An Eulerian joint velocity-concentration PDF method for reactive transport in highly heterogeneous porous media

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Outline

- Dispersion in heterogeneous porous media
- Existing methods
- PDF method
- Validation PDF method with Monte Carlo data:
  - Tracer dispersion:
    Caroni, E. and V. Fiorotto, Analysis of Concentration as Sampled in Natural Aquifers. Transport in Porous Media, 2005. 59(1): p. 19-45.
  - Bimolecular reaction:
    Cirpka, O.A., Choice of dispersion coefficients in reactive transport calculations on smoothed fields. Journal of Contaminant Hydrology, 2002. 58(3-4): p. 261-282.

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Uncertainty Assessment of Tracer Dispersion in Heterogeneous Porous Media

uncertain

$$\frac{\partial C_\alpha}{\partial t} + u_i \frac{\partial C_\alpha}{\partial x_i} = \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial C_\alpha}{\partial x_j} \right) + S_\alpha(\mathbf{C})$$

uncertain

$$\mathbf{u} = -\tfrac{1}{n} K \nabla h$$

uncertain

$$Y = \ln(K)$$

log-conductivity Y(**x**) modeled by multivariate Gaussian field with l_Y, σ_Y^2 (unconditional, no Y measurements)

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Existing Methods

- Monte Carlo, sample over $Y(\mathbf{x})$ realizations
  - \+ general
  - – expensive
- moment methods, solve for $\langle C_\alpha \rangle$ and $\sigma_{C\alpha}^2$
  - \+ evolution equations are easy to derive
  - – closure problems, $\langle S_\alpha(\mathbf{C}) \rangle = ?$
  - – what about concentration PDF, $p(\mathbf{c};\mathbf{x},t)$?
- low order approximations, $Y = \langle Y \rangle + Y'$
  - \+ analytical expressions for $\langle C_\alpha \rangle$ and $\sigma_{C\alpha}^2$ as $f(\sigma_Y^2)$
  - – valid for small σ_Y^2

➡ similar to turbulent flows, propose a PDF method

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Particle Evolution Equations

Each particle represents a fluid volume
in a porous medium realization

$$
\begin{aligned}
dX_i &= \underbrace{u_i(t)\,dt}_{\text{advection}} + \underbrace{\sqrt{2D_i}\,dW(t)}_{\text{PSD}} \\
du_i &= \underbrace{a(u_i)\,dt}_{\text{drift}} + \underbrace{b(u_i)\,dW(t)}_{\text{diffusion}} \\
dC_\alpha &= [\underbrace{M_\alpha(\mathbf{C},\mathbf{X},\mathbf{u})}_{\text{dilution}} + \underbrace{S_\alpha(\mathbf{C})}_{\text{reaction}}]\,dt
\end{aligned}
$$

