Topic:
Global random walk stochastic simulations for the assessment of the contamination risk in groundwater systems

Summary

The predictability of contamination in groundwater systems will be investigated via stochastic simulations using the Global Random Walk method (GRW). To this aim, statistical ensembles of transport realizations, computed by GRW simulations on high performance parallel computers, will be used to estimate ergodicity ranges. The latter are defined by the root mean square deviation of actual observables from predictions provided by stochastic models and quantify the ergodicity in a large sense. The investigations will focus on pre-asymptotic regime and on memory effects induced by the nonlinear dependence of transport on the shape and dimensions of the initial solute plumes. Stochastic analyses based on Fokker-Plank and Itô equations will be developed and used for the interpretation of the stochastic simulations results. To increase the computational efficiency, the algorithm GRW also will be used as part of an ergodic simulations procedure. This approach exploits the ergodicity of the geo-statistical model of the groundwater velocity field with finite correlation range by inferring transport statistics from space averages over simulations done for a single velocity realization.
State of the art

Considering advection-dispersion as the principal mechanism and assuming constant porosity, the transport of solutes in time stationary groundwater flows can be described at a macroscopic scale by the local partial derivative balance equation for the concentration field $c(x,t)$,

$$\partial_t c + \nabla(Vc) = \nabla(D\nabla c). \tag{1}$$

The tensor of the “local dispersion coefficients” $D$ describes the molecular diffusion and the hydrodynamic dispersion caused by the spatial variability of the velocity at scales smaller than those resolved by the velocity vector field $V(x)$ [Sposito et al., 1986]. The latter is governed by the Darcy law $V(x) = -K(x)\nabla h(x)$, where $h$ is the hydraulic head and $K$ the hydraulic conductivity field, and by a local conservation law which in absence of sources is given by the incompressibility condition for the velocity field, $\nabla V = 0$.

It is convenient to rewrite (1) as

$$\partial_t c + \nabla [(V + \nabla D)c] = \nabla^2 (Dc), \tag{1'}$$

which has the form of a Fokker-Planck (or Kolmogorov “forward”) equation describing the transition probabilities of the advection-dispersion process. For constant $D$, there is no difference between (1) and (1’) and the transport in divergence-free flows is described by the equation

$$\partial_t c + V\nabla c = D\nabla^2 c, \tag{1''}$$

on which most of the theoretical and numerical approaches are based. For given initial conditions, $c(x,t)$ is the one time probability of the advection-dispersion process, i.e. a normalized concentration, and (1’’) is strictly equivalent to the Itô stochastic equation

$$X(t) = X(0) + \int V(X(t'))dt' + \int dW(t'), \tag{2}$$

where $X(t)$ is a trajectory of the process starting at $X(0)$ and $W$ is a Wiener process of mean zero and variance $<W^2> = 2tD$ [Gardiner, 1985].

The heterogeneity of the hydraulic conductivity is efficiently described as a realization of a random space function [Sposito et al. 1986; Hassan et al., 1998] which is based on geo-statistical models of field data [Chilès and Delfiner, 1999]. The corresponding advection velocity field also becomes a random function and the transport in natural porous media is described by a stochastic model consisting of a diffusion process in a random velocity field [Matheron and de Marsily, 1980; Dagan, 1984; McLaughlin et al., 1985; Oelschläger, 1988; Avellaneda and Majda, 1992]. Different stochastic approaches, based on a master equation describing the solute transport at local scale [Berkowitz and Scher, 2001], or using a Fokker-Planck equation in velocities-positions phase space [Kurbanmuradov et al., 2003], were also proposed and are very promising, since the parameters of the model can, in principle, be derived from measured data.

