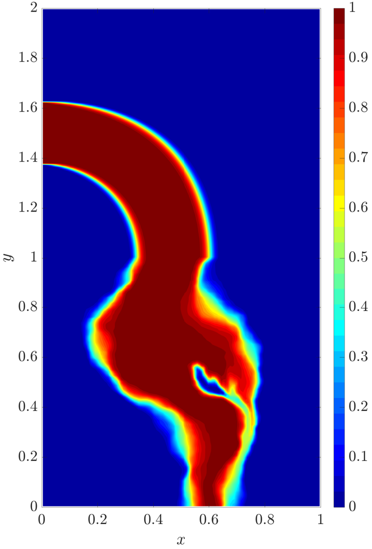
$$\phi \frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{u} - \mathbb{D}\nabla c) = \phi f^t$$
$$c = c_0 \quad \text{in} \quad t = 0.$$

Boundary condition

$$(c\mathbf{u} - \mathbb{D}\nabla c)\cdot\mathbf{n} = (c_{in}\mathbf{u})\cdot\mathbf{n} \quad \text{inflow boundary}$$
$$\mathbb{D}\nabla c \cdot \mathbf{n} = 0 \quad \text{outflow boundary}$$

Discontinuous inflow condition

$$c_{in}(0, y, t) = 1, \quad \text{for} \quad |y - 1.5| \leq 1/8, \quad t \geq 0$$



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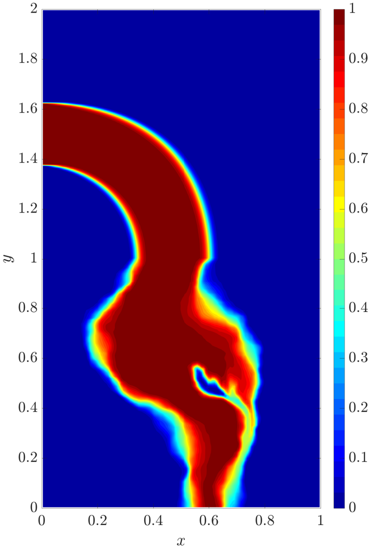
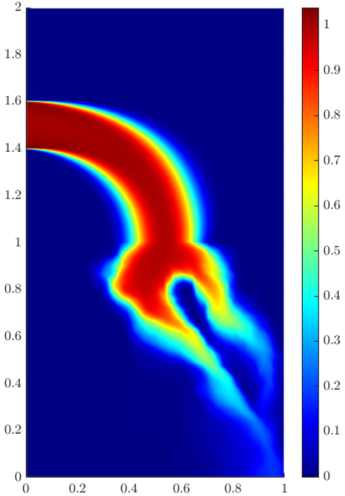


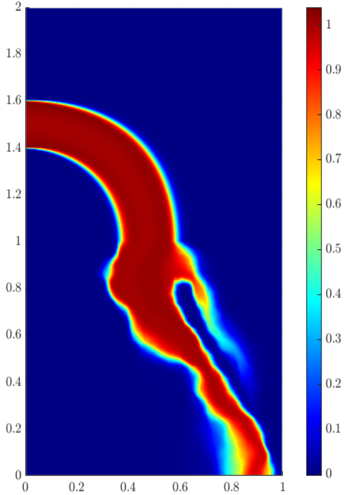
Discretization: Quadratic upwinding combined with ADI time-stepping

Sensitivity to numerical diffusion

First order upwind $c(x, y, t = 6.0)$



Flux limited QUICK[1] $c(x, y, t = 6.0)$



Quadratic Upwind Interpolation for Convective Kinematics (QUICK), B.P.Leonard, 1979

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Multigrid

$$\boxed{L_h u_h = f_h, \quad u_h^m \to u_h^{m+1}}$$

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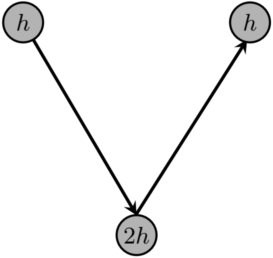
Pre-smoothing: $\overline{u}_h^m = \mathcal{S}_h u_h^m$