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PDF Transport Equation

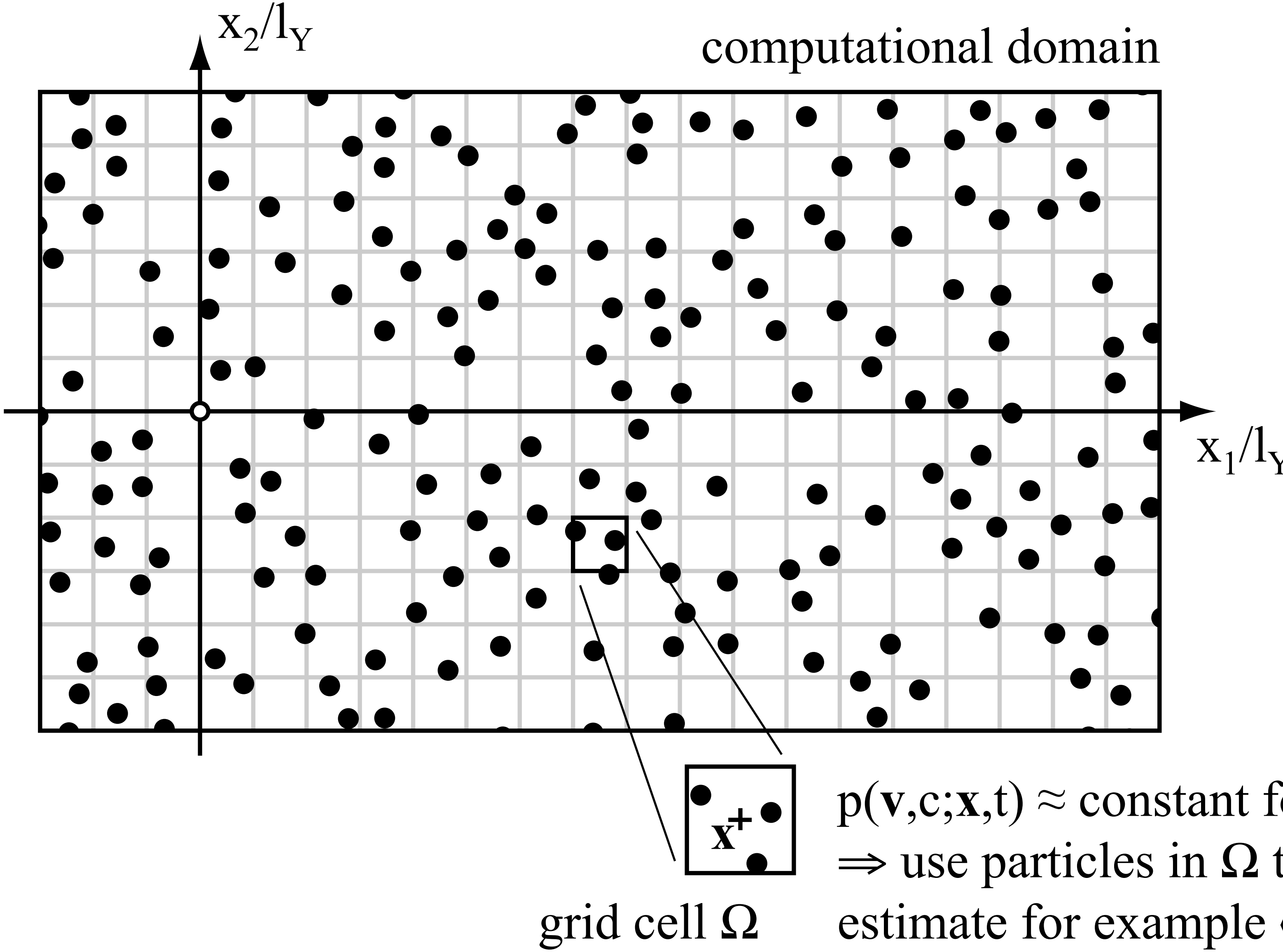
equation for joint PDF p(**v**,**c**;**x**,t) equivalent to the stochastic differential equations

$$\frac{\partial p}{\partial t} = -v_i \frac{\partial p}{\partial x_i} + D_i \frac{\partial^2 p}{\partial x_i^2} - \frac{\partial}{\partial v_i}\left[a(v_i)\, p\right] + \tfrac{1}{2}\frac{\partial^2}{\partial v_i^2}\left[b(v_i)^2\, p\right] - \frac{\partial}{\partial c_\alpha}\{[M_\alpha(\mathbf{c},\mathbf{x},\mathbf{v}) + S_\alpha(\mathbf{c})]\, p\}$$

$$p(\mathbf{c};\mathbf{x},t) = \int_{-\infty}^{\infty} p(\mathbf{v},\mathbf{c};\mathbf{x},t)\, d\mathbf{v}$$

Gardiner, C.W., Handbook of stochastic methods for physics, chemistry and the natural sciences. Third ed. 2004, Berlin: Springer. 415.

Numerical Solution with Particles



$p(\mathbf{v},c;\mathbf{x},t) \approx$ constant for $\mathbf{x}$ in Ω
$\Rightarrow$ use particles in Ω to estimate for example $\langle C(\mathbf{x},t)\rangle$

Pope, S.B., A Monte-Carlo Method for the Pdf Equations of Turbulent Reactive Flow. Combustion Science and Technology, 1981. 25(5-6): p. 159-174.

