Filtered density function approach for reactive transport in groundwater

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG
NATURWISSENSCHAFTLICHE FAKULTÄT

Nicolae Suciu[1,2] Lennart Schüler[3,4], Sabine Attinger[3,4], Peter Knabner[2]
[1]Tiberiu Popoviciu Institute of Numerical Analysis, Romanian Academy, Cluj-Napoca
[2]Chair of Applied Mathematics I, Friedrich-Alexander University of Erlangen-Nuremberg
[3]Institute of Geosciences, Friedrich Schiller University of Jena
[4]Department of Computational Hydrosystems, UFZ Centre for Environmental Research Leipzig

seit 1558

PDF/FDF evolution equations

Random species concentrations C_α transported in a statistically homogeneous random velocity field $\mathbf{V}$ with divergence-free samples are governed by the stochastic balance equations

$$\frac{\partial C_\alpha}{\partial t}+V_i\frac{\partial C_\alpha}{\partial x_i}=D\frac{\partial^2 C_\alpha}{\partial x_i \partial x_i}+S_\alpha, \qquad (1)$$

where $\alpha=1,\ldots,N_\alpha$, D is a constant diffusion coefficient, S_α are the reaction rates.
The **probability density function** (PDF) $f(\mathbf{c};\mathbf{x},t)$ of the random field $\mathbf{C}$ solving (1) satisfies

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial x_i}(\mathcal{V}_i f)-\frac{\partial^2}{\partial x_i \partial x_j}(\mathcal{D}_{ij} f)=-\frac{\partial^2}{\partial c_\alpha \partial c_\beta}(\mathcal{M}_{\alpha\beta} f)-\frac{\partial}{\partial c_\alpha}(S_\alpha f). \qquad (2)$$

- $\boldsymbol{\mathcal{V}}$ and $\boldsymbol{\mathcal{D}}$ are stochastically upscaled drift and diffusion coefficients and
- $\boldsymbol{\mathcal{M}}$ is the conditional average dissipation rate accounting for mixing by molecular diffusion.

The **filtered density function** (FDF) is defined by the spatial average

$$f(\mathbf{c};\mathbf{x},t)_\lambda=\int_{\Omega_x}\prod_{\alpha=1}^{N_\alpha}\delta[c_\alpha-C_\alpha(\mathbf{x}',t)]G(\mathbf{x}'-\mathbf{x})d\mathbf{x}'=\left\langle\prod_{\alpha=1}^{N_\alpha}\delta[c_\alpha-C_\alpha(\mathbf{x}',t)]\right\rangle_\lambda ,$$

where $G(\mathbf{x}'-\mathbf{x})$ is a filter function of width λ, spatially invariant, non-negative and normalized to unity, $\int_{\Omega_x}G(\mathbf{x}'-\mathbf{x})d\mathbf{x}'=1$, which commutes with differentiation.
The FDF is the PDF of subgrid (i.e., filtered) fluctuations and solves the same evolution equation (2), with coefficients defined by spatial filtering [Suciu et al., 2016].

The Fokker-Planck solution approach

A **stochastic process** in the concentration-position space $\{\mathbf{C}(t),\mathbf{X}(t)\}$ with the **one-time** joint PDF $p(\mathbf{c},\mathbf{x},t)$ is consistent with the **random function** $\mathbf{C}(\mathbf{x},t)$ if for some conserved scalar $\Theta(\mathbf{c})$ the corresponding PDFs are related by

$$\Theta(\mathbf{c})f(\mathbf{c};\mathbf{x},t)=p(\mathbf{c},\mathbf{x},t). \qquad (3)$$

The weighted concentration PDF is then given by the the solution of the Fokker-Planck equation verified by $p(\mathbf{c},\mathbf{x},t)$ [Suciu et al., 2015].

Illustration of the FDF approach for passive transport in aquifers

The weighted PDF/FDF of the concentration averaged over the transverse dimension L_y of a 2-dimensional domain, $C(x,t)=\int_0^{L_y}c(x,y,t)dy/L_y$, estimated on the trajectory $x=Ut$ of the mean flow velocity U is constructed, via (3) with $\Theta(c)=c$, from the solution of the Fokker-Planck equation

$$\partial_t p+\mathcal{V}\frac{\partial p}{\partial x}+\mathcal{V}_c\frac{\partial p}{\partial c}=\mathcal{D}\frac{\partial^2 p}{\partial x^2}+\mathcal{D}_c\frac{\partial^2 p}{\partial c^2}. \qquad (4)$$

The Monte Carlo estimation of $p(\mathbf{c},\mathbf{x},t)$ is obtained by solving the associated system of Itô equations,