Compute: $\overline{r}_h^m = f_h - L_h \overline{u}_h^m$

Restriction: $\overline{r}_{2h}^m = \mathcal{I}_h^{2h} \overline{r}_h^m$



Solve: $L_{2h} \overline{e}_{2h}^m = \overline{r}_{2h}^m$

Interpolate: $\overline{e}_h^m = \mathcal{I}_{2h}^h \overline{e}_{2h}^m$

Correct: $\overline{u}_h^{m+1} = \overline{u}_h^m + \overline{e}_h^m$

Post-smoothing: $u_h^{m+1} = \mathcal{S}_h \overline{u}_h^{m+1}$

Saddle point system

Discretization of the Darcy-Stokes system

$$\begin{bmatrix} \mathcal{A}_h & \mathcal{B}_h^T \\ \mathcal{B}_h & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}_h \\ p_h \end{bmatrix} = \begin{bmatrix} \mathbf{g}_h \\ f_h \end{bmatrix}$$

- $\mathcal{B}_h^T$: discrete gradient
- $\mathcal{B}_h$: minus discrete divergence
- $\mathcal{A}_h$: discrete $-\eta\Delta$ for the Stokes equation
  discrete $K^{-1}I_h$ for the Darcy equation

Uzawa smoothing

Splitting the saddle point system:

$$\begin{bmatrix} \mathcal{A}_h & \mathcal{B}_h^T \\ \mathcal{B}_h & 0 \end{bmatrix} = \begin{bmatrix} \mathcal{M}_h & 0 \\ \mathcal{B}_h & -\zeta_h^{-1} I_h \end{bmatrix} - \begin{bmatrix} \mathcal{M}_h - \mathcal{A}_h & -\mathcal{B}_h^T \\ 0 & -\zeta_h^{-1} I_h \end{bmatrix}$$

- ζ_h : some positive parameter
- $\mathcal{M}_h$: a suitable smoother corresponding to operator $\mathcal{A}_h$

Uzawa, 1958

Uzawa smoother

Define an iteration $\mathbf{u}_h^{k-1}, p_h^{k-1} \to \mathbf{u}_h^k, p_h^k$

$$\left[\begin{array}{cc} \mathcal{M}_h & 0 \\ \mathcal{B}_h & -\zeta_h^{-1} I_h \end{array}\right] \left[\begin{array}{c} \mathbf{u}_h^k \\ p_h^k \end{array}\right] = \left[\begin{array}{cc} \mathcal{M}_h - \mathcal{A}_h & -\mathcal{B}_h^T \\ 0 & -\zeta_h^{-1} I_h \end{array}\right] \left[\begin{array}{c} \mathbf{u}_h^{k-1} \\ p_h^{k-1} \end{array}\right] + \left[\begin{array}{c} \mathbf{g}_h \\ f_h \end{array}\right]$$

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Symmetric Gauss-Seidel iteration for velocity

$$\mathbf{u}_h^k = \mathbf{u}_h^{k-1} + \mathcal{M}_h^{-1} \left(\mathbf{g}_h - \mathcal{A}_h \mathbf{u}_h^{k-1} - \mathcal{B}_h^T p_h^{k-1} \right)$$

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Symmetric Gauss-Seidel iteration for velocity

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Richardson iteration for pressure

$$p_h^k = p_h^{k-1} + \zeta_h (\mathcal{B}_h \mathbf{u}_h^k - f_h)$$

Optimal Richardson parameter

Local Fourier Analysis (LFA) is used to obtain optimal ζ_h

$$\zeta_h(i,j) = \begin{cases} \eta \text{ (viscosity)} & \text{in} \qquad \text{Stokes domain} \\ \frac{\eta h^2}{5\overline{K}_h(i,j)} & \text{in} \qquad \text{Darcy domain} \end{cases}$$

where

$$\overline{K}_h(i,j) = \frac{1}{8}[4K_{i,j} + K_{i-1,j} + K_{i+1,j} + K_{i,j-1} + K_{i,j+1}]$$

P. Luo, C. Rodrigo, F. J. Gaspar and C.W. Oosterlee, 2017

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Optimized w.r.t random field

– fluctuations in permeability is incorporated via $\overline{K}_h(i,j)$

– ζ_h is modified on each grid level

P. Luo, C. Rodrigo, F. J. Gaspar and C.W. Oosterlee, 2017

Benchmarking

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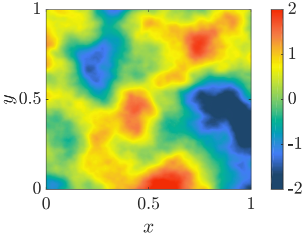