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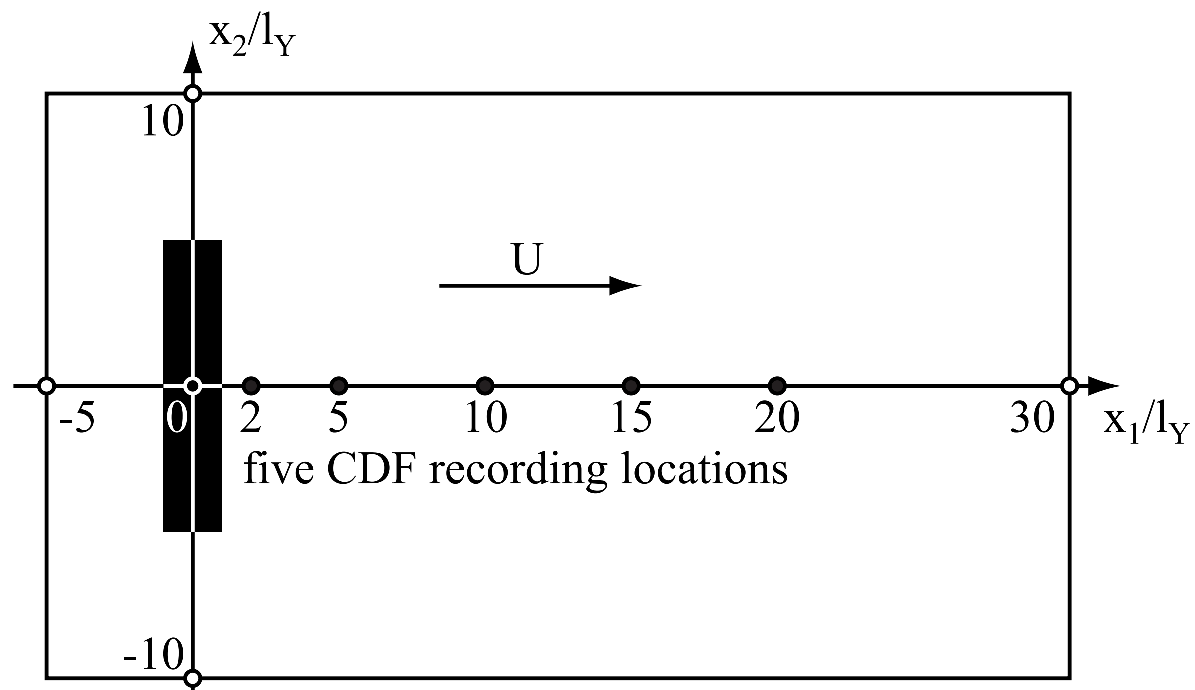
Tracer Dispersion with σ_Y^2 up to 2

- Monte Carlo:
  Caroni, E. and V. Fiorotto, Analysis of Concentration as Sampled in Natural Aquifers. Transport in Porous Media, 2005. 59(1): p. 19-45.
- log-conductivity variances σ_Y^2=0.05, 1, and 2
- Péclet numbers Pe=10...10^4
- rectangular initial tracer cloud
- D_2/D_1=0.05



