Status Report

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Stochastic simulations of groundwater contamination

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HPC System
JURECA

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Contents

1 Work accomplished and results obtained

The project for the granting period 01.05.2015-30.04.2016 had two objective: GRW simulations for passive transport and MFEM solutions for reactive transport in groundwater, which were part of the DFG Project AT 102/7-1, KN 229/15-1, SU 415/2-1,"Filtered density function uncertainty assessments for reactive transport in groundwater" (2013-2015).

Monte Carlo GRW simulations provided the numerical support for the development of probability density function (PDF) and filtered density function (FDF) approaches for groundwater systems. The results were used to validate the PDF (Suciu et al., 2015a, 2015b) and FDF (Suciu et al., 2016) approaches as well as a new mixing model, governing PDF transport in concentration spaces, (Schüler et al., 2016). Mixing models were also inferred from concentration time series (Suciu et al., 2015a, 2016). Hydrological time series, with power-law behavior (Suciu at al., 2015c) decomposed into intrinsic components by an automatic algorithm (Vamoş et al., 2015) can be used to derive reliable mixing models.

MFEM simulations of reactive transport were done to test various numerical schemes and to design a problem of reactive transport suitable for testing numerical solutions to PDF/FDF equations. An illustration of the new MFEM code for bimolecular reactive transport which will be used in the following investigations is given below, in Section 3.

2 Publications with project results

Schüler, L., N. Suciu, P. Knabner, and S. Attinger (2016), Building a Bridge from Moments to PDF's: A new approach to finding PDF mixing models, submitted to Adv. Water Resour. (under review), arXiv:1602.01353vl [physics.flu-dyn] 3 Feb 2016.

Suciu, N., F.A. Radu, S. Attinger, L. Schüler, P. Knabner (2015a), A Fokker-Planck approach for probability distributions of species concentrations transported in heterogeneous media, Journal of Computational and Applied Mathematics, 289, 241-252, doi:10.1016/j.cam.2015.01.030.

Suciu, N., L. Schüler, S. Attinger, C. Vamoş, and P. Knabner (2015b), Consistency issues in PDF methods, Analele Stiintifice ale Universitatii Ovidius Constanta-Seria Matematica, 23(3), 187-208, doi: 10.1515/auom-2015-0055.

Suciu, N., S. Attinger, F. A. Radu, C. Vamos, J. Vanderborght, H. Vereecken, and P. Knabner (2015c), Solute transport in aquifers with evolving scale heterogeneity, Analele Stiintifice ale Universitatii Ovidius Constanta- Seria Matematica, 23(3), 167-186, doi:10.1515/auom-2015-0054.

Suciu, N., L. Schüler, S. Attinger, C. Vamoş, and P. Knabner (2016), Towards a filtered density function approach for groundwater, submitted to Adv. Water Resour., 90, 83–98, doi:10.1016/j.advwatres.2016.02.016.

Vamoş, C., M. Crăciun, and N. Suciu (2015), Automatic algorithm to decompose discrete paths of fractional Brownian motion into self-similar intrinsic components, Eur. Phys. J. B, 88, 250, doi:10.1140/epjb/e2015-60515-5.