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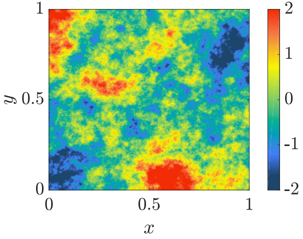

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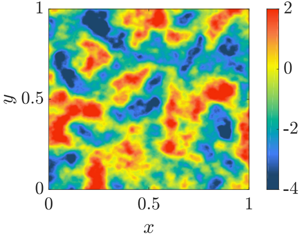

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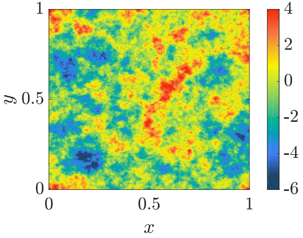

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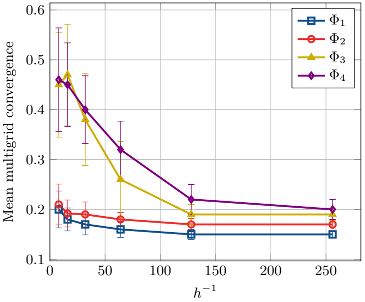
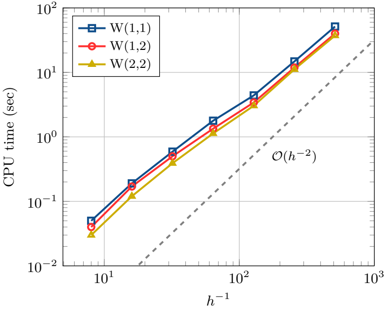
Multigrid performance for W(2,2)-cycle





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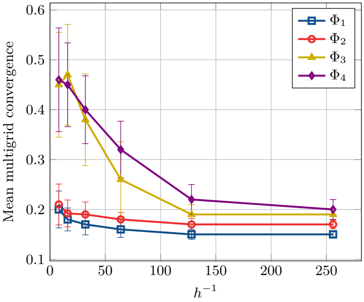

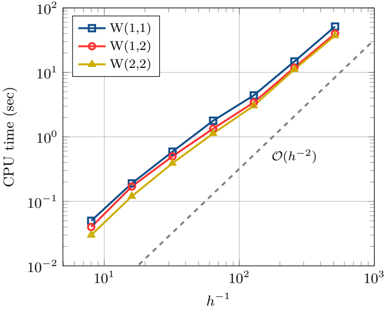

– Efficiency matches with constant permeability case after certain refinement

Alternating Direction Implicit (ADI) time-stepping

Semi-discrete formulation for transport equation

$$\frac{\partial c_h}{\partial t} + \mathcal{L}_h c_h = f_h$$

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$$\left(I_h + \tfrac{\Delta t}{2}\mathcal{L}_h^x\right) c_h^{m-1/2} = \tfrac{\Delta t}{2} f_h^{m-1/2} + \left(I_h - \tfrac{\Delta t}{2}\mathcal{L}_h^y\right) c_h^{m-1}$$ x-Implicit, y-Explicit

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$$\left(I_h + \tfrac{\Delta t}{2}\mathcal{L}_h^y\right) c_h^{m} = \tfrac{\Delta t}{2} f_h^{m} + \left(I_h - \tfrac{\Delta t}{2}\mathcal{L}_h^x\right) c_h^{m-1/2} \qquad \text{y-Implicit, x-Explicit}$$

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Benefits:

- Requires inverting two tridiagonal matrices
- Second-order accurate in time
- Unconditionally stable (coarser time-step can be used in MLMC)

Monte Carlo for stochastic transport model

Monte Carlo estimator

$$\mathbb{E}[c_h] \approx \mathcal{E}_N^{MC}[c_h] := \frac{1}{N}\sum_{i=1}^{N} c_h(\omega_i)$$

Monte Carlo for stochastic transport model

Monte Carlo estimator

$$\mathbb{E}[c_h] \approx \mathcal{E}_N^{MC}[c_h] := \frac{1}{N}\sum_{i=1}^{N} c_h(\omega_i)$$

- Balance discretization error $\mathcal{O}(h^\alpha)$ with sampling error $\sqrt{\frac{\mathbb{V}[c]}{N}}$