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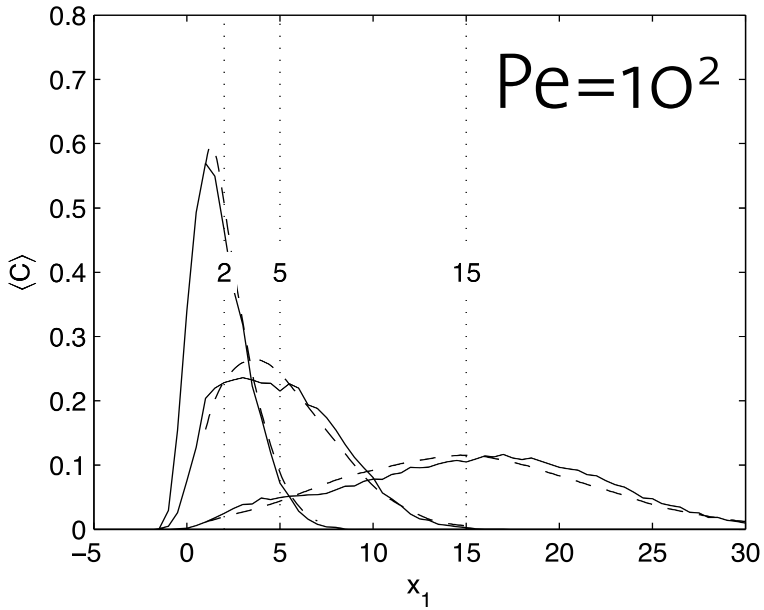
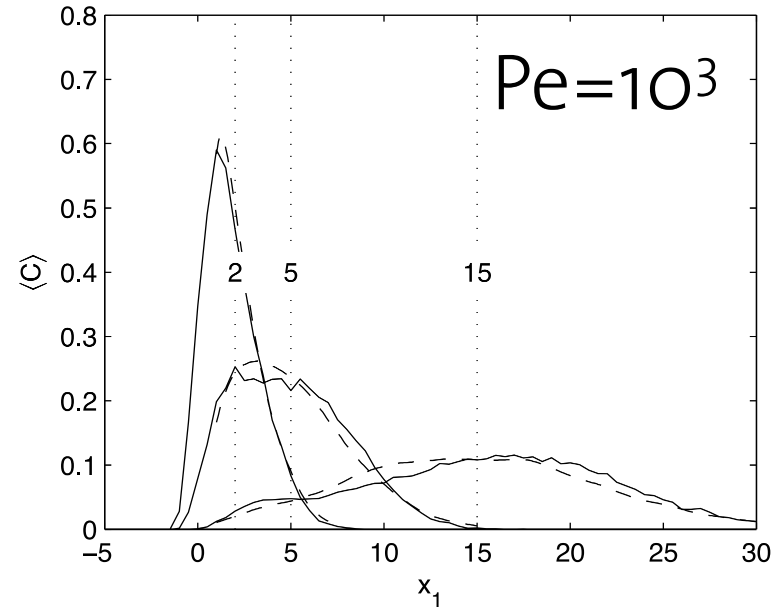
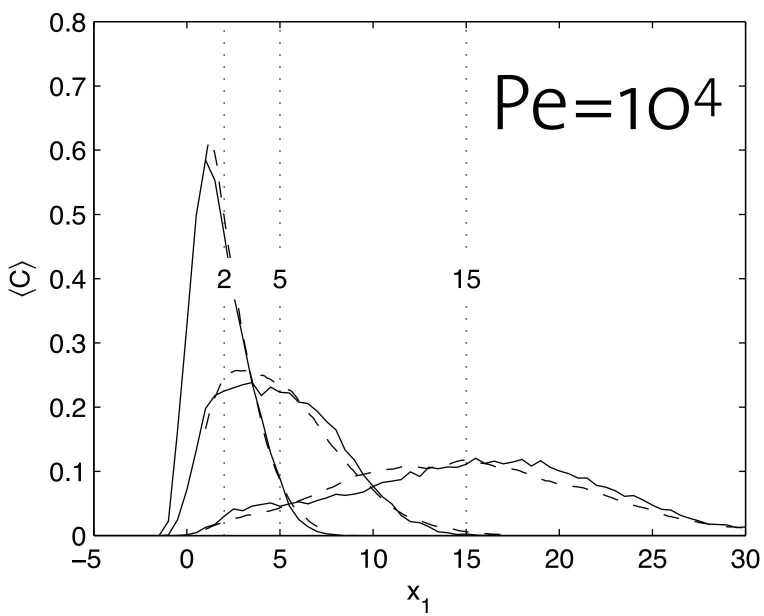
Comparison MC vs. PDF Method







