Computation of macro spreading in 3D porous media with uncertain data

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joint work with
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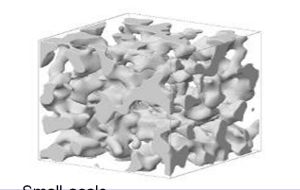
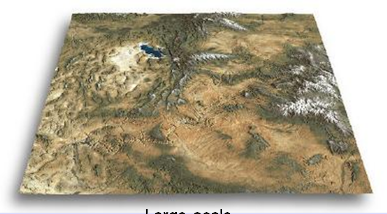
Heterogeneous porous media



Small scale



Large scale

Meso scale

- Heterogeneity at all scales
- Lack of data

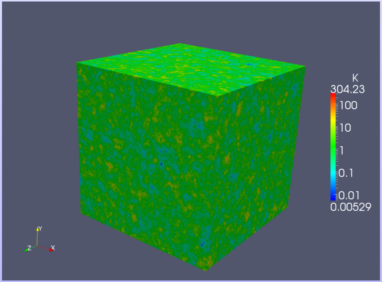
Models and methods must deal with uncertainty: **random data**

A. Beaudoin et al., WRR 2007, WRR 2008, WRR 2010, WRR 2013

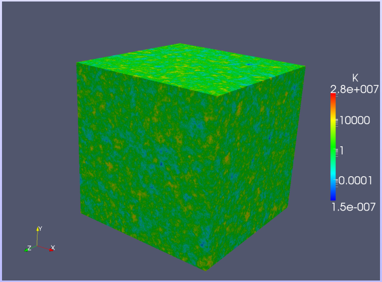
Random conductivity field

$$\begin{cases} a(\omega, x) = \exp(Y(\omega, x)) \text{ in } \Omega \times O, \\ cov[Y](x,y) = \sigma^2 \exp(-(\frac{\|x-y\|}{l})^\delta) \text{ in } O, \end{cases} \quad (1)$$

with O open domain in $\mathbb{R}^2$ or $\mathbb{R}^3$,
Ω probability space,
Y a gaussian field with mean μ and covariance $cov[Y]$



$\sigma = 1, l = 5$, 5 orders or magnitude



$\sigma = 3, l = 5$, 14 orders of magnitude

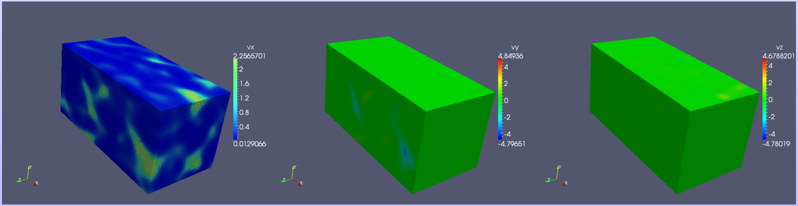
Flow equations

Single-phase steady-state flow in a saturated porous medium

Darcy's law and mass conservation law

$$\begin{cases} \theta(x)v(\omega,x) = -a(\omega,x)\nabla p(\omega,x) \text{ in } \Omega \times O, \\ \nabla.(\theta(x)v(\omega,x)) = 0 \text{ in } \Omega \times O, \\ \text{Boundary conditions}, \end{cases} \quad (2)$$

with θv the Darcy velocity, p the hydraulic head, θ the porosity, a the hydraulic conductivity.



Domain $L_x = 64, L_y = 32, L_z = 32,$ Gaussian covariance $l = 5, \sigma = 2$

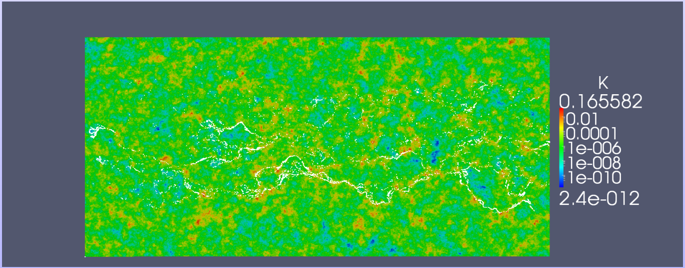
Transport by advection-diffusion-dispersion

