Stochastic groundwater simulations for highly heterogeneous porous media

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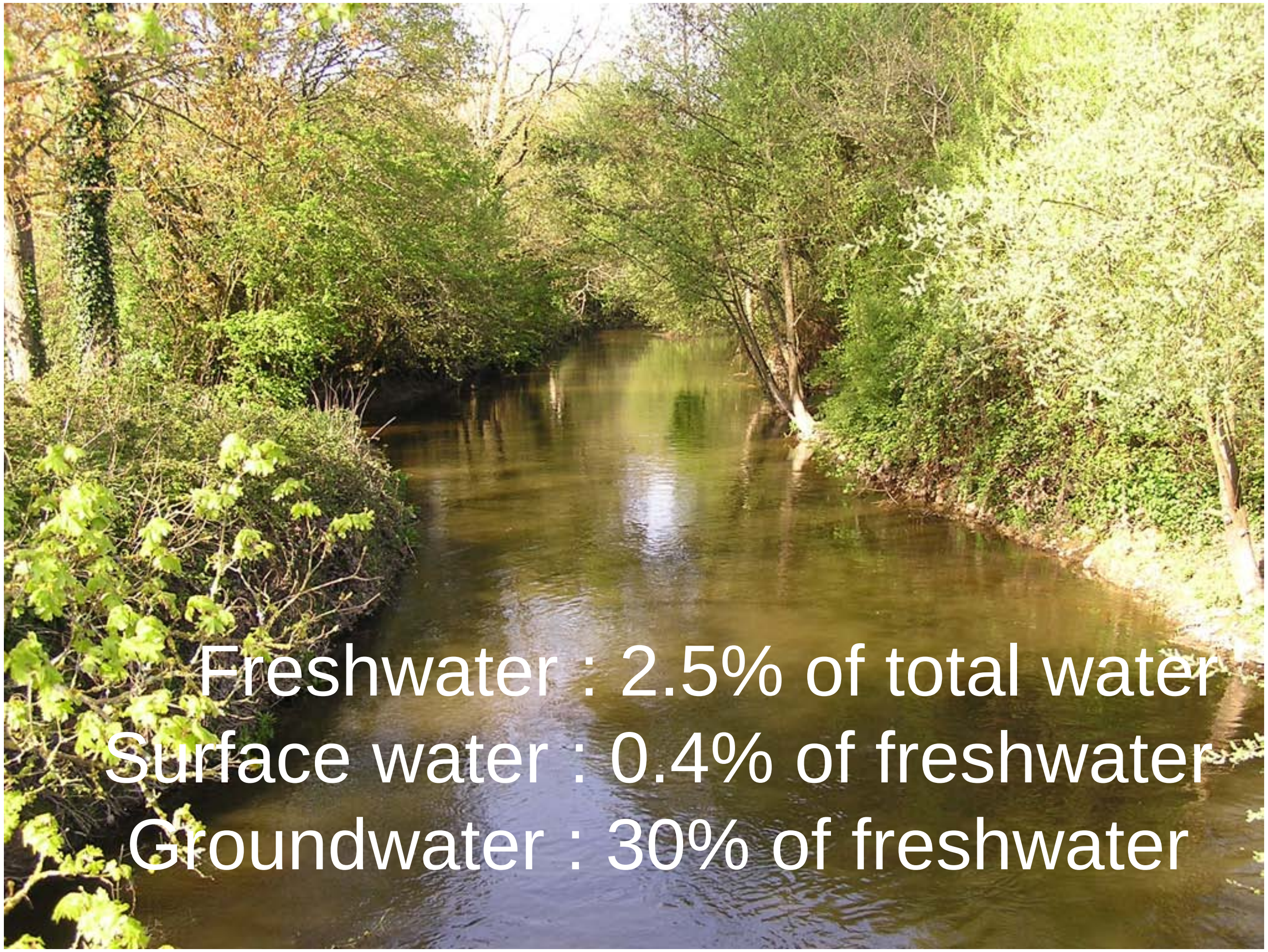
Surface water and groundwater



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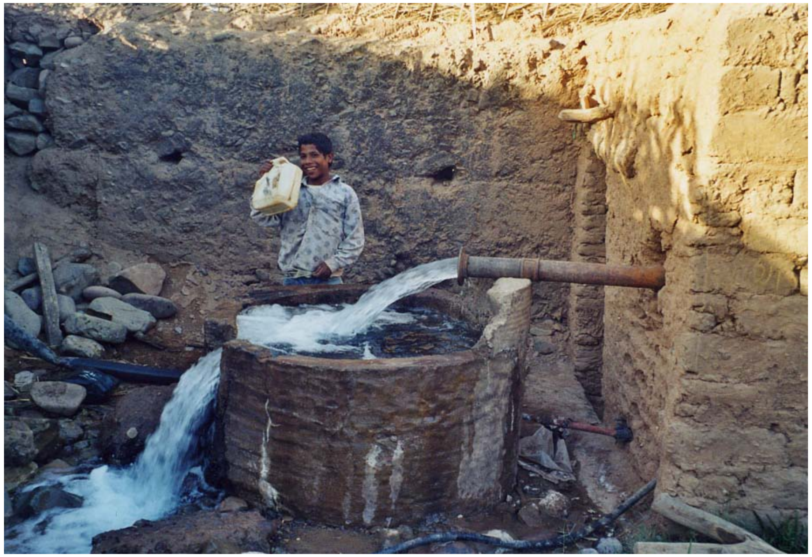
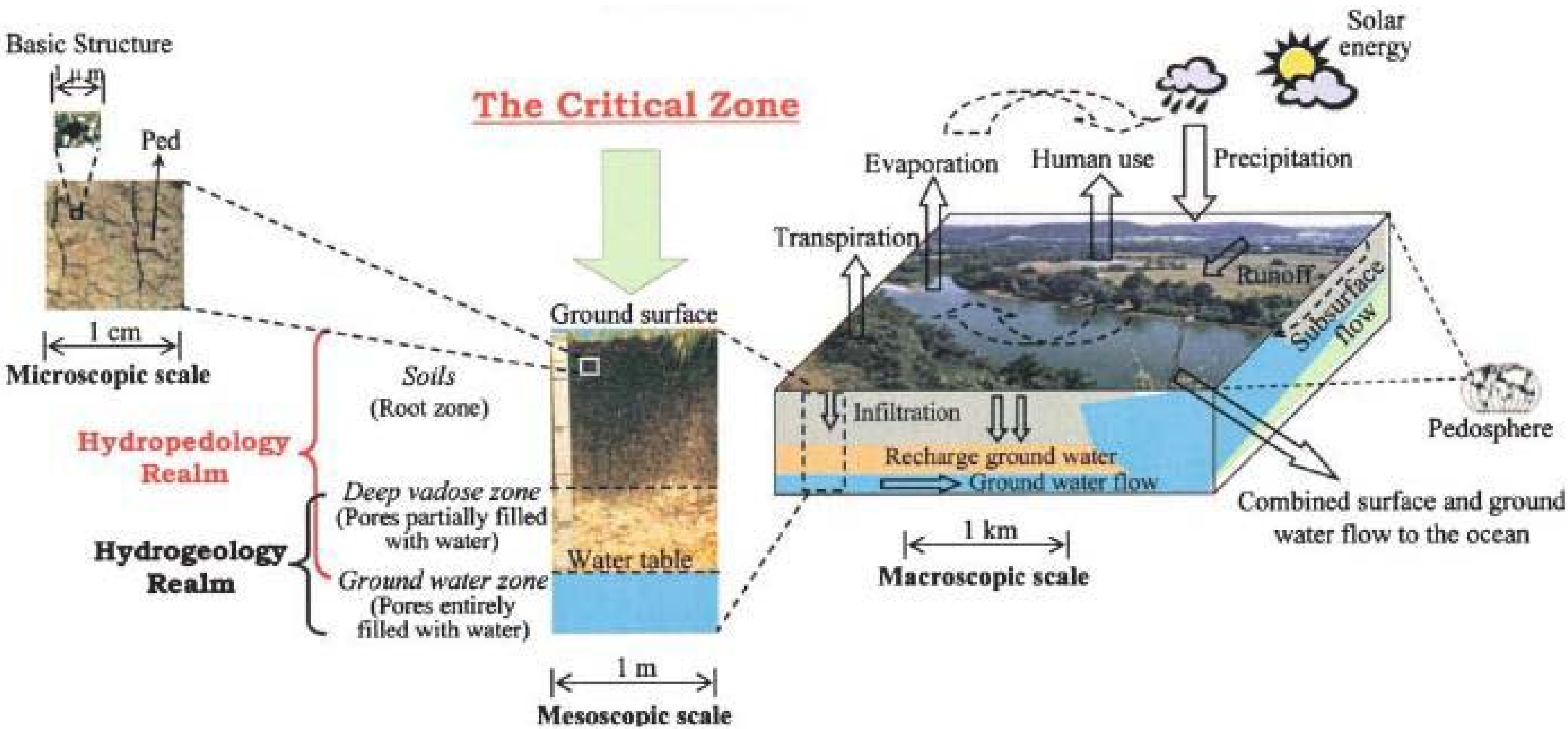
sustainable use of groundwater



Groundwater numerical models

- **Understand physical phenomena**
- **Manage water resources**
- **Prevent risks of pollution**
- **Help in remediation**