concentration mean

$\sigma_Y^2=2$

dashed MC

solid PDF method

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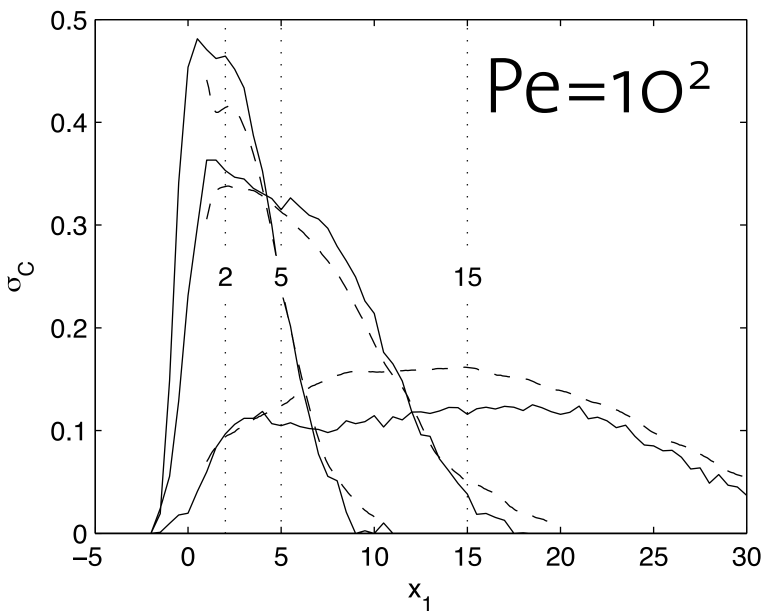
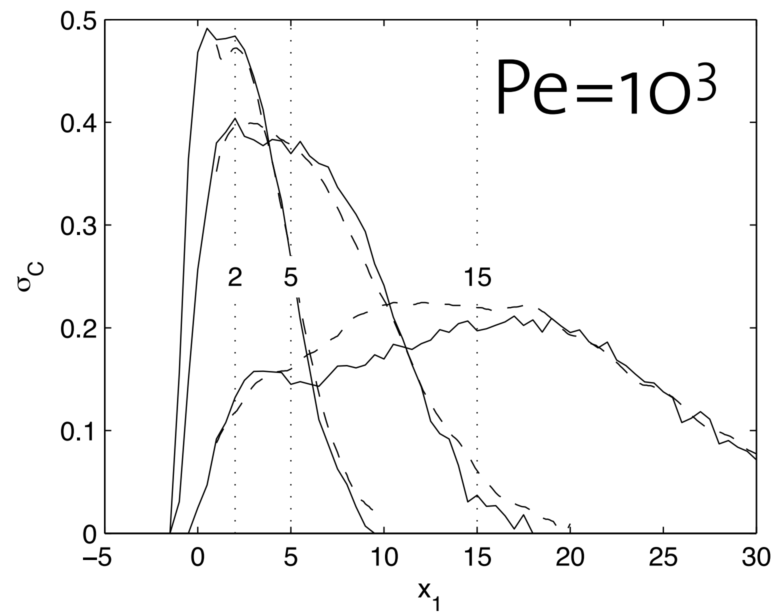
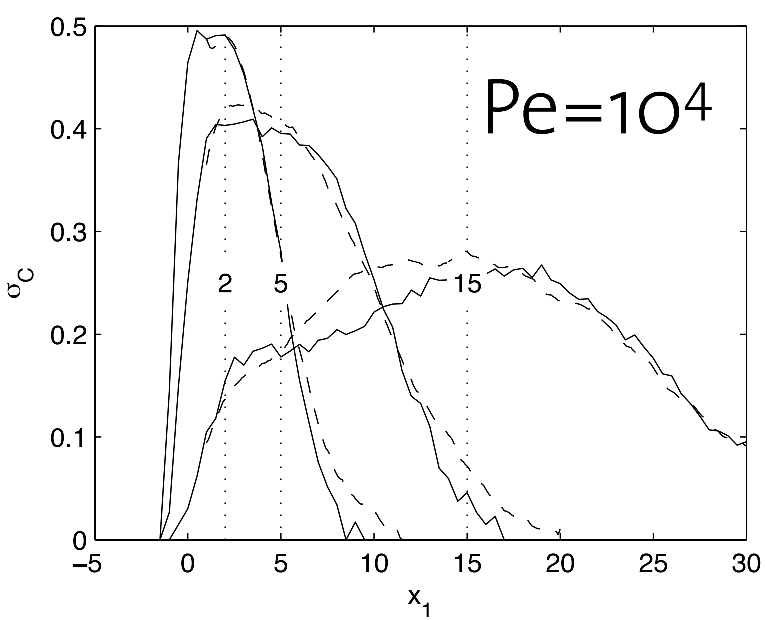
Comparison MC vs. PDF Method







concentration stand. dev.