$$\begin{cases} \frac{\partial(\theta(x)c(\omega,x,t))}{\partial t} + \nabla.(\theta(x)v(\omega,x)c(\omega,x,t)) - \nabla.(\theta(x)D_v(\omega,x)\nabla c(\omega,x,t)) = 0, \\ \text{boundary conditions,} \\ \text{initial condition,} \end{cases} \quad (3)$$

with c the solute concentration, D_v the dispersion tensor given by

$$D_v(\omega,x) = (\alpha_T(x)\,\|v(\omega,x)\| + D_m(x))I + (\alpha_L(x) - \alpha_T(x))\frac{v(\omega,x)v(\omega,x)^T}{\|v(\omega,x)\|}, \quad (4)$$

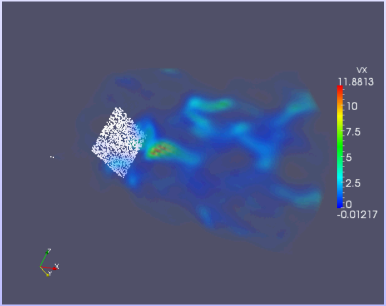
with $D_m(x)$ the isotropic molecular diffusion coefficient,
$\alpha_T(x)$ and $\alpha_L(x)$ the transversal and longitudinal dispersion coefficients.



Evolution of the plume in a log-normal exponentially correlated field in the pure advection case($\sigma = 3$, $l = 10$, $\mu = -13.8155$)

Simulation of flow and transport with random input data

- PARADIS software integrated in H2OLab platform, with Graphical User Interface
- Large scale 2D and 3D computations, using High Performance Computing
- Experimental computation of statistical quantities of interest



Evolution of the plume by advection-diffusion($D_m = 0.005, \sigma = 1, l = 5$)

Quantities of interest

Spreading and macro-dispersion

$$\begin{cases} G_k(\omega,t) = \int_O c(\omega,x,t)x_k dx, \\ S_k(\omega,t) = \int_O c(\omega,x,t)(x_k - G_k(\omega,t))^2 dx, \\ D_k(\omega,t) = \frac{1}{2}\frac{dS_k(\omega,t)}{dt}. \end{cases}$$

with G_k the center of mass in direction k, $k = 1,2,3$,
S_k the spreading, D_k the macro-dispersion.

Mean spreading and mean macro-dispersion

$$\begin{cases} S_k(t) = \mathbb{E}_\omega[S_k(\omega,t)], \\ D_k(t) = \mathbb{E}_\omega[D_k(\omega,t)]. \end{cases}$$

Asymptotic values for $t \to \infty$

Stochastic method

Monte-Carlo method

- Finite number of samples $S_k(t) \simeq \frac{1}{N} \sum_{i=1}^{N} S_{i,k}(t)$,
- Discretization in the physical space for flow and transport computations,
- non intrusive and parallel simulations,
- a priori large number N of simulations, but fast convergence in an ergodic case (observed in numerical experiments)

Erhel et al., ParCFD, 2010; A. Beaudoin et al., ESAIM Proc., to appear

$a = \exp(\mu + \sigma Z)$ with Z normal field with a given covariance function.

Truncated K-L expansion

- Discretization of the probability space,
- $Z(\omega, x) = \sum_{n=1}^{P} \sqrt{\lambda_n} b_n(x) Z_n(\omega)$
- Analytical or approximate computation of eigenvalues λ_n and eigenvectors b_n

Spectral simulation

- Discretization of the physical space,
- regular mesh of a domain, mesh step Δx
- compute the discrete spectral density, using a DFT of the covariance,
- compute the discrete normal field Z, using an inverse FFT

G. Pichot, Inria preprint, 2012; M. Oumouni et al., Inria preprint, in preparation

Flow method

Mixed hybrid finite element method

- local and global mass conservation,
- can deal with anisotropic conductivity,
- can deal with unstructured mesh,
- equivalent to a finite volume method in a regular case,
- sparse symmetric positive definite matrix,
- mesh step Δx and approximate velocity $\tilde{v}$