Groundwater cycle



scale

Observations

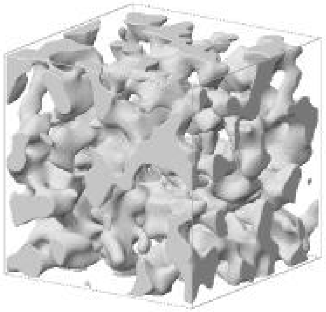
macroscopic

Variable geology

mesoscopic

Variable layers

microscopic

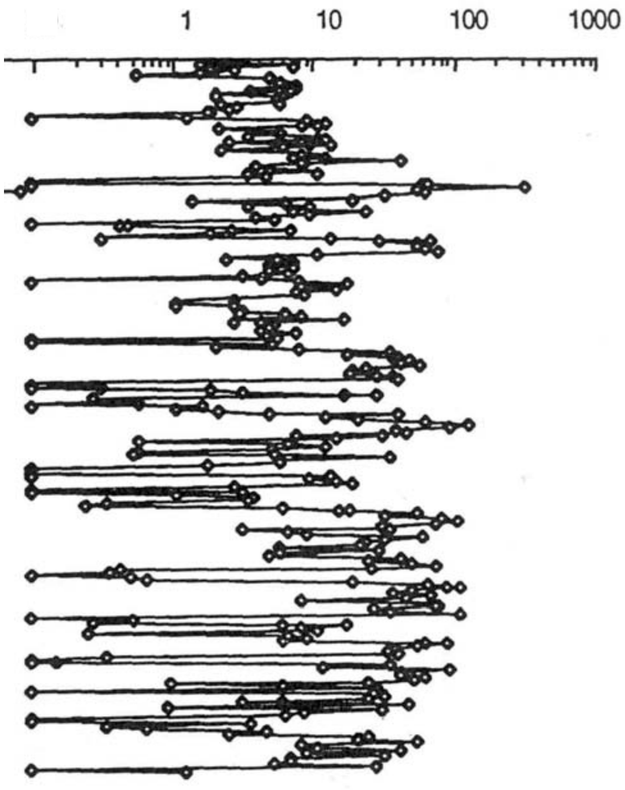


Variable pores

Heterogeneity at all scales

(Freeze et al., 1979; Koltermann et al., 1996)

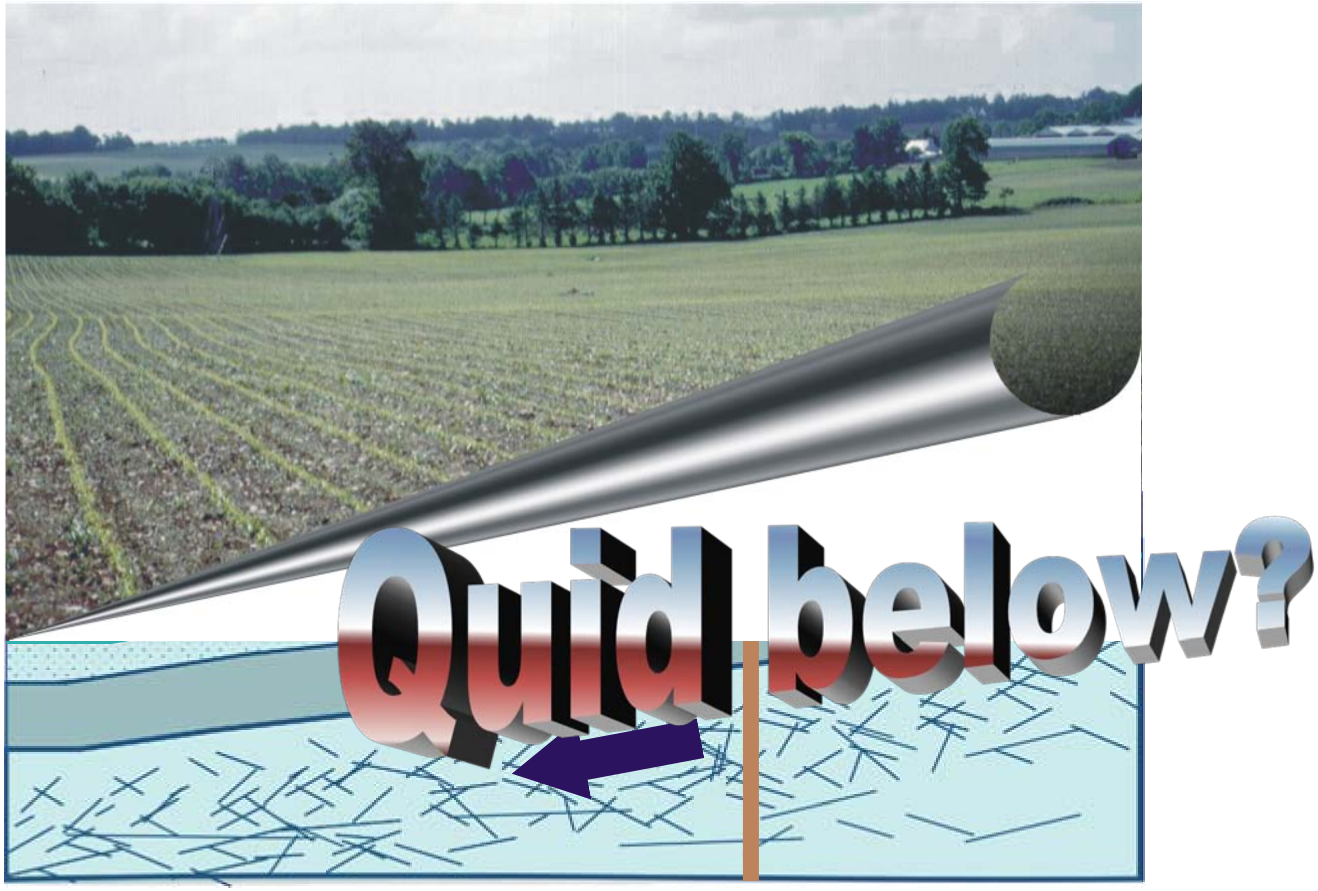
Heterogeneous porous media



permeability (md)

Sand and gravel deposits in Switzerland, Gelhar [1993]

The real world of hydrogeology



Numerical models of porous media

Porous geological media   Spatial heterogeneity   Lack of observations

↓

Stochastic models of flow and solute transport

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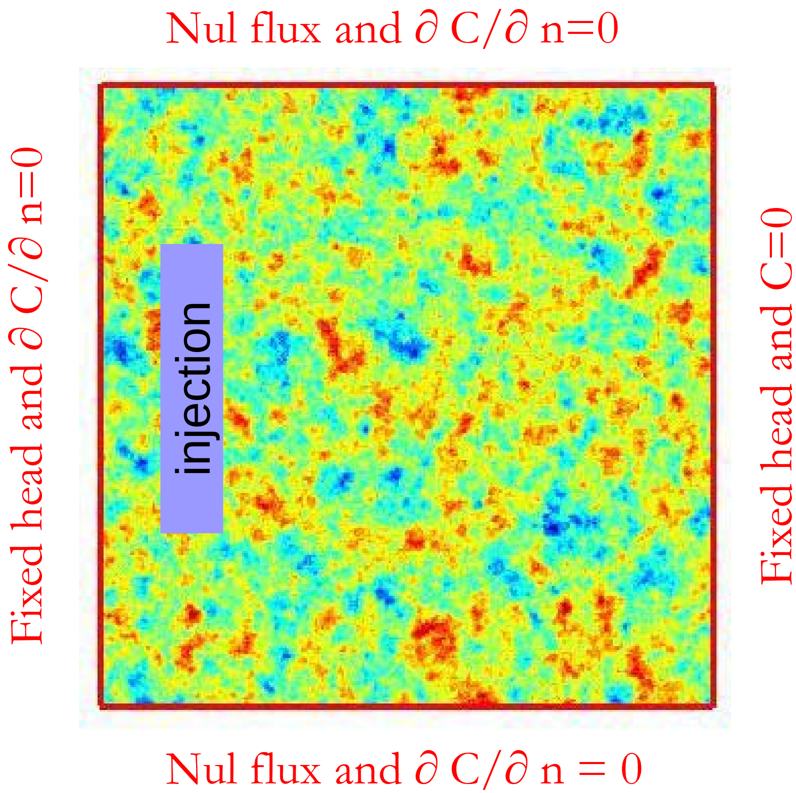
-random velocity field

-random solute transfer time and dispersivity

Physical assumptions

- Saturated medium: one water phase
- Constant density: no saltwater
- Constant porosity and constant viscosity
- Linear equations
- Steady-state flow or transient flow
- Inert transport: no coupling with chemistry
- No coupling between flow and transport
- No coupling with heat equations
- No coupling with mechanical equations
- Classical boundary conditions
- Classical initial conditions

Flow and transport equations in porous media



- Flow equations

$$\epsilon V = -K \nabla h, \nabla . V = 0$$

- Advection-dispersion equations

Boundary conditions

Initial condition

$$\frac{\partial (\epsilon c)}{\partial t} + \nabla.(\epsilon c V) - \nabla.(\epsilon d \nabla c) = 0$$

Macro-dispersion

Total mass $M(t)=\int c(x,t)dx$

Center of mass $X(t)=1/M(t) \int c(x,t)xdx$

Spread of mass around center of mass $S(t)= 1/M(t) \int c(x,t)(x-X)(x-X)^T dx$

Dispersion $D(t)=dS/dt$

Study of asymptotic behaviour

Need for large scale computations in space and time

Stochastic equations

Random permeability field $K(\omega;x)$

Example: log-normal correlated field

$$Y=\log(K),\ C(r)=\sigma^2 \exp(-|r|/\lambda)$$

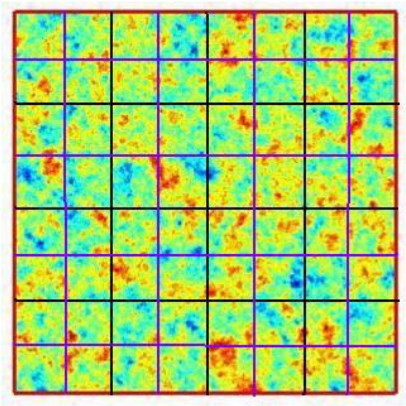
Random hydraulic head $h(\omega;x)$ and velocity field $V(\omega;x)$
Random concentration $c(\omega;x,t)$