A basic concept in stochastic modeling is the “macrodispersion”, i.e. an up-scaled Gaussian process which describes the average of the concentration over the realizations of the velocity field at sufficiently large scales. Besides heuristic arguments, assuming that a central limit...
For the pre-asymptotic regime of transport it is even more intricate to assess the reliability of the stochastic modeling. The macrodispersion concept makes no sense for small and intermediate times, as the ensemble average predictor of the dispersive flux \( \mathbf{J} = \mathbf{V} c - \mathbf{D} \nabla c \) corresponding to processes described by (1) is non-local in space-time and non-Fickian. Even if localized forms can be derived under some restrictive conditions, the localized dispersion coefficients still depend on space and time [Morales-Casique et al., 2006]. Moreover, since the velocity field is highly variable and actually known mainly in a mean (statistical) sense, the equations (1) and (2) cannot
be in general solved to provide a complete description of the transport for given velocity realizations. Some information about the behavior of the transport is supplied by the second spatial central moments of the plume (or by their rate of increase with time, which defines dispersion coefficients). Such dispersion quantities can be derived by different approximation techniques, without solving the transport equations and regardless the Fickian or non-Fickian behavior of the process [Suciu et al., 2006b]. They are usually given as ensemble averaged quantities [Dagan, 1984; Dentz et al., 2002, 2003] but they can also be computed for single realizations of the velocity [Eberhard, 2004].

The dispersion of a swarm of diffusing particles is defined by their mean square displacement and, due to the equivalence between (2) and (1), it is identical to the second central spatial moment of the actual concentration \( c(x,t) \). The average of the dispersion tensor over the realizations of the velocity field, \( S_{ij} \), \( i,j = 1,2,3 \), is related with the second moment of the ensemble averaged concentration \( <c> \), denoted by \( \Sigma_{ij} \), and with the variance of the plume center of mass, \( R_{ij} \), by the well known relation [see e.g. Kitanidis, 1988]

\[
S_{ij}(t) = \Sigma_{ij}(t) - R_{ij}(t).
\]

Using a simplified Lagrangian model and the argument of “Lagrangian stationarity” of the plume moments, Dagan [1990] has found a similar relation,

\[
S_{ij}(t) = S_{ij}(0) + X_{ij}(t) - R_{ij}(t),
\]

where \( X_{ij} \) is independent of the initial conditions and equals the moment \( \Sigma_{ij} \) of the ensemble averaged concentration for a point like instantaneous injection at the origin of the coordinates system. The vanishing centroid variance, \( R_{ij} \approx 0 \), is referred to as “ergodicity condition” which ensures the reliability of the estimations of the actual moments \( S_{ij}(t) \) by “the second moment of an ergodic plume” \( X_{ij} \) [Dagan, 2004; Zhang and Seo, 2004].

The relations (3) and (4) are often confounded and cited together as “the fundamental relation of Kitanidis [1988] and Dagan [1990]”. While (3) was derived by Kitanidis [1988] under the only requirement of finiteness of the first two moments of the plume and is a simple identity [Suciu et al., 2006a, Section 4.3], the relation (4) is not valid in general. Sposito and Dagan [1994] warned that unless strong assumptions as the ergodicity of the plume moments are allowed, (4) have to be supplemented by the ensemble average of the cross-correlation between initial positions and velocity fluctuations along trajectories. Recent numerical investigations [Suciu et al., 2006a] have also shown that, for large transverse sources, (3) and (4) written for the transverse dispersion are not equivalent, i.e. \( \Sigma_{22}(t) - S_{22}(0) \) strongly depends on the plume dimension and therefore cannot be equated to an ergodic moment \( X_{22} \).