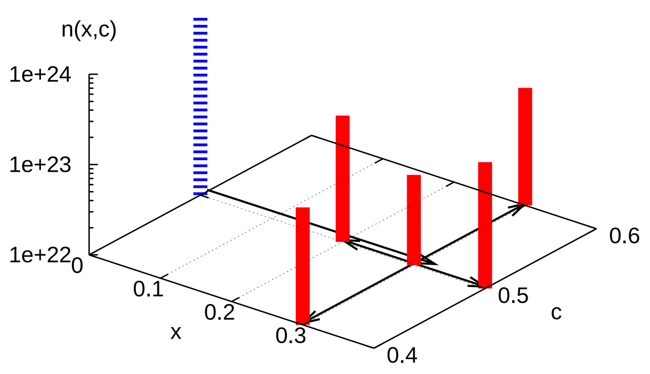
$$dX(t)=\mathcal{V}dt+\sqrt{2\mathcal{D}}dW_1(t), \qquad (5)$$

$$dC(t)=\mathcal{V}_c dt+\sqrt{2\mathcal{D}_c}dW_2(t), \qquad (6)$$

where $W_1(t)$ and $W_2(t)$ are two independent standard Wiener processes.

GRW solutions

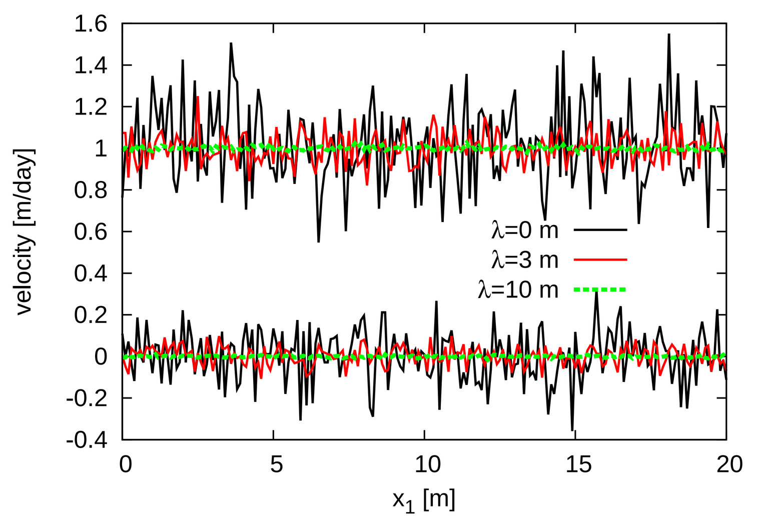
The global random walk algorithm (GRW) is equivalent to a superposition of large numbers of weak Euler schemes for the system of Itô equations (5-6) which moves the $n(i,j,k)$ particles from a lattice site $(x,c)=(i\delta x, j\delta c)$ at $t=k\delta t$ according to



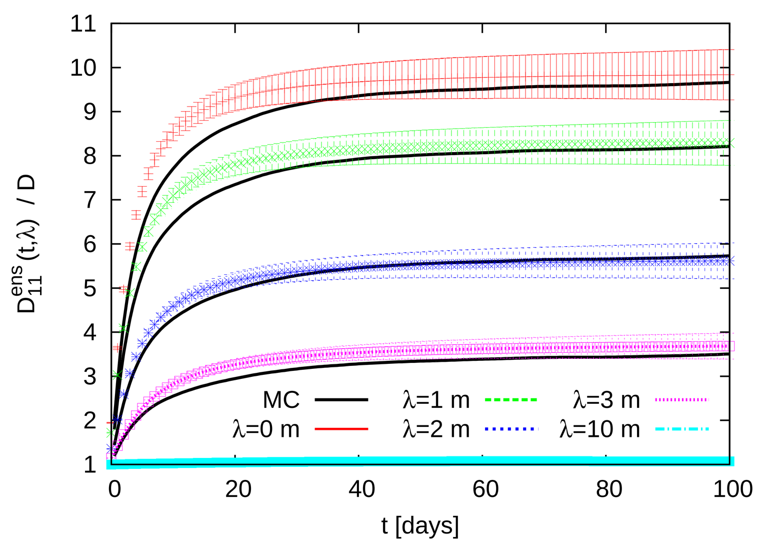
$$\begin{aligned} n(i,j,k) &= \delta n(i+v_i,j+v_j \mid i,j,k) \\ &+ \delta n(i+v_i+d_i,j+v_j \mid i,j,k) \\ &+ \delta n(i+v_i-d_i,j+v_j \mid i,j,k) \\ &+ \delta n(i+v_i,j+v_j+d_j \mid i,j,k) \\ &+ \delta n(i+v_i,j+v_j-d_j \mid i,j,k), \\ n(l,m,k+1) &= \delta n(l,m,k)+\sum_{i\neq l,j\neq m}\delta n(l,m \mid i,j,k), \end{aligned}$$

where v_i, v_j, d_i, d_j are discrete versions of the drift and diffusion coefficients in (4) [Suciu, 2015].