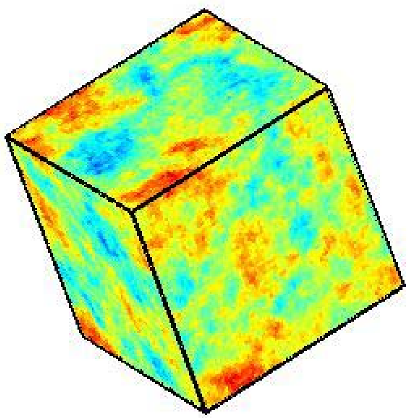
Study of statistics of results
Need for uncertainty quantification methods

Monte-Carlo simulations

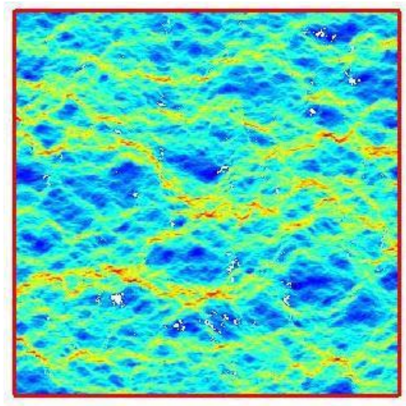
For $j=1,\ldots,N_s$

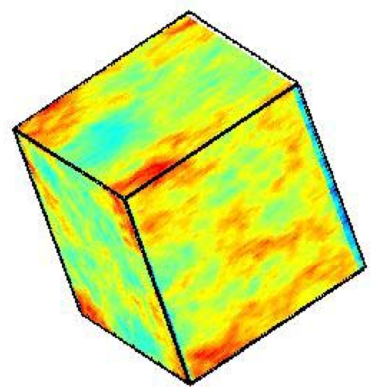
generate permeability field $K(\omega_j,x)$ using a regular mesh



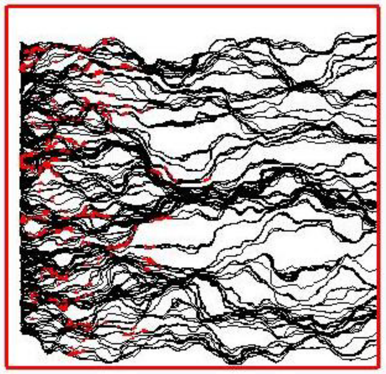


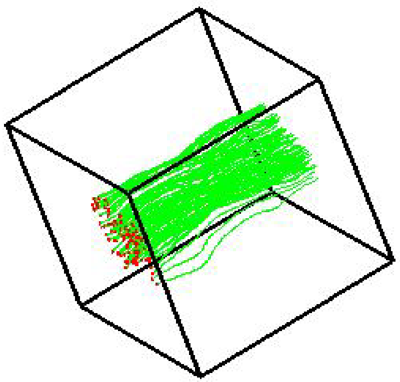
Compute $V(\omega_j,x)$ using a finite volume method





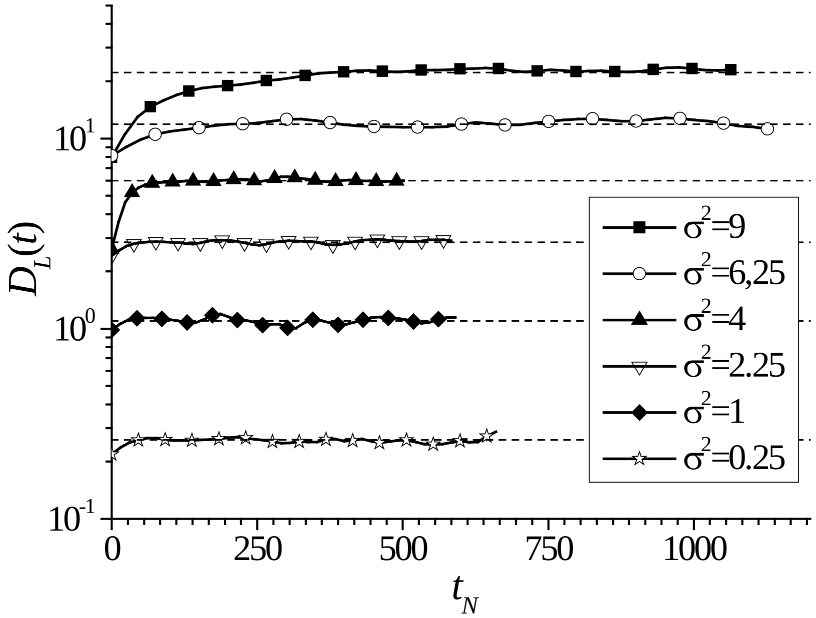
Compute $D(\omega_j,t)$ using a random walker method