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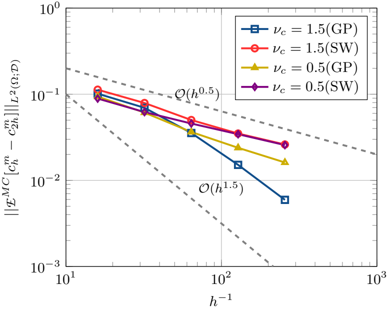
- Balance discretization error $\mathcal{O}(h^\alpha)$ with sampling error $\sqrt{\frac{\mathbb{V}[c]}{N}}$
- Cost scales as $\sim \mathcal{O}(h^{-(2\alpha+\gamma)})$ where $\mathcal{O}(h^{-\gamma})$ is cost of one sample

Discretization error (α)



Inflow boundary conditions: Gaussian plume (GP) and Square wave (SW)

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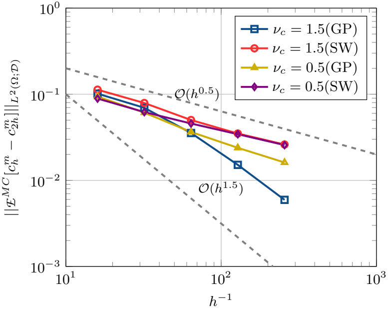

Inflow boundary conditions: Gaussian plume (GP) and Square wave (SW)

For "hardest" case: $\nu_c = 0.5$ (SW)
$\alpha = \nu_c = 0.5$ (rough permeability field)
$\gamma = 3$ (optimal solver for 2D unsteady problems)

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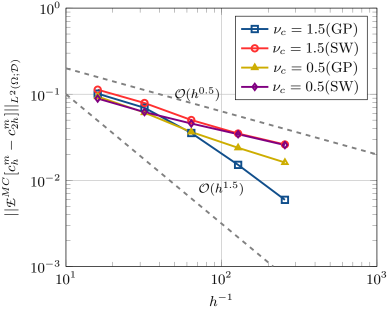

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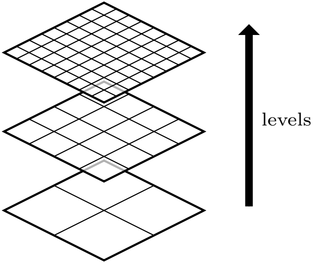
– To get an error reduction of factor 2 $\rightarrow$ cost grows by a factor of 256

Multilevel Monte Carlo (MLMC)

Distribute the cost on a hierarchy of levels:

$$\mathbb{E}[c_L] = \mathbb{E}[c_0] + \sum_{\ell=1}^{L} \mathbb{E}[c_\ell - c_{\ell-1}]$$



M.B. Giles, 2008

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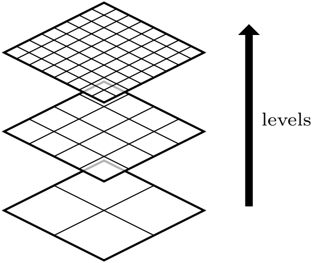

Inexpensive to compute

- $\mathbb{E}[c_0]$ due to coarse grid
- $\mathbb{E}[c_\ell - c_{\ell-1}]$ due to small sample variance $\mathbb{V}[c_\ell - c_{\ell-1}]$

M.B. Giles, 2008

MLMC estimator

Standard Monte Carlo estimator for each expectation

$$\mathcal{E}_L^{ML}[c_L] := \mathcal{E}_{N_0}^{MC}[c_0] + \sum_{\ell=1}^{L} \mathcal{E}_{N_\ell}^{MC}[c_\ell - c_{\ell-1}]$$

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The associated MSE can be decomposed as

$$\left|\left|\mathbb{E}[c] - \mathcal{E}_L^{ML}[c_L]\right|\right|_{L^2(\Omega,\mathcal{D})}^2 \leq \mathcal{O}(h_L^{2\alpha}) + \sum_{\ell=0}^{L} \frac{\mathcal{V}[c_\ell - c_{\ell-1}]}{N_\ell},$$

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– Best possible MSE is $\sim \mathcal{O}(h_L^{2\alpha}) = TOL^2$

Sampling strategy

- Fix number of samples on finest level, $N_L \sim \mathcal{O}(10)$

Mishra and Schwab, 2012

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- Assuming $\mathcal{V}[c_\ell - c_{\ell-1}] = \mathcal{O}(h_\ell^\beta)$, we get $N_\ell = N_L 2^{\beta(L-\ell)}$