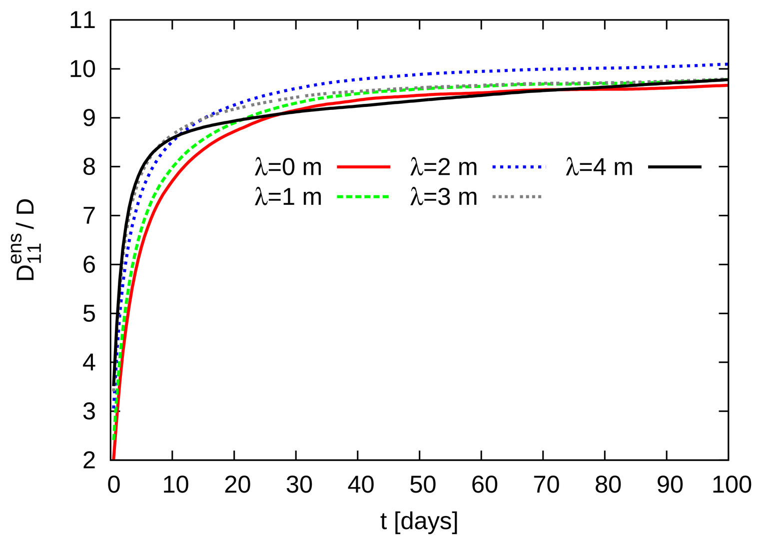
Coarse-grained simulations

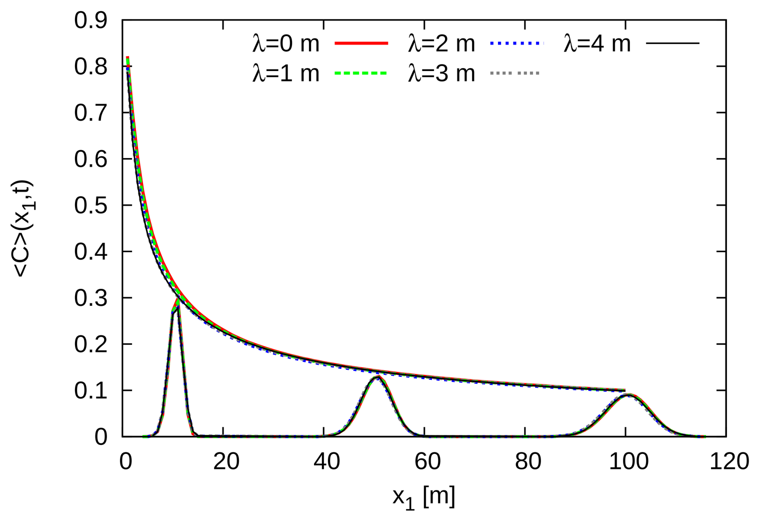


Filtered velocity fields $(\tilde{V}_1,\tilde{V}_2)$ are computed by applying a Gaussian spatial filter of width λ to velocity fields (V_1,V_2) obtained with a Kraichnan random field generator [Suciu et al., 2016, Appendix A]. Monte Carlo ensembles of realizations are obtained by GRW solutions to Eq. (1).



Filtered longitudinal "ensemble dispersion coefficients" $D_{11}^{ens}=\langle(X_1-\langle X_1\rangle)^2\rangle/(2t)$, resulted from Monte Carlo GRW simulations (solid black lines) are close to estimations done on a single trajectories $\{X_1(t),X_2(t)\}$ [Suciu, 2016, Appendix B] (represented with errorbars).





Coarse-grained simulations (CGS) of transport in groundwater are solutions to Eq. (1) with filtered velocities $(\tilde{V}_1,\tilde{V}_2)$ and corrected diffusion coefficients $D_{11}^{CG}=D+\delta D_{11}^{ens}$, with $\delta D_{11}^{ens}=D_{11}^{ens}(\mathbf{V})-D_{11}^{ens}(\tilde{\mathbf{V}})$, $D_{22}^{CG}=D$. For moderately large $\lambda\gtrsim 4$ m, estimates from 256 GRW-CGS retrieve the ensemble dispersion coefficient $D_{11}^{ens}(\mathbf{V})$ computed with fine grained velocities (left) as well as the cross-section concentration $C(x_1,t)$ recorded at $t=10$, 50, and 100 days and the concentration at the expected center of mass $C(x_1=Ut,t)$ (monotonous curves) (right).