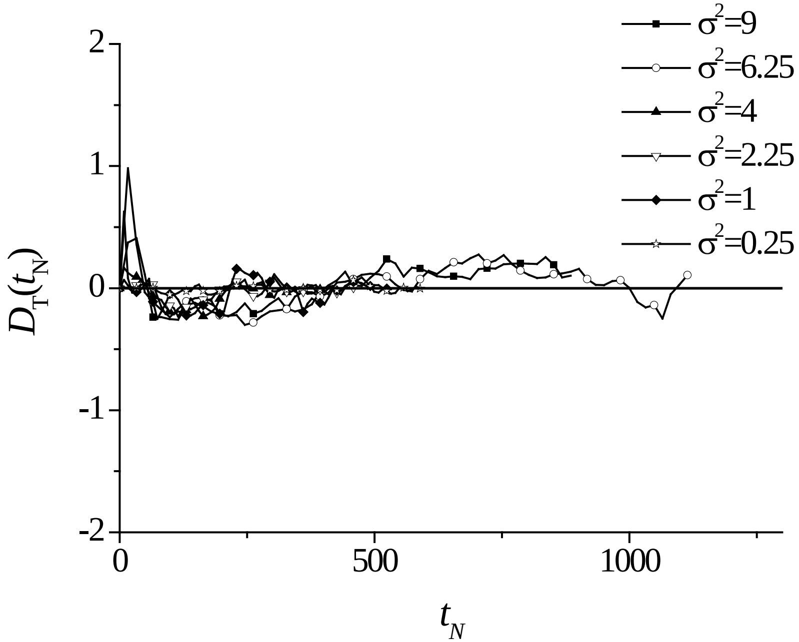


End For

Results with 2D domains

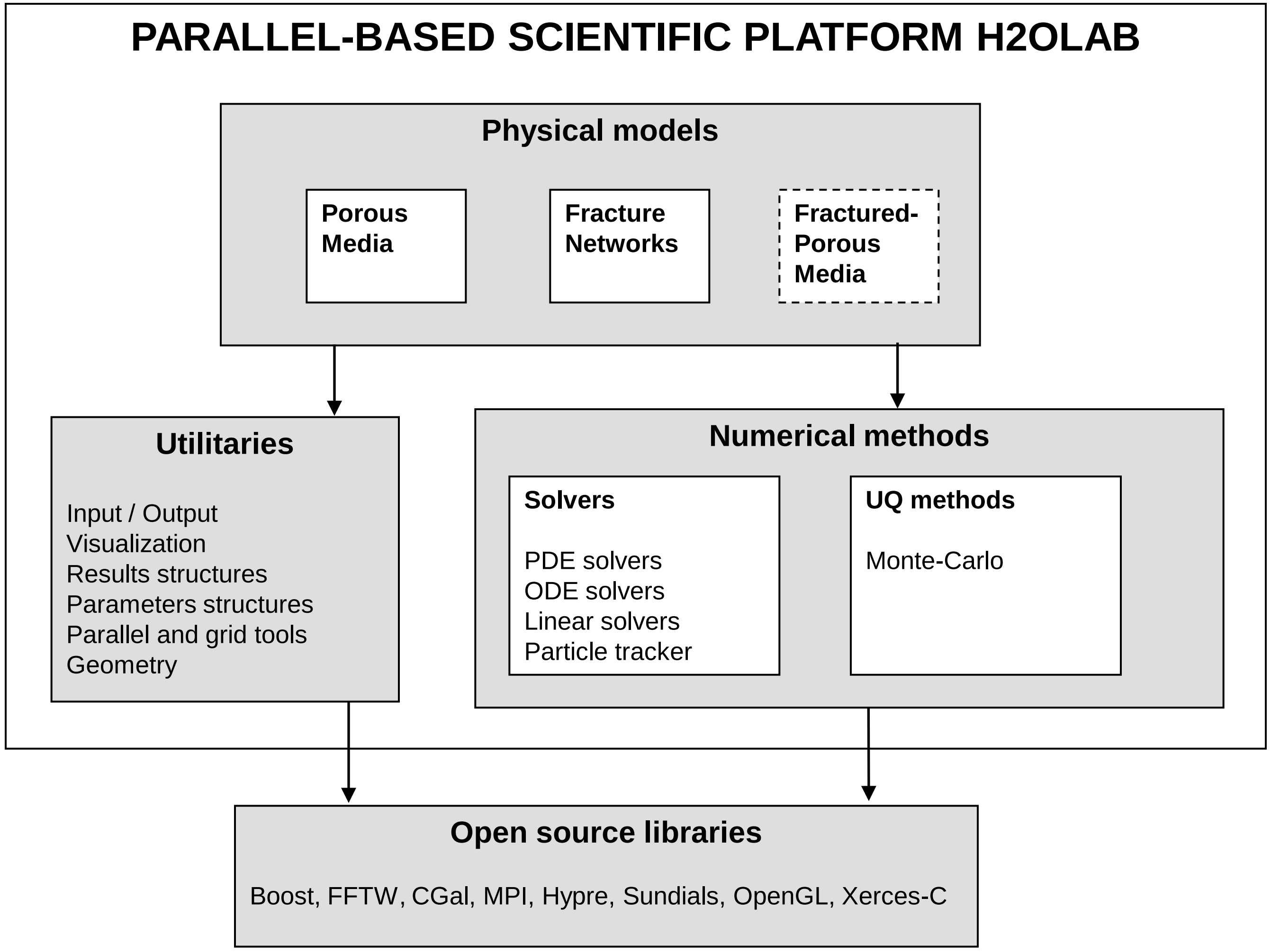


Longitudinal dispersion



Transversal dispersion

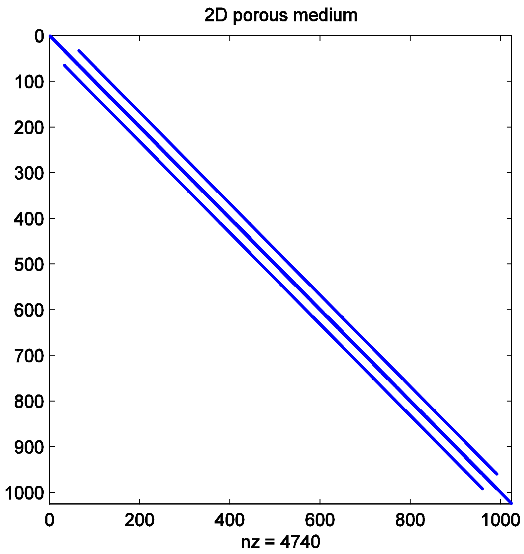
Each curve represents 100 simulations
on domains with 67.1 millions of unknowns
high performance computing is required



Object-oriented and modular with C++
Parallel algorithms with MPI
Efficient numerical libraries

Discrete flow numerical model

Finite volume method
with a regular orthogonal mesh



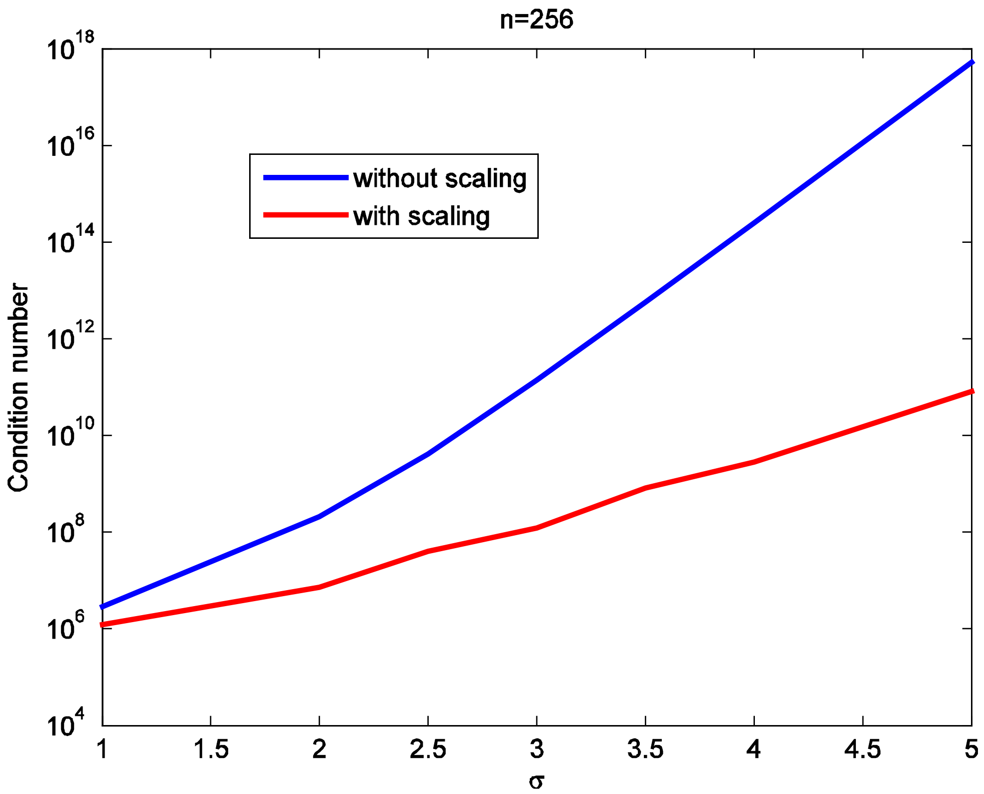
Linear system
$A(\omega;\Delta x)\, H(\omega;\Delta x)=b(\omega;\Delta x)$

b: boundary conditions and source term
A is a sparse matrix : NZ coefficients
Matrix-Vector product : O(NZ) opérations

Regular 2D mesh : $N=n^2$ and $NZ=5N$
Regular 3D mesh : $N= n^3$ and $NZ=7N$

Need for parallel sparse linear solvers

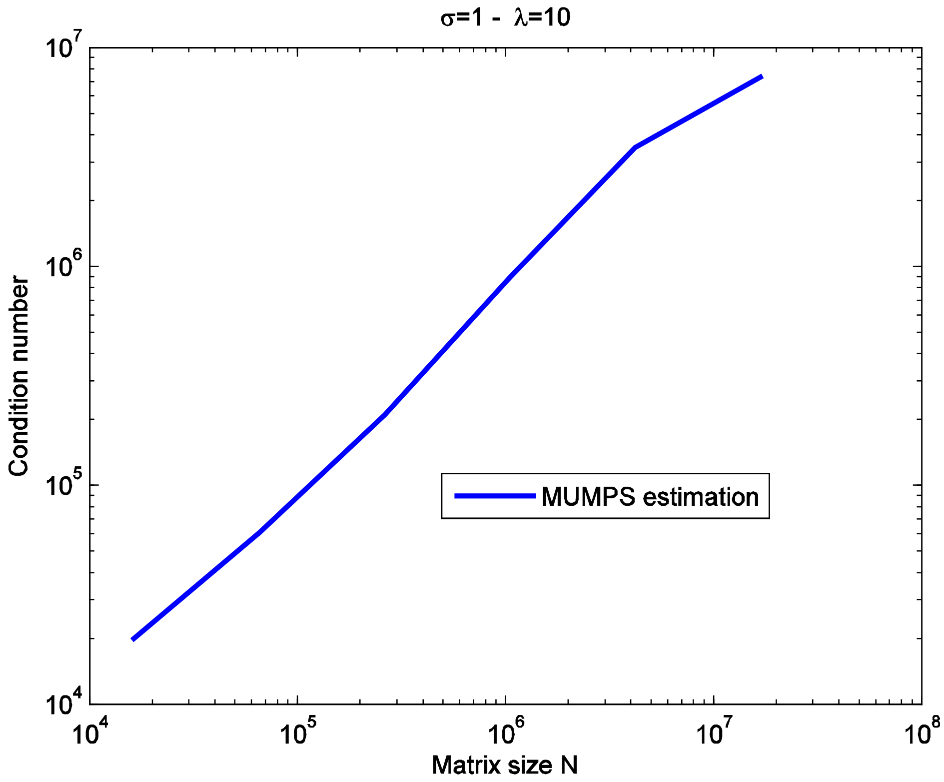
Accuracy: condition number and variance



Estimation with Matlab without scaling and with scaling

Scaled condition number in $O(\exp(\sigma))$ as expected

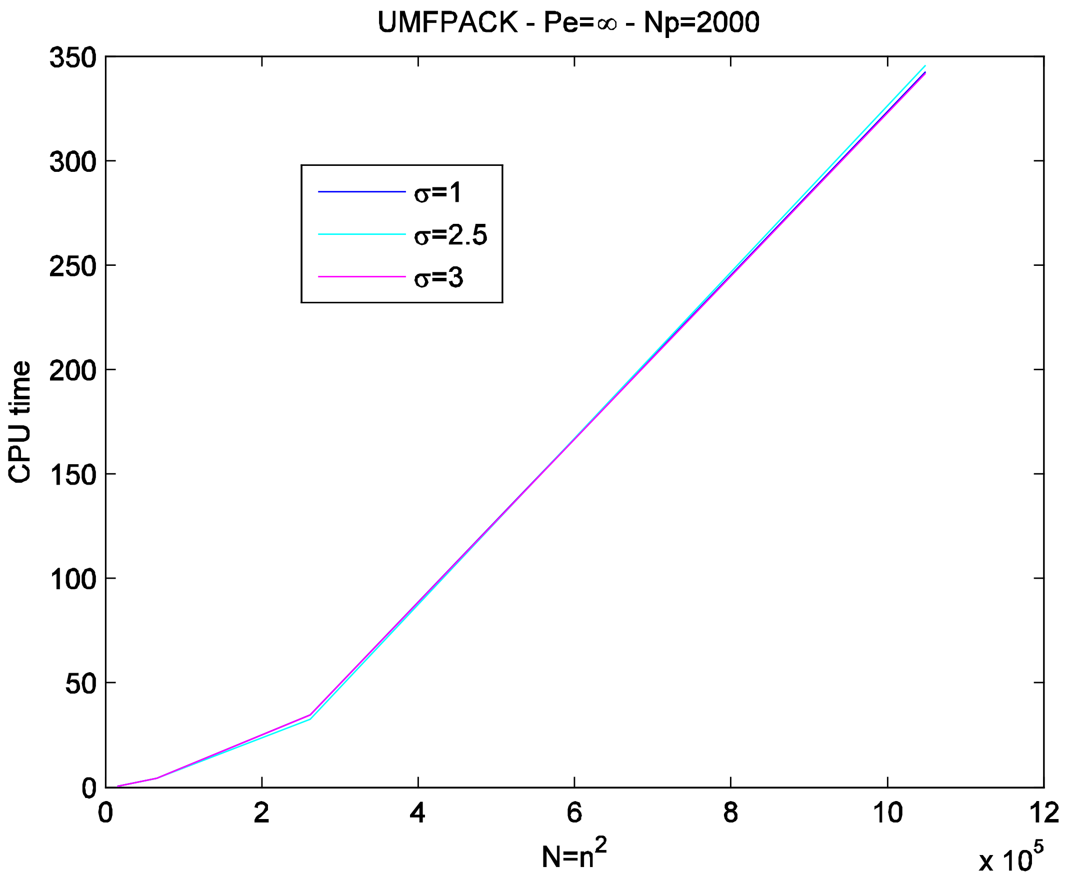
Accuracy: condition number and system size