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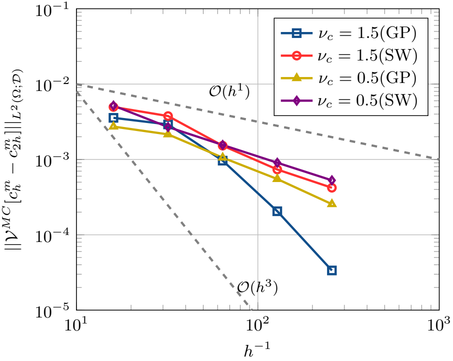
– *Asymptotically optimized*

Mishra and Schwab, 2012

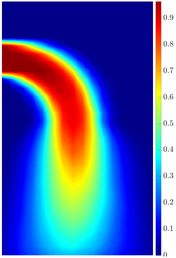
Level-dependent variance (β)



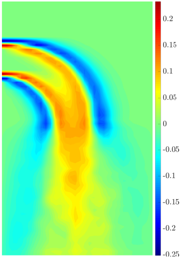
– Typically, variance decays 2x faster than the discretization error, i.e. $\beta = 2\alpha$

– From this, we can deduce $N_\ell = N_L 2^{\beta(L-\ell)}$

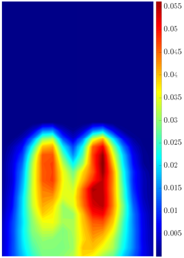
2-level MLMC: Concentration field at $t = 6.00$



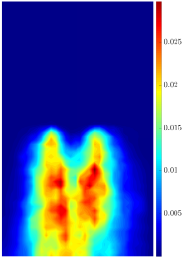
$\mathbb{E}[c_0]$ | $h_0 = \nabla t_0 = 1/16$ | $N_0 = 512$