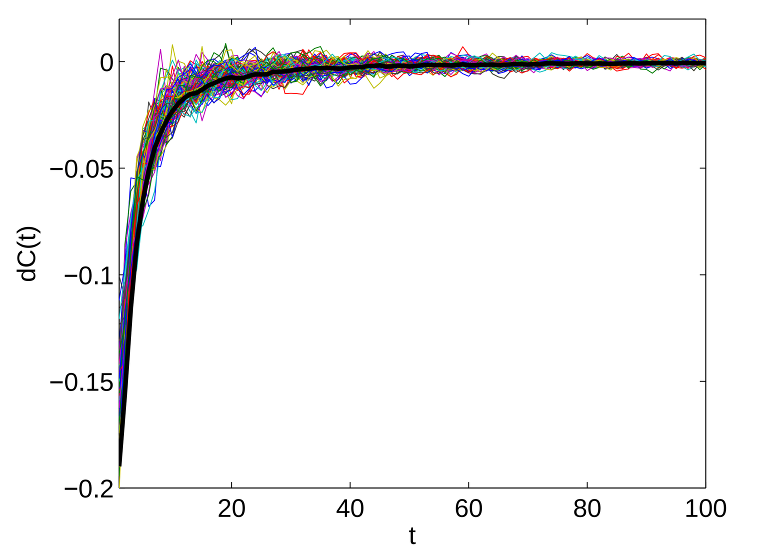
Parameterization of the PDF/FDF equations

Parameterization of PDF/FDF transport in physical space

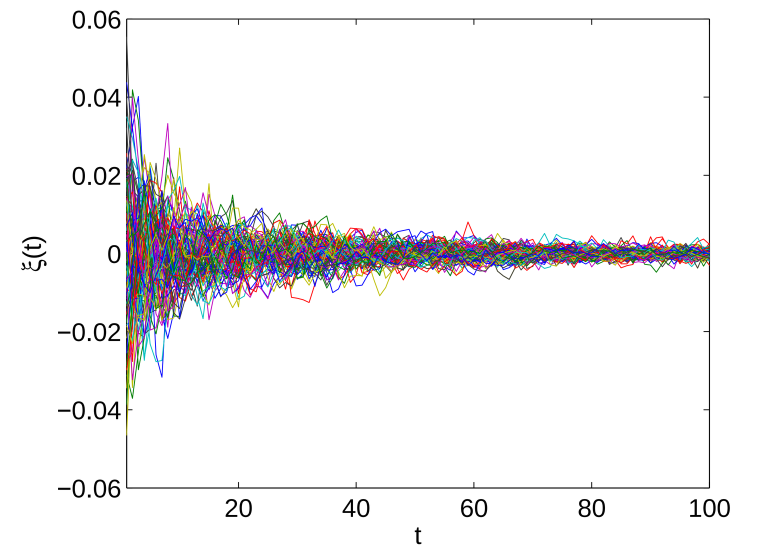
- Drift coefficients in Eq. (5): $\mathcal{V}=U=1$ m/day, for PDF, and $\mathcal{V}=\tilde{V}_1$, for FDF simulations;
- Diffusion coefficients: $\mathcal{D}=D_{11}^{ens}$, for PDF, and $\mathcal{D}=D_{11}^{CG}=D+\delta D_{11}^{ens}$, for FDF simulations.

Parameterization of PDF/FDF transport in concentration space

The stochastic analysis of 500 time series $C(t)=C(x=Ut,t)$ of simulated concentrations provided a Time Series (TS) mixing model for PDF simulations:



Drift coefficients $\mathcal{V}_c^{TS}$ in Eq. (6) are given by the ensemble average of the increments $dC(t)=C(t+1)-C(t)$.



Diffusion coefficients $\mathcal{D}_c^{TS}$ are inferred from the noisy part $\xi(t)$ of the increments $dC(t)$.