Estimation with MUMPS for $\sigma=1$

Cond(A) in O(N) as expected

Sparse direct linear solver

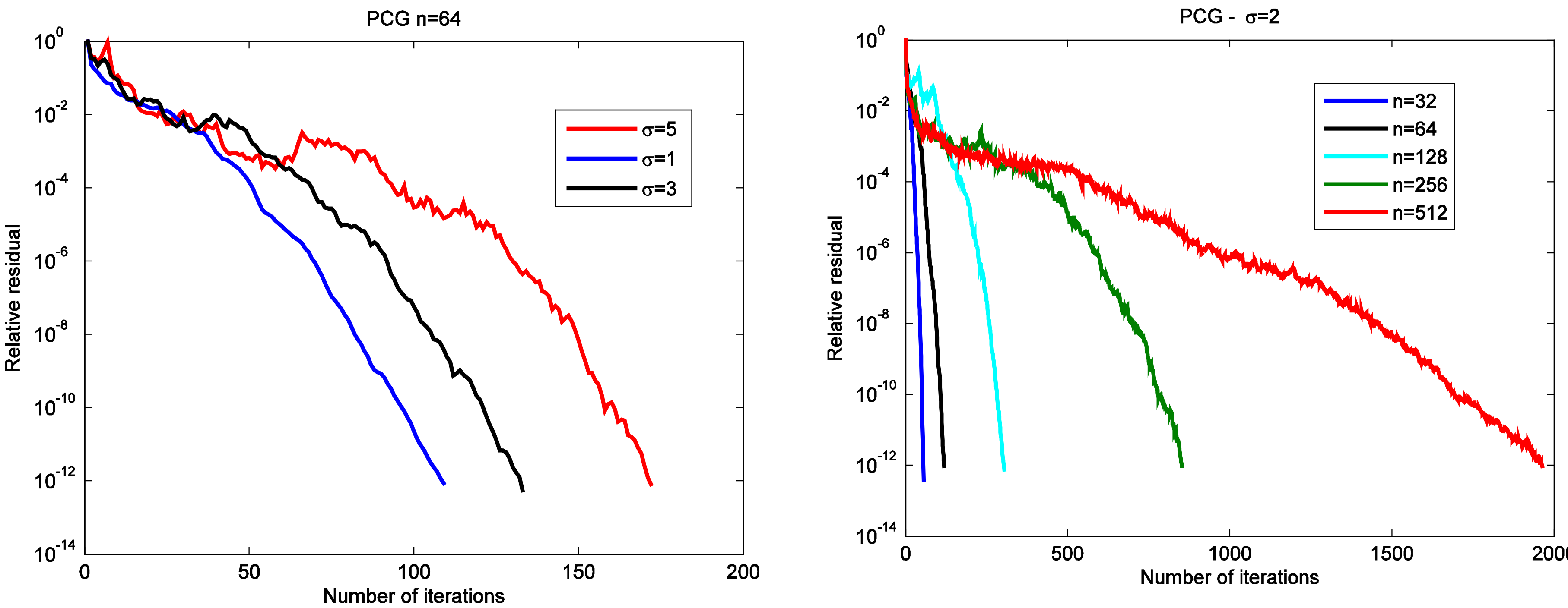


UMFPACK multifrontal solver

Robust to variance σ but CPU time in $O(N^{1.5})$

As expected

Preconditioned Conjugate Gradient

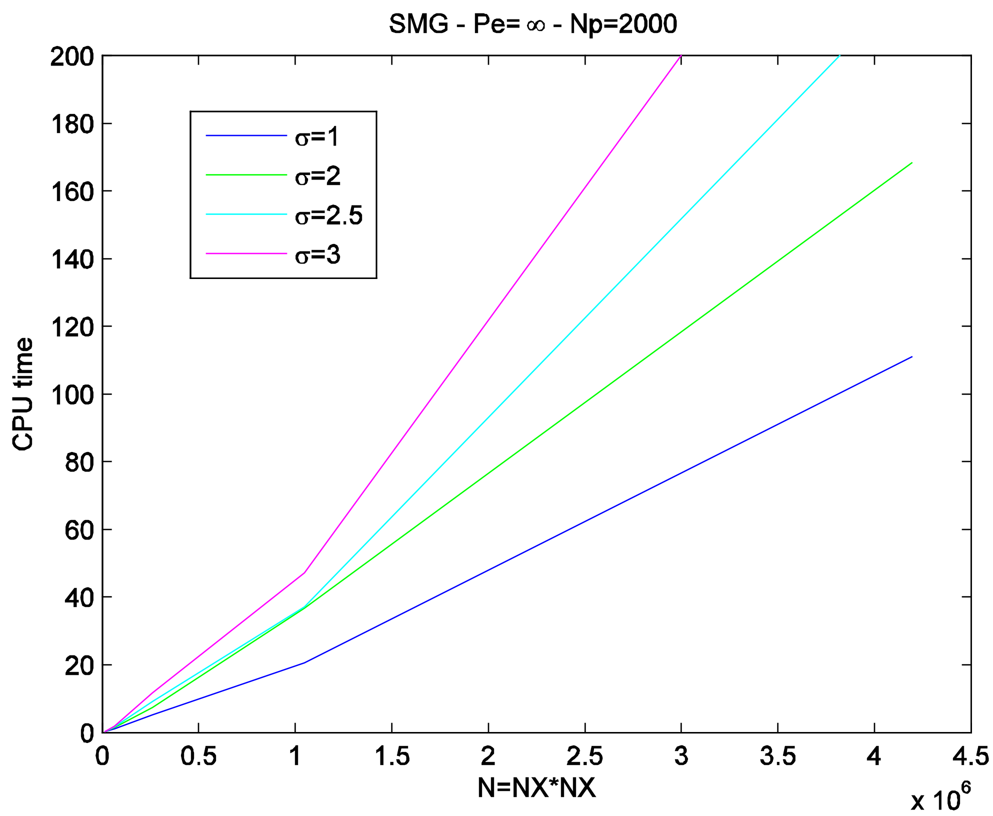


PCG with IC(0) slightly sensitive to variance σ

But very sensitive to size N

Need for a multilevel preconditioner

Geometric multigrid

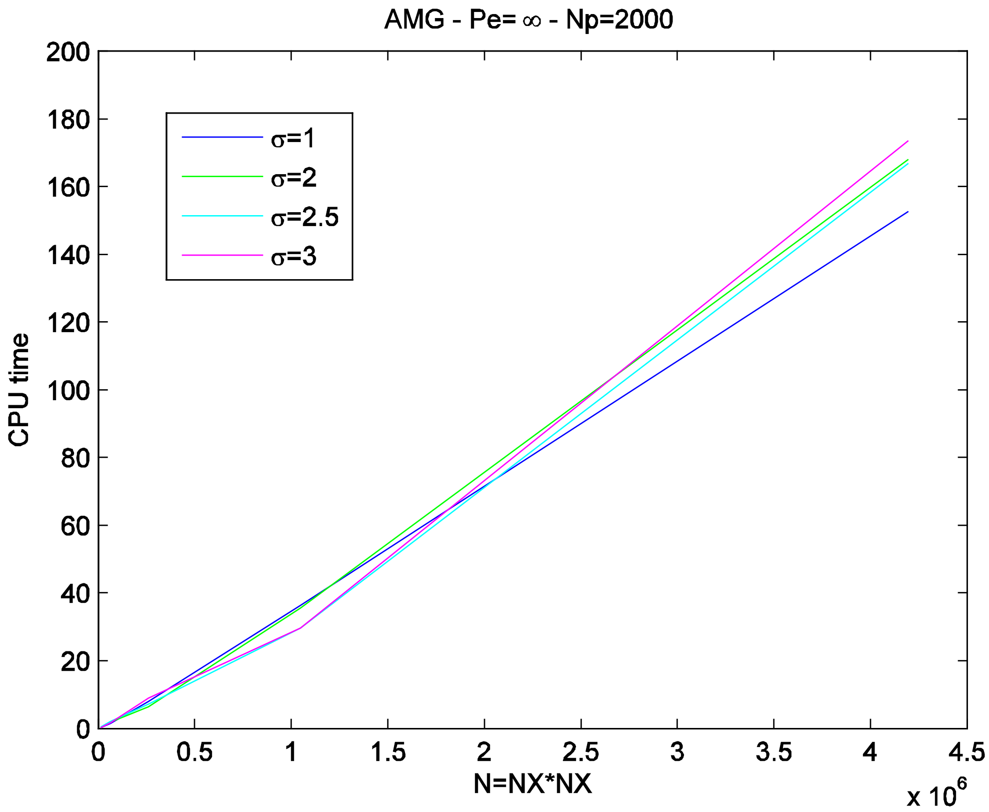


HYPRE Solver SMG

Linear CPU time in O(N) but sensitivity to variance

As expected

Algebraic multigrid

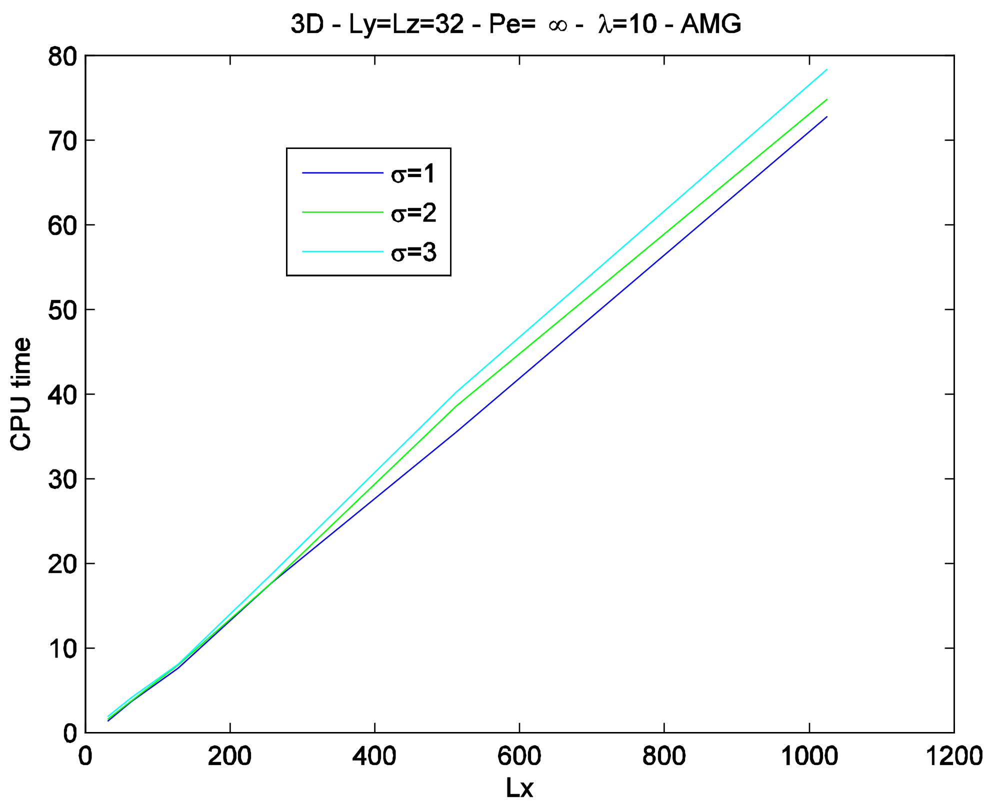


HYPRE Solver AMG

Robust to variance and linear CPU time in O(N)