$\sigma_Y^2=2$

dashed MC

solid PDF method

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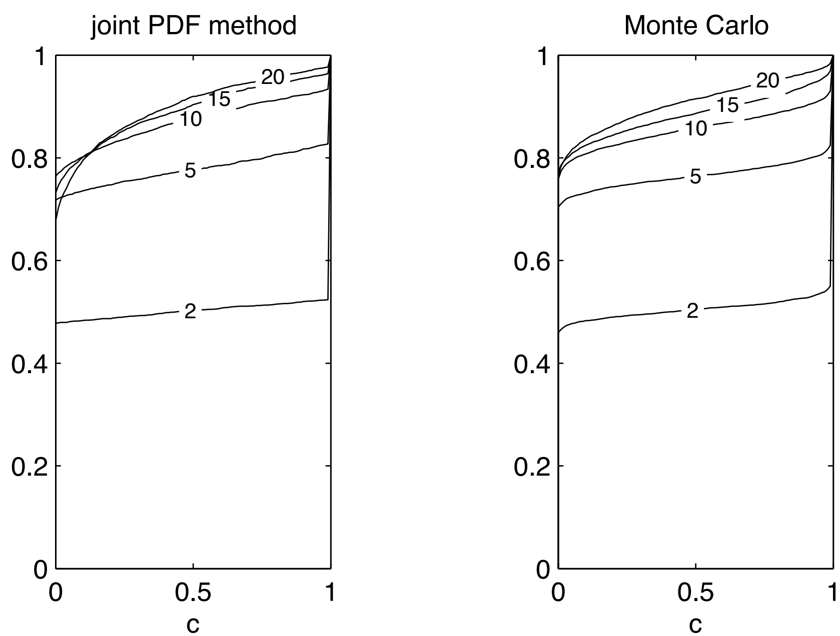
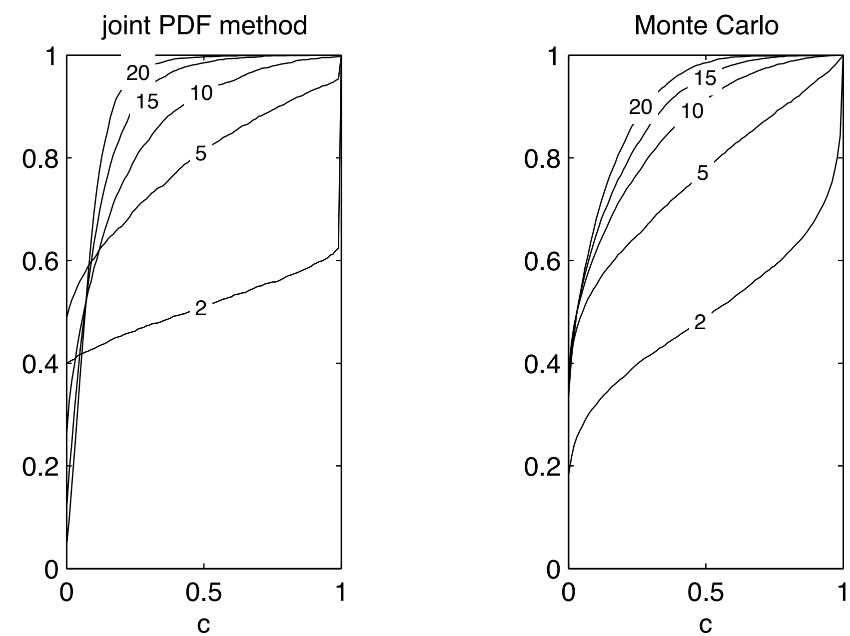
Comparison MC vs. PDF Method

concentration cumulative density functions, $\sigma_Y^2=2$

$Pe=10^4$



$Pe=10^2$



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Bimolecular Reaction with σ_Y^2=1/4

- Monte Carlo (10 realizations):
  Cirpka, O.A., Choice of dispersion coefficients in reactive transport calculations on smoothed fields. Journal of Contaminant Hydrology, 2002. 58(3-4): p. 261-282.
- $A + B \rightarrow C$: $S_A = -\gamma C_A C_B$, $S_B = -\gamma C_A C_B$, $S_C = +\gamma C_A C_B$
- grid resolution: 20 cells per Y correlation length l_Y
- domain size: 50 l_Y x 25 l_Y
- Péclet number $Pe=U\,l_Y/D=500$
- Damköhler number $\mathrm{Da} = \frac{\gamma l_Y^2 \sqrt{C_A^0 C_B^{\mathrm{in}}}}{D} = 500$
- initial condition: $C_A = C_A^0$, $C_B = C_C = 0$
- inflow boundary: $C_B = C_B^{in}$, $C_A = C_C = 0$