Sparse linear solver

- parallel direct solver for large systems,
- parallel algebraic multigrid for very large systems,
- convergence of AMG independent of heterogeneity,
- almost linear complexity of AMG

Erhel et al., ParCFD, 2009; A. Beaudoin et al., ESAIM Proc., to appear

Transport method

Random walker method

- Lagrangian method,
- Pure advection case: characteristic method,
- Pure diffusion case: Monte-Carlo method,
- No numerical diffusion,
- Efficient parallel algorithm

Erhel et al., Europar, 2007

Fokker-Planck equation

with $D_v = D_m I$ and $\theta(x) = 1$, infinite domain

$$\begin{cases} \frac{\partial c(x,t))}{\partial t} + v(x)\nabla c(x,t) - D_m \Delta c(x,t)) = 0, \\ c(x,0) = c_0(x) \end{cases} \tag{5}$$

Stochastic Differential Equation

$$\begin{cases} dX_t = v(X_t)dt + \sqrt{2D_m}dW_t, \\ X_0 \text{ given} \end{cases} \tag{6}$$

If X_0 admits $c_0(x)$ as density, then $X(t)$ admits $c(x)$ as density.

Spreading and macro dispersion

$$\begin{cases} G_k(t) = \mathbb{E}_\xi\left[X_{t,k}\right], \\ S_k(t) = \mathbb{E}_\xi\left[(X_{t,k} - G_k(t))^2\right], \\ \\ V_k(t) = \mathbb{E}_\xi\left[v_k(X_t)\right], \\ D_k(t) = \text{trace}(D_m) + \mathbb{E}_\xi\left[X_{t,k} v_k(X_t)\right] - G_k(t)V_k(t). \end{cases}$$

Approximation of macro-dispersion for one simulation

J. Erhel joint work with A. Beaudoin , J.-R. de Dreuzy , G. Pichot , J. Charrier , A. Debussche , M. Oumouni , Z. Mghazli

Simulation i, $i = 1, \dots, N$

Discrete Flow equation with random data a_i and approximate velocity $\widetilde{v}_i$

Euler scheme with approximate velocity $\widetilde{v}_i$

M particles $j = 1, \dots, M$ and time step Δt

$$\begin{cases} \widetilde{X}_{i,j}(t+\Delta t) = \widetilde{X}_{i,j}(t) + \widetilde{v}_i(\widetilde{X}_{i,j}(t))\Delta t + \sqrt{2D_m\Delta t}\widetilde{W}_{i,j}(t), \\ \widetilde{X}_{i,j}(0) \text{ given.} \end{cases} \tag{7}$$

Particle Monte-Carlo applied to simulation i

$$\begin{cases} \widetilde{G}_{i,k}(t) = \frac{1}{M}\sum_{j=1}^{M} \widetilde{X}_{i,j,k}(t), \\ \widetilde{S}_{i,k}(t) = \frac{1}{M}\sum_{j=1}^{M} (\widetilde{X}_{i,j,k}(t) - \widetilde{G}_{i,k}(t))^2, \\ \widetilde{V}_{i,k}(t) = \frac{1}{M}\sum_{j=1}^{M} \widetilde{v}_{i,k}(\widetilde{X}_{i,j}(t)), \\ \widetilde{D}_{i,k}(t) = \text{trace}(D_m) + \frac{1}{M}\sum_{j=1}^{M} \widetilde{X}_{i,j,k}(t)\widetilde{v}_{i,k}(\widetilde{X}_{i,j}(t)) - \widetilde{G}_{i,k}(t)\widetilde{V}_{i,k}(t). \end{cases}$$

Approximation of mean macro dispersion

N Monte-Carlo simulations

$$\begin{cases} \widetilde{S}_k(t) = \frac{1}{N}\sum_{i=1}^{N} \widetilde{S}_{i,k}(t), \\ \widetilde{D}_k(t) = \frac{1}{N}\sum_{i=1}^{N} \widetilde{D}_{i,k}(t), \\ \text{with Finite Differences:} \widehat{D}(t) = \frac{1}{2}(\widetilde{S}(t+\Delta s) - \widetilde{S}(t))/\Delta s, \end{cases}$$