As expected Less efficient than SMG for small variance

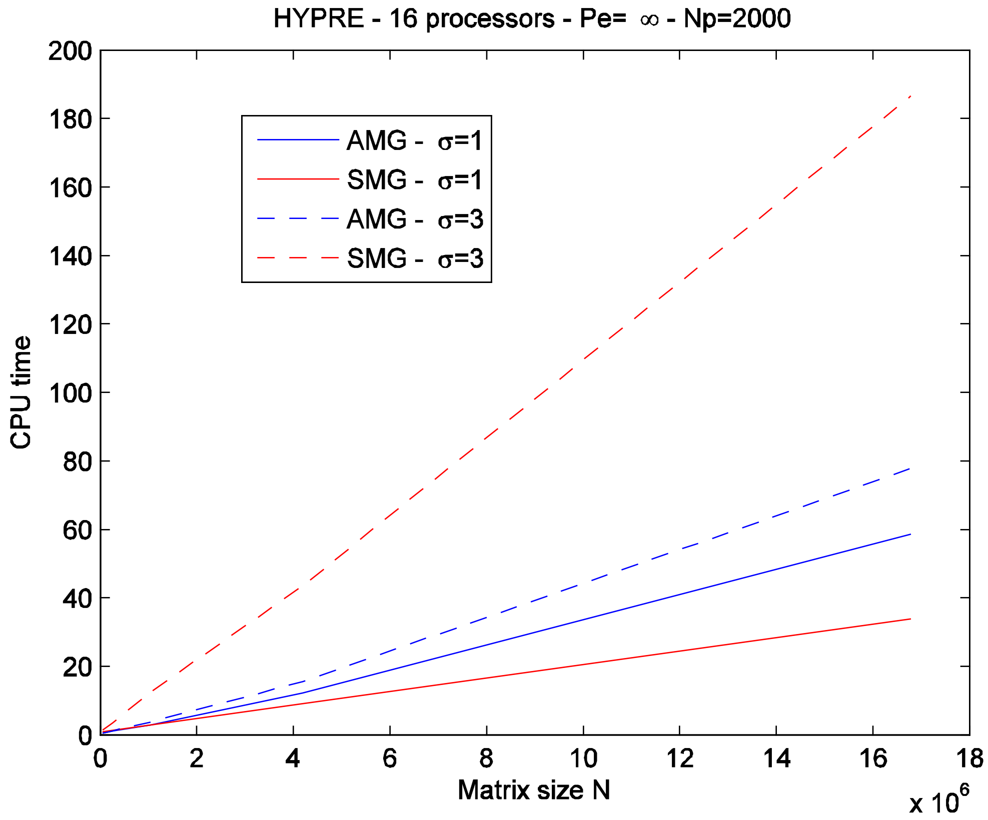
Algebraic multigrid with 3D domains



Robust to variance and CPU time in O(N)

Same properties as in 2D

Parallel performances with 2D domains



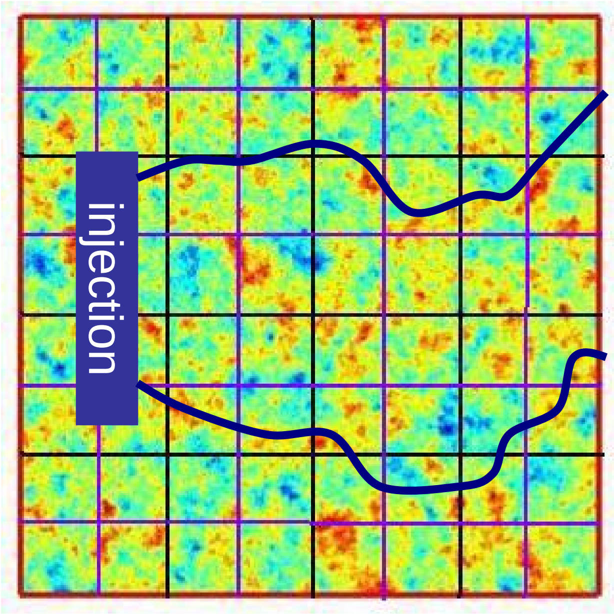
Parallel CPU time in O(N)

SMG more efficient than AMG for small σ

AMG much more efficient than SMG for large σ

Solute transport : random walker

Particle tracker does not induce artificial diffusion
But random walker expensive for diffusion approximation



Homogeneous molecular diffusion
Stochastic differential equation
First-order explicit scheme

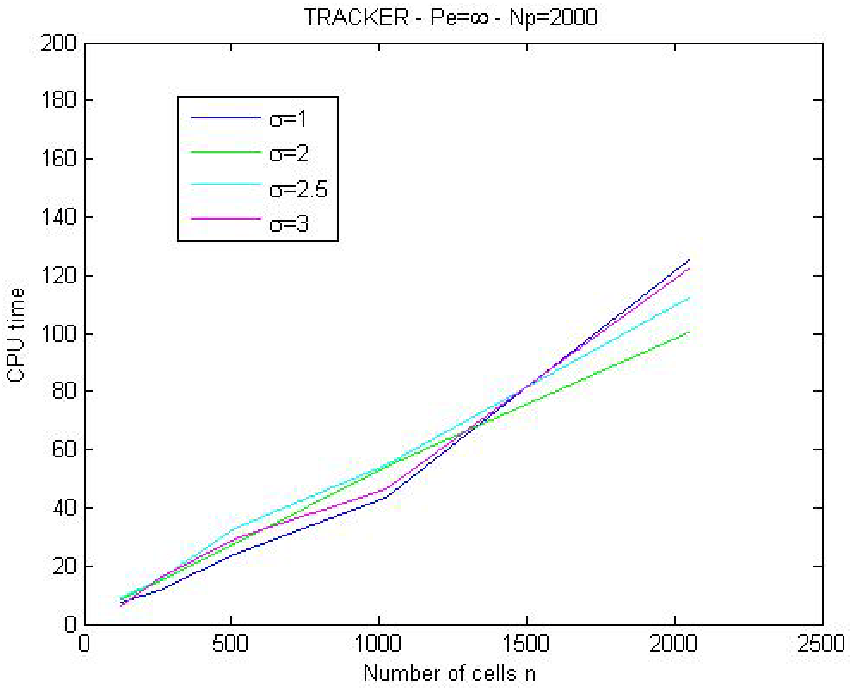
$d = d_m I$, $U = \text{mean}(V)$, $Pe = \lambda U / d_m$