$\mathbb{E}[c_1 - c_0]$ | $h_1 = \nabla t_1 = 1/32$ | $N_1 = 256$

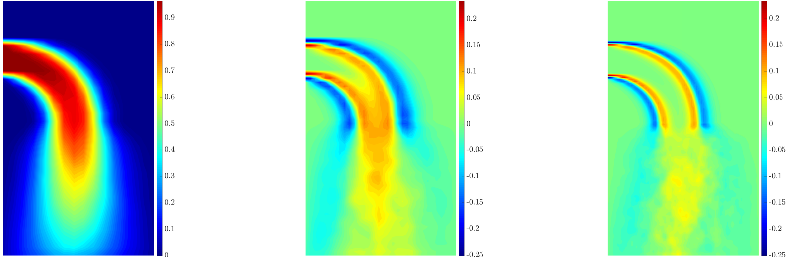


$\mathbb{V}[c_0]$ | $h_0 = \nabla t_0 = 1/16$ | $N_0 = 512$

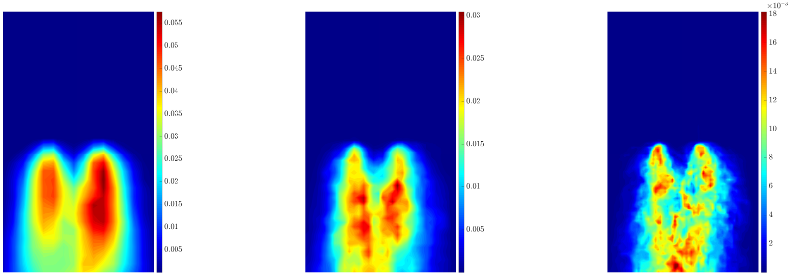


$\mathbb{V}[c_1] - \mathbb{V}[c_0]$ | $h_1 = \nabla t_1 = 1/32$ | $N_1 = 256$

3-level MLMC: Concentration field at $t = 6.00$

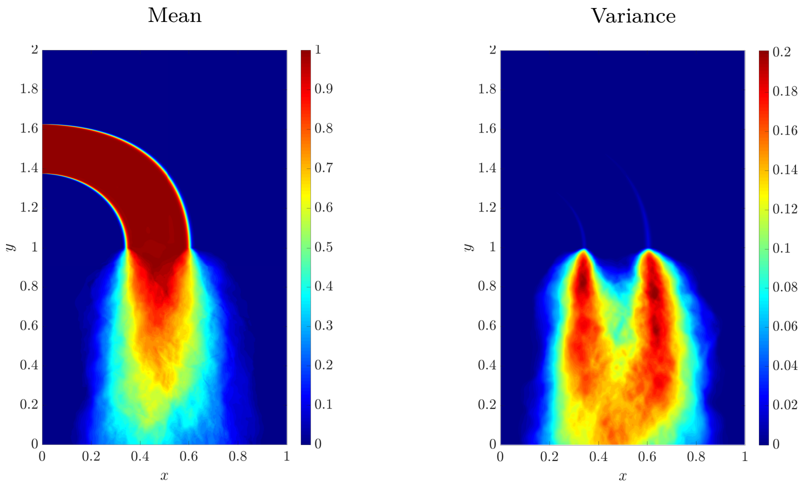


$\mathbb{E}[c_0]$ $\mathbb{E}[c_1 - c_0]$ $\mathbb{E}[c_2 - c_1]$



$\mathbb{V}[c_0]$ $\mathbb{V}[c_1] - \mathbb{V}[c_0]$ $\mathbb{V}[c_2] - \mathbb{V}[c_1]$

6-level MLMC estimate: Concentration field $c(x, y, T = 6.00)$

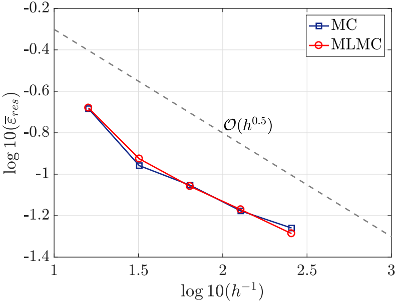


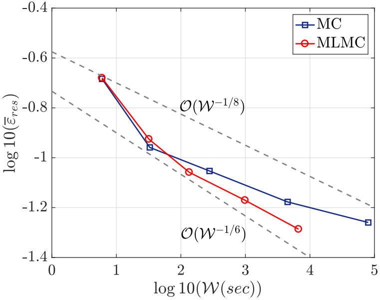
– Finest level: $h_L = \nabla t_L = 1/512$

– Sampling sequence: $N_\ell = N_L 2^{(L-\ell)}$ with $N_L = 16$

– Uncertainty dimension: 512×512

Accuracy vs cost





– *Asymptotically optimal MLMC estimator*

Conclusion

Presented a multigrid MLMC method for transport in Darcy-Stokes flow

- Uzawa smoothers in multigrid can result in a fast solver for Darcy-Stokes flow
- Transport in random porous media is very sensitive to numerical diffusion
- ADI method is highly suitable for MLMC due to stability, accuracy and fast time-stepping
- For rough problems, MLMC estimator has same computational complexity as its deterministic counterpart

Thank you for your attention!

Questions?

1. P. Kumar, C. W. Oosterlee, R. P. Dwight, *A Multigrid Multilevel Monte Carlo method using high-order finite-volume scheme for lognormal diffusion problem*, International Journal for Uncertainty Quantification 7 (1) (2017) 57-81.
2. P. Kumar, P. Luo, F. J. Gaspar, C. W. Oosterlee, *A multigrid multilevel Monte Carlo method for transport in the Darcy-Stokes system*, Journal of Computational Physics (to appear)
3. P. Kumar, C. Rodrigo, F. J. Gaspar, C. W. Oosterlee, *On cell-centered multigrid methods and Local Fourier Analysis for PDEs with random coefficients*, arXiv preprint arXiv:1803.08864

MLMC complexity

Cost of MLMC estimator

$$\mathcal{W}_L^{ML} = \sum_{\ell=0}^{L} N_\ell \mathcal{W}_\ell$$

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$\beta > \gamma$

$- - - - - - - - - - -$

- Dominant cost from the coarsest level

$$\begin{aligned}\mathcal{W}_L^{ML} &= \mathcal{O}(N_0 \mathcal{W}_0) \\ &= \mathcal{O}(\mathrm{TOL}^{-2})\end{aligned}$$

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- All levels equally contribute

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- Dominant cost from the finest level

$$\mathcal{W}_L^{ML} = \mathcal{O}(N_L \mathcal{W}_L) = \mathcal{O}(\mathrm{TOL}^{-2-(\gamma-\beta)/\alpha})$$

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$$\mathcal{W}_L^{ML} = \mathcal{O}(N_L \mathcal{W}_L) = \mathcal{O}(\mathrm{TOL}^{-2-(\gamma-\beta)/\alpha})$$

– Standard MC: $\mathcal{W}^{MC} = \mathcal{O}(\mathrm{TOL}^{-2-\gamma/\alpha})$