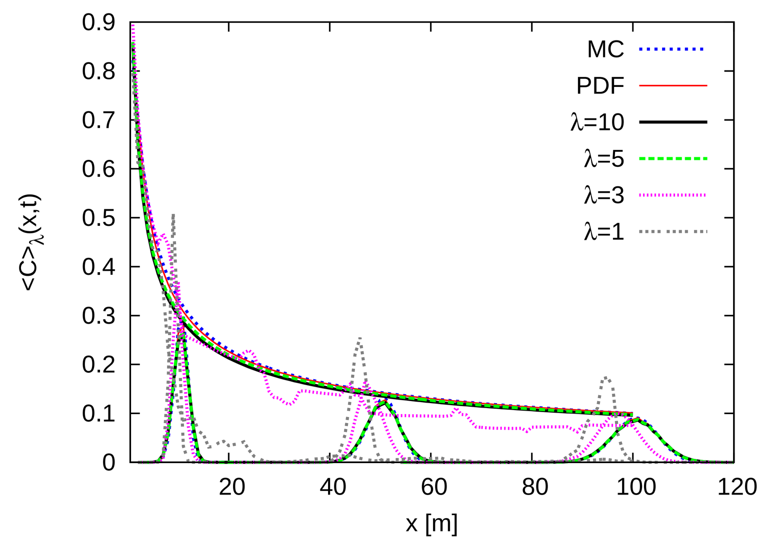
FDF simulations were performed with the linear combination of models for $\mathcal{V}_c$

$$\mathcal{V}_c^{TS-IEM}(t)=\frac{T-t}{T}\mathcal{V}_c^{TS}(t)+\frac{t}{T}\mathcal{V}_c^{IEM}(t),\quad \mathcal{V}_c^{IEM}=-\frac{\mathcal{D}}{(\lambda_{\ln K}+\lambda)^2}(C-\langle C\rangle),$$

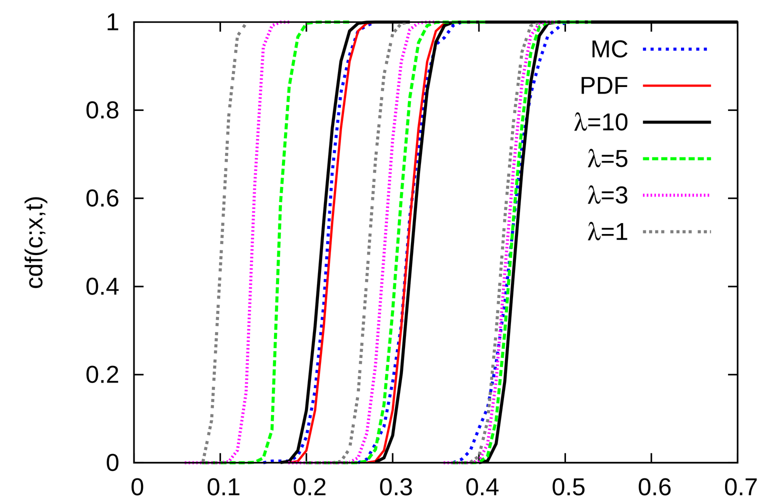
where $\mathcal{V}_c^{IEM}$ is a drift given by the Interaction by Exchange with the Mean mixing model, $\lambda_{\ln K}$ is the correlation length of the log-hydraulic conductivity, and T is the total simulation time.

FDF solutions converge with increasing λ to PDF solutions

The mean concentration $\langle C\rangle(x,t)$ is the position PDF $p_x(\mathbf{x},t)$ obtained by integrating Eq. (3) for $\Theta(c)=c$ over the concentration space Ω_c. It is obtained in the GRW simulation by summing up $p_x(c,x,t)$ over the c-axis.



$\langle C\rangle(x,t)$ at t =10, 50, and 100 days as well as $\langle C\rangle(t)$ recorded at on the mean flow trajectory $x=Ut$ converge with increasing λ to the PDF solution.



Cumulative distribution functions (cdf) estimated at $x=Ut$, t =5, 10, and 20 days obtained in FDF simulations converge with increasing λ to the PDF solution.

Affiliation:
Tiberiu Popoviciu Institute of Numerical Analysis, Romanian Academy, nsuciu@ictp.acad.ro;
Chair of Applied Mathematics I, University of Erlangen-Nuremberg, {suciu, knabner}@math.fau.de;
Institute of Geosciences, Friedrich Schiller University of Jena and UFZ Centre for Environmental Research Leipzig {lennart.schueler, sabine.attinger}@ufz.de

References:
N. Suciu, L. Schüler, S. Attinger, P. Knabner, *Towards a filtered density function approach for reactive transport in groundwater*, Adv. Water Resour. 90 (2016) 83–98, doi:10.1016/j.advwatres.2016.02.016.
N. Suciu, F.A. Radu, S. Attinger, L. Schüler, P. Knabner, *A Fokker-Planck approach for probability distributions of species concentrations transported in heterogeneous media*, J. Comput. Appl. Math. 289 (2015) 241–252, doi:10.1016/j.cam.2015.01.030.