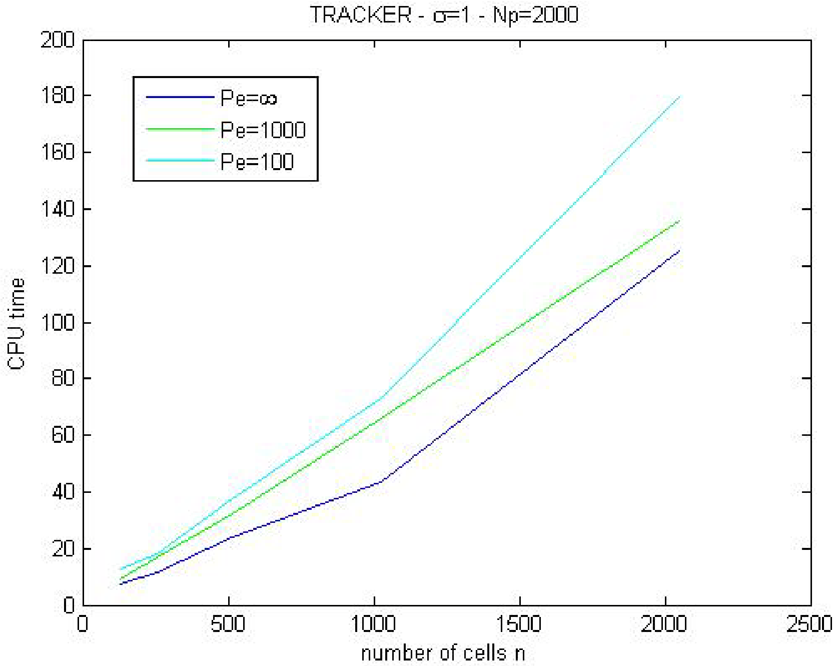
$$dX = V\,dt + \sqrt{2d_m}\,dW$$
$$X(t+\Delta t) = X(t) + V\Delta t + \sqrt{2d_m}\,Zw\sqrt{\Delta t}$$

Particle-in-cell approach:
Bilinear interpolation for V to ensure local mass balance

Independent particles X_k , $k=1,\ldots N_p$

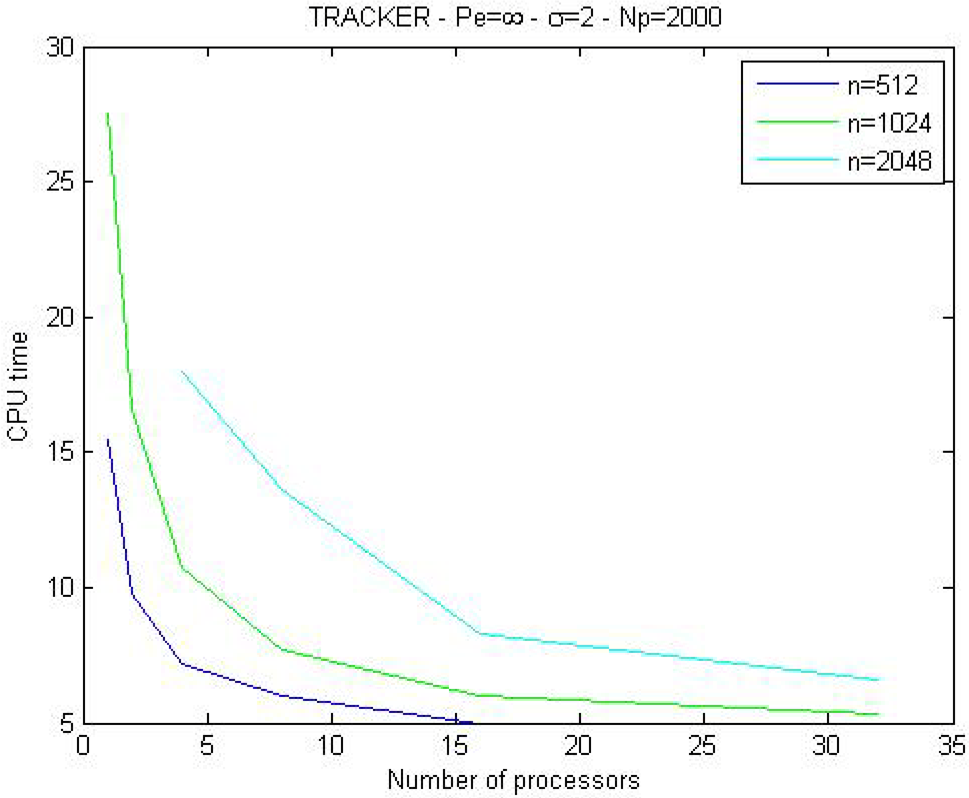
Random walker : impact of diffusion and heterogeneity





Not very sensitive to heterogeneity
More efficient in pure advective case
Linear complexity with the number of cells in each direction

Parallel performances of solute transport



Good speed-up and good scalability

Estimation of macro dispersion

Total mass $M(t)=\int c(x,t)dx = M$

Center of mass $X(t)=1/M \int c(x,t)xdx \simeq 1/N_p \sum_k X_k$

Spread of mass $S(\omega, t)= 1/M \int c(x,t)(x-X)(x-X)^T dx \simeq 1/N_p \sum_k (X_k-X) (X_k-X)^T$

Dispersion $D(\omega, t)=dS/dt \simeq (S(t+\Delta t)-S(t)) / \Delta t$

Mean spread of mass $E[S(\omega,t)] \simeq 1/N_s \sum_l S(\omega_l, t)$

Mean dispersion $E[D(\omega, t)] \simeq 1/N_s \sum_l D(\omega_l, t)$

Error estimation

Several assumptions of regularity

Error $E = E[S(\omega,t)] - 1/N_s \, 1/N_p \sum_l \sum_k (X_k - X)(X_k - X)^T$

$\| E \| \leq C \, (1/\sqrt{Ns} + 1/\sqrt{Np} + \Delta t + \Delta x \, |\ln(\Delta x)|)$