Theoretical approaches based on approximations could be inadequate tools to capture the subtle difference between (3) and (4). For instance it can be shown that the first order approximations render the two relations strictly equivalent. Therefore numerical approaches are not only attractive but possibly unavoidable. Appropriate algorithms for advection-dominated transport problems can be built in a Lagrangian-Eulerian approach, for instance by solving the advection step separately with the method of characteristics. In this way it is possible to obtain accurate numerical solutions, uniformly convergent with respect to the Péclet number, and stable with respect to the initial data [Bause and Knabner, 2002]. This approach can be successfully applied to real cases of contamination when the problem parameters can be supplied by measurements and inverse modeling. Numerical solutions of partial derivative equations have especially proved their strength for multiphase transport with many different reactant species.
As for non-reactive transport, mainly in synthetic velocity fields which show sharp contrasts in their spatial variability [Schwarze et al., 2001; Dentz et al., 2002, 2003; Eberhard, 2004; Suciu et al., 2004a, 2006a], the approaches based on random walk methods are easier and more accurate to implement [Chorin, 1978; Ghoneim and Sherman, 1985; Sun, 1996; Delay et al., 2005].

The mostly used random walk methods which track particles in the space domain, generically called “particle tracking” (PT) methods, are numerical schemes for the Itô stochastic equation (2) [Kloeden and Platen, 1995]. Their main limitation is due to the enormous number of particles necessary to achieve the accuracy in real life problems [Sun, 1996]. The “global random walk” algorithm (GRW) overcomes the difficulties encountered by PT since the number of particles can be as large as supported by the double-precision representation on a given computing platform [Vamoş et al., 2003]. GRW has been recognized as a general method of “walks on lattices” [Bakalis et al., 2006] of cellular automata (CA) type which, unlike PT, moves groups of particles [Delay et al., 2005]. A drawback of the random walk methods, of both PT of CA type, is that, in order to calculate concentrations, the particles belonging to one cell often have to be gathered at its center (or projected on the grid), a procedure which may yield artificial dispersion [Delay et al., 2005]. In this respect, GRW has the advantage that being a “walk on lattice”, and not a “grid-free” procedure like PT, the particles density is simply given by the number of particles at grid nodes. Moreover, the squared space steps divided by the time step are proportional to the diffusion coefficients. The mean square displacement in a time step of the particles jumping from any grid site is also strictly equal to the dispersion of the simulated diffusion process (which, in fact, defines the diffusion coefficients). Therefore, GRW is completely free of numerical diffusion. As the number of particles at grid sites is not limited, GRW is self-averaging and has no random fluctuations of the computed concentration like the usual PT method [Vamos et al., 2003].

An issue which has received much less attention in reviews on random walk methods [Ghoniem and Sherman, 1985; Delay et al., 2005] is that of the “overshooting”. The overshooting errors occur when the computational particles overpass cells with different velocities or diffusion coefficients. The overshooting can be managed by refining the time discretization in the PT scheme and solving the advection step, separately, by a Runge-Kutta method [Roth and Hammel, 1996]. However, as long as the particles jump over more than one space step, the overshooting errors cannot be completely removed. By imposing that the particles move only to the nearest grid sites, the advective flux should be modeled by a method different from the translation-like advective step used in PT and GRW. This can be achieved when the jumps of the particles are described by spatially biased probabilities. In this way, a biased GRW algorithm (BGRW) has been obtained. BGRW is a cellular automaton which preserves the self-averaging property of GRW, solves exactly the advection-dispersion equation (1), i.e. it is free of overshooting errors, and is by itself a consistent numerical model for transport in complex systems such as natural porous media [Suciu et al., 2005a]. Because it requires much finer grids, BGRW is computationally more expensive than GRW in the case of large scale simulations. Nevertheless, it could be more adequate for multispecies and reactive transport at small and intermediate scales. Besides, BGRW can also be used to evaluate the overshooting of the unbiased GRW algorithm [Suciu and Vamoş, 2006, Suciu et al., 2006b].

To summarize, the assessment of the contamination risk in groundwater systems requires not only investigations on macrodispersion and asymptotic ergodicity but also focusing on the pre-asymptotic transport behavior. The latter implies theoretical investigations on the plume spatial moments as well as stochastic simulations by efficient and validated numerical methods. The encouraging results obtained with the GRW algorithm indicate that it is an appropriate tool to be used in stochastic simulation approaches.
**Progress report:** Stage at the end of month 14 of the DFG Project SU