Theoretical results

with some assumptions

$$\left\| D(t) - \widetilde{D}(t) \right\|_{L^2_{\omega,\xi}} \leq C(\Delta t^{\frac{1+\alpha}{2}} + \Delta x \left|\log(\Delta x)\right| + \frac{1}{\sqrt{N}} + \frac{1}{\sqrt{M}})$$

with Finite Differences:

$$... + \frac{1}{\sqrt{M\Delta s}})$$

J. Charrier, Inria preprint 2011 and Marseille Univ. preprint, 2013

M. Oumouni, Ph-D, 2013

Small 2D numerical experiments

Physical parameters

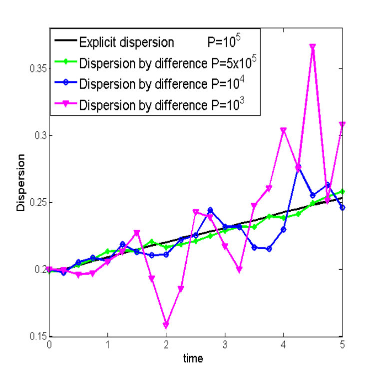
- 2D square of size $L = 10$,
- conductivity $a = exp(\mu + \sigma Z)$ with $\mu = 0$,
- exponential covariance $cov[Z](x, y) = \exp(-\frac{\|x-y\|}{l})$, with $l = 1$,
- truncated K-L expansion of Z,
- homogeneous Neumann transversal boundary conditions for flow and transport,
- Dirichlet longitudinal boundary conditions for flow:$p = p_{in}$ at inflow and $p = p_{out} = 0$ at outflow,
- initial injection $c_0(x) = 1_B/\|B\|$, with $B = [2.85, 3] \times [5, 5.15]$
- advection-diffusion with $D_v = D_m I$, and $D_m = 0.1$

Numerical parameters

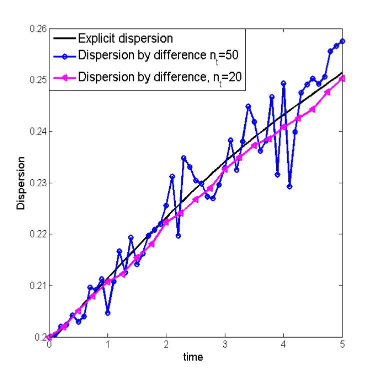
- uniform triangular mesh and mixed finite element method with Δx,
- flow computed with FreeFem++,
- transport: final time T and timestep $\Delta t = T/50$

Explicit $\widetilde{D}$ versus Finite Difference $\hat{D}$ computations

$\sigma = 1, p_{in} = 4, p_{out} = 0, \Delta x = L/20, T = 5, \Delta t = 1/10, N = 200$



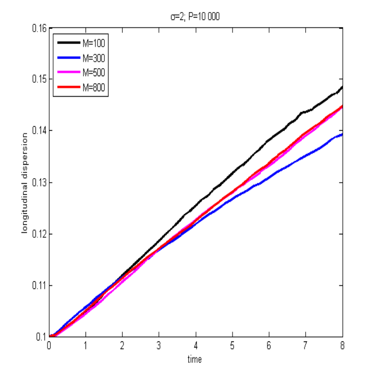
$\Delta s = 1/10$



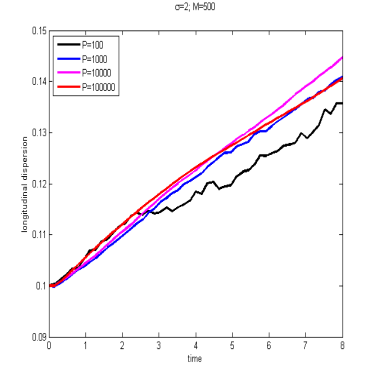
$M = 10^5, \Delta s = 1/4$ and $\Delta s = 1/10$