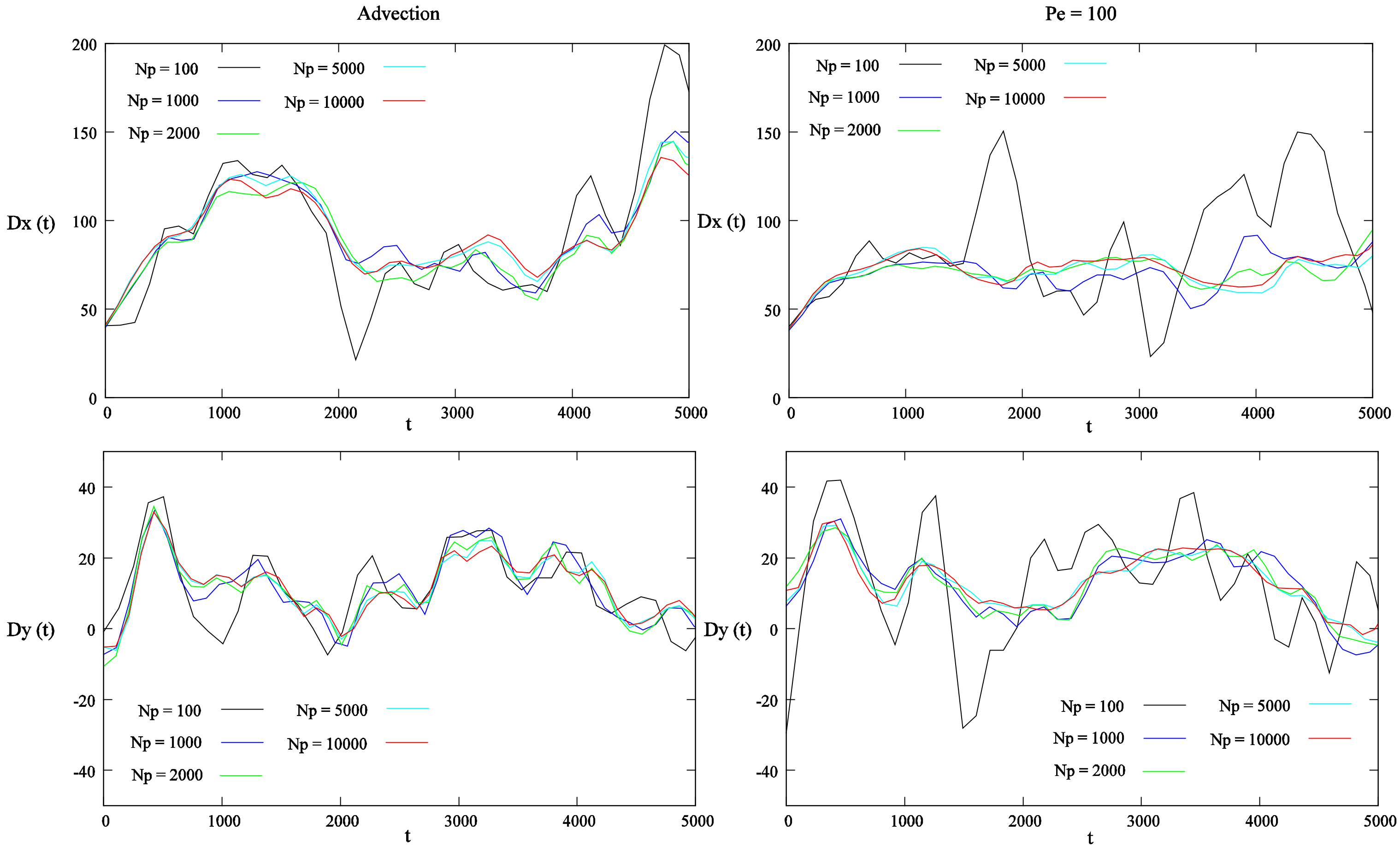
Random walker : convergence analysis

Pure advection

Advection-diffusion with Pe=100

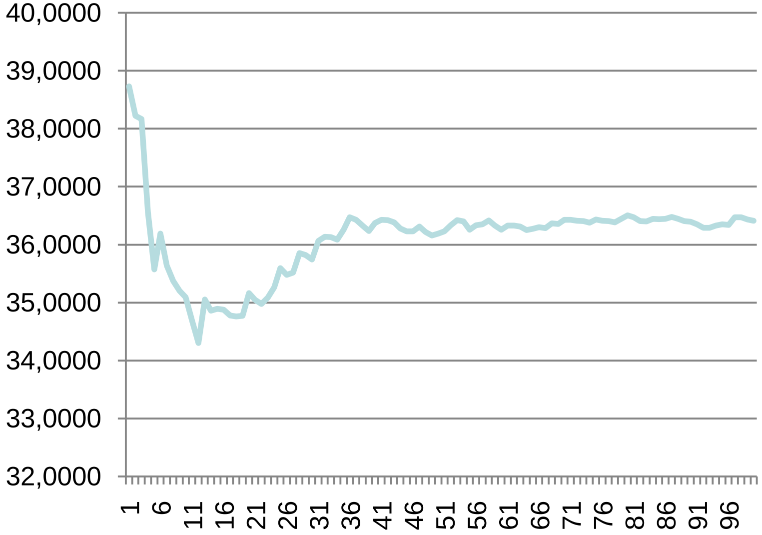
Longitudinal dispersion

Transversal dispersion

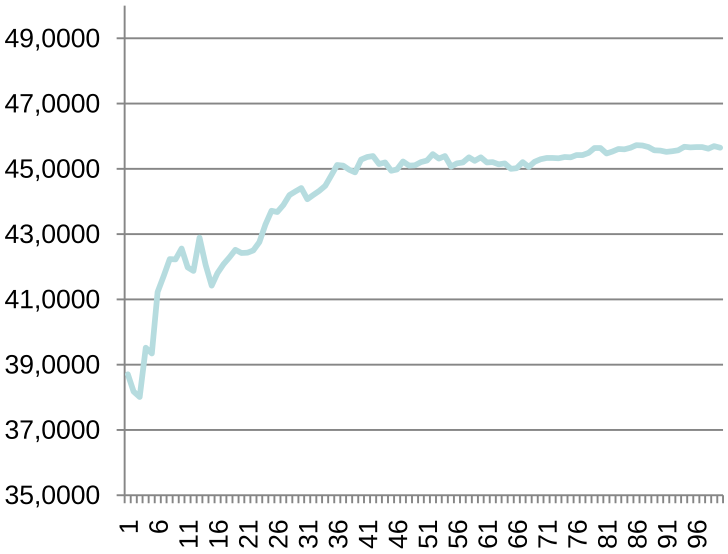


N_p = 2000 is a good trade-off between efficiency and convergence

Monte carlo simulations: convergence analysis

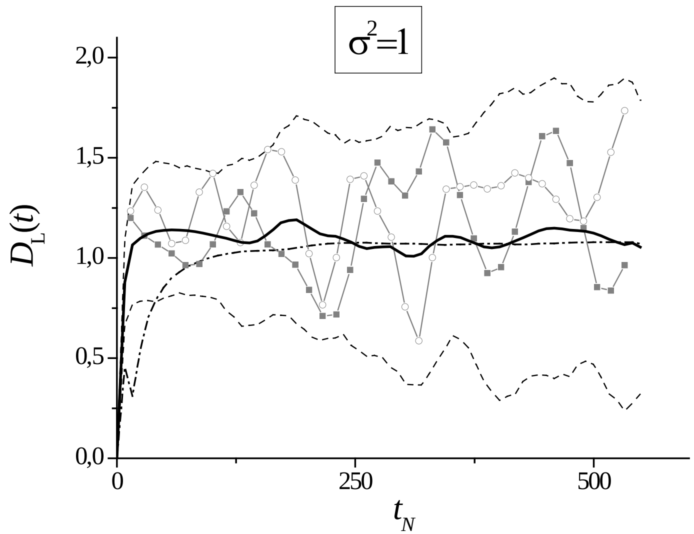


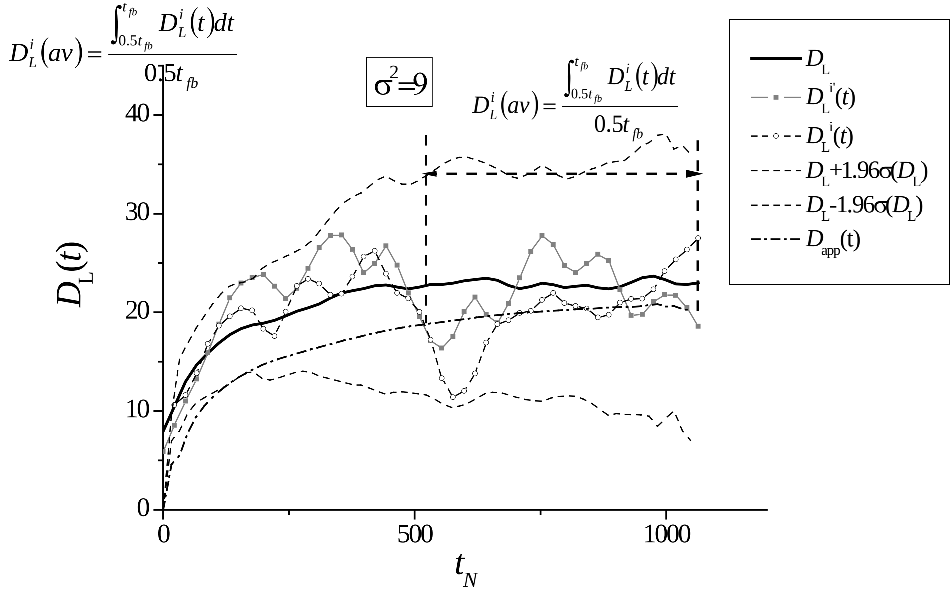
Pure advection

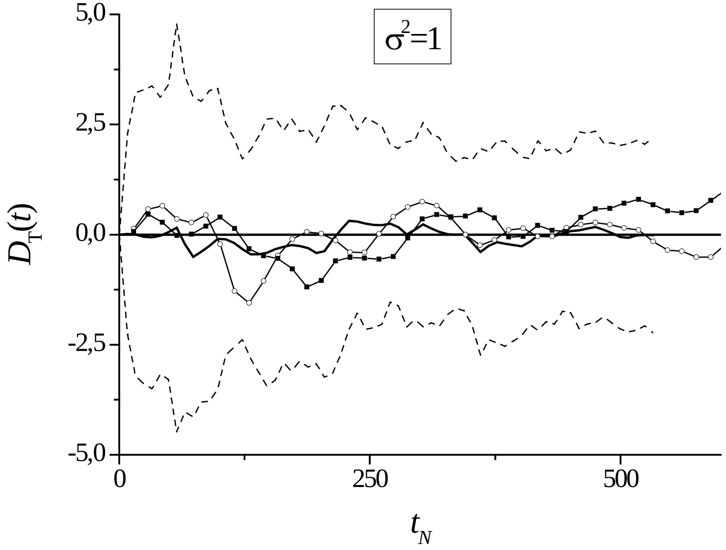


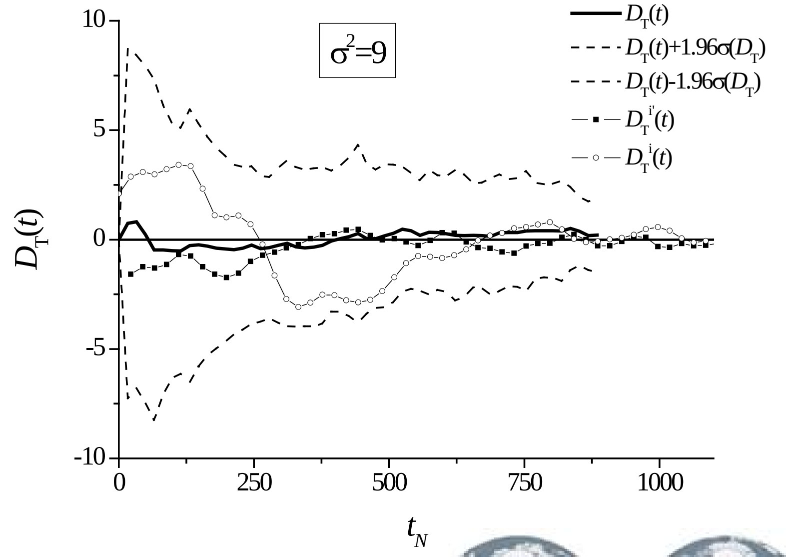
Pe=1000

Monte-Carlo simulations: convergence analysis









Conclusion

Summary

- Efficient and accurate algebraic multigrid solver for groundwater flow in heterogeneous porous media
- Efficient random walker solver for solute transport
- Macro-dispersion analysis in 2D domains

Current and Future work

- 3D heterogeneous porous media
- Grid computing and parametric simulations
- Dispersion due to velocity
- Mathematical and numerical analysis
- Tuning of numerical parameters
- Other non intrusive UQ methods