3 Material suitable for the general public

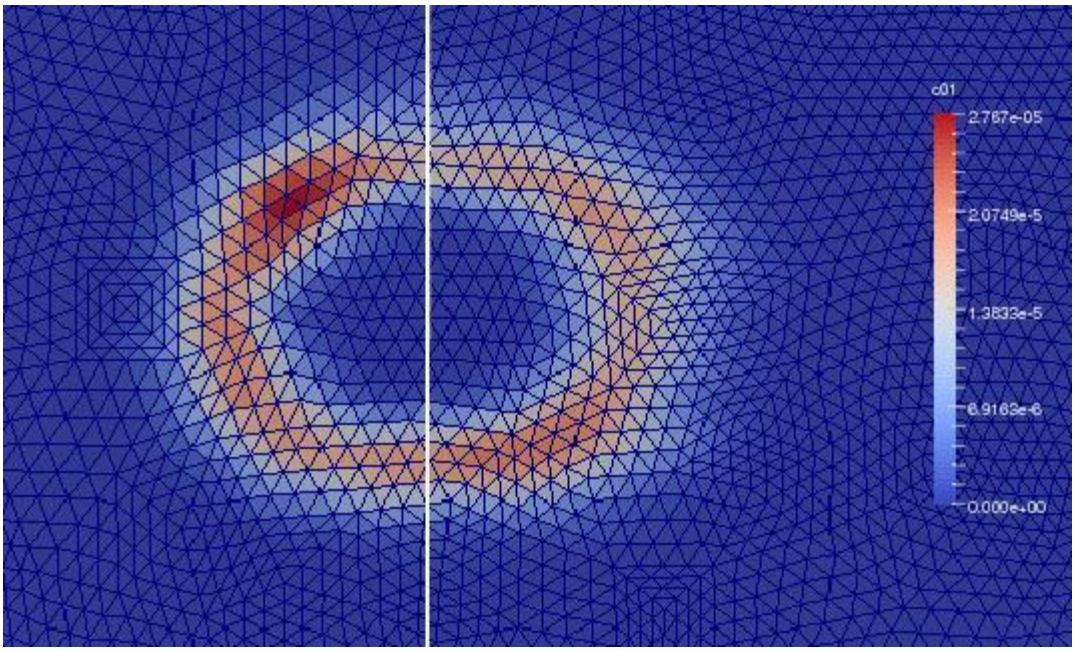

Figure 4.1. MFEM solution to a bimolecular reactive transport problem at t=100 days. The initial condition for the two chemical species was a uniform distribution with $c_1 = c_2$ in a small rectangle located close to the left boundary of a two-dimensional domain. The corresponding reaction rates are given by c_1c_2 and $-c_1c_2$, respectively. The flow, oriented from left to right, solves the Darcy and continuity equations for a realization of a lognormal hydraulic conductivity field. At t=100 days the c_2 species is completely consumed.

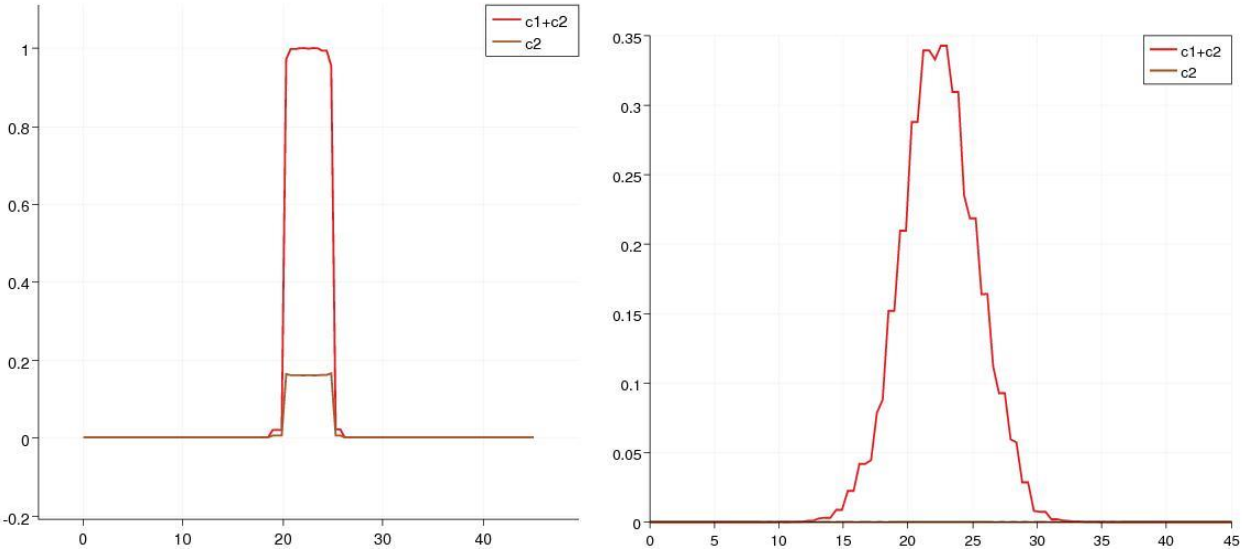

Figure 4.2. The sum of species concentrations and the c_2 concentration, sampled in a cross section through the solution (white line in Figure 1) at t=2 days and at t=100 days.