Convergence with N and M

$\sigma = 2, p_{in} = 2, \Delta x = L/30, T = 8, \Delta t = T/50$



Convergence with the number of simulations (10000 particles)



Convergence with the number of particles (500 simulations)

Physical parameters

- 3D domain of size $1024 \times 256 \times 256$
- Log-normal conductivity field Gaussian covariance and $\mu = 0, \sigma = 1, l = 10$
- Periodic transversal boundary conditions for flow and transport
- Dirichlet longitudinal flow boundary conditions: $p_{in} = 1024$, $p_{out} = 0$
- Inflow homogeneous Neumann and outflow homogeneous Dirichelt transport boundary condition
- Molecular diffusion $D_m = 10^{-3}$

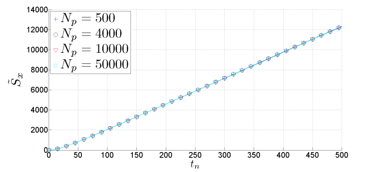
Numerical parameters

- Computations with PARADIS software using HPC
- Regular mesh with square cells of size $\Delta x = 1$
- Injection window of transversal size 0.8×256 and longitudinal size Δx
- Local time step

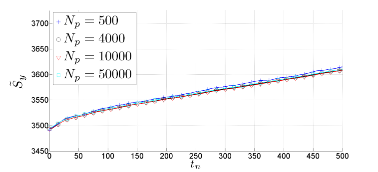
A. Beaudoin et al., ESAIM Proceedings, to appear

Convergence of spreading with the number of particles

$N = 500$ simulations



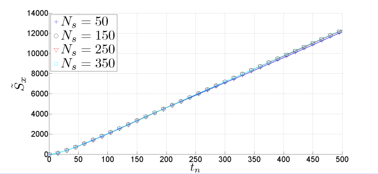
Longitudinal spreading



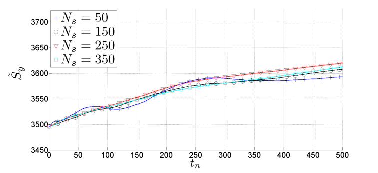
Transversal spreading

Monte-Carlo convergence of spreading

50000 particles



Longitudinal spreading



Transversal spreading

Large 3D numerical experiments

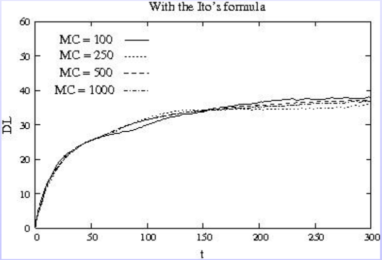
Physical parameters

- 3D domain of size $1024 \times 128 \times 128$
- Log-normal conductivity field Gaussian covariance and $\mu = 0, \sigma = 1.5, l = 10$
- Periodic transversal boundary conditions for flow and transport
- Dirichlet longitudinal flow boundary conditions: $p_{in} = 1024$, $p_{out} = 0$
- Inflow homogeneous Neumann and outflow homogeneous Dirichelt transport boundary condition
- Molecular diffusion $D_m = 10^{-1}$

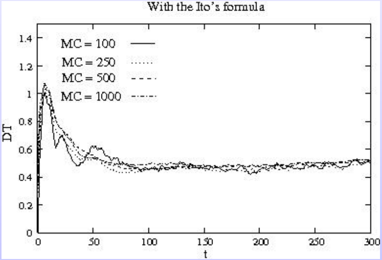
Numerical parameters

- Regular mesh with square cells of size $\Delta x = 1$
- Injection window of transversal size 0.2×256 and longitudinal size Δx
- Local time step

10000 particles



Longitudinal macro-dispersion



Transversal macro-dispersion

Concluding remarks

Current results

- Macro-dispersion in 3D domains with advection-diffusion
- Theoretical and experimental convergence analysis
- Fast Monte-Carlo convergence

Current and future work

- Random walker with discontinuous dispersion tensor (joint work with A. Lejay)
- Theoretical analysis of asymptotic spreading
- Domain decomposition for very large 3D domains (joint work with D. Tromeur-Dervout)