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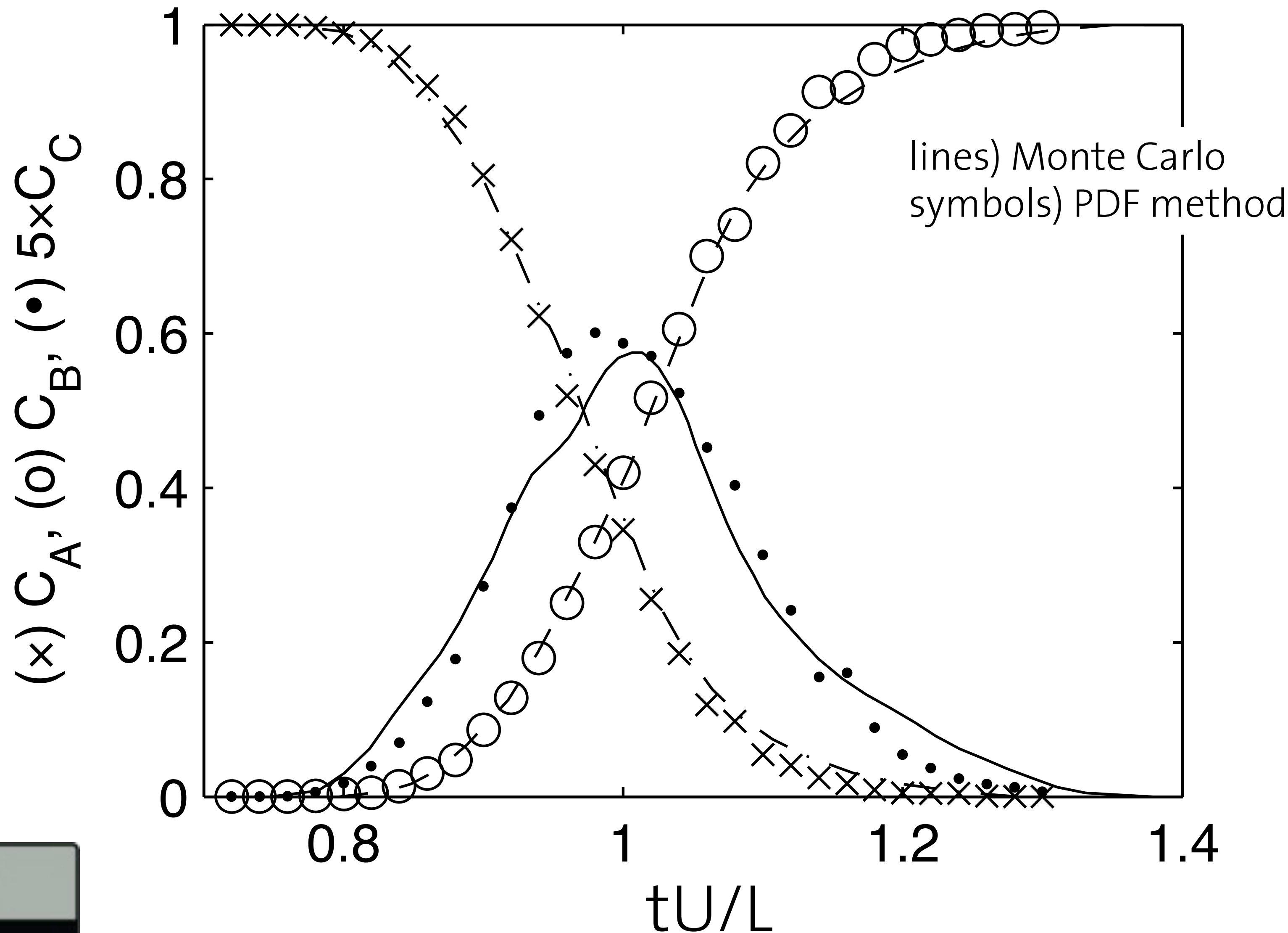
Mean Breakthrough Curves



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Summary

- A new joint velocity-concentration PDF method was outlined where the reactive source term is closed.
- The PDF method includes models to account for advective transport and pore-scale dilution.
- The PDF method produces results at considerably lower computational cost compared to MC.
- Dispersion tests involving a tracer in heterogeneous media and reactive scalars in mildly heterogeneous media were conducted.
- For more details:

Meyer, D.W., P. Jenny, and H.A. Tchelepi, Water Resour. Res., 2010. 46(12): p. W12522
Meyer, D.W. and H.A. Tchelepi, Water Resour. Res., 2010. 46(11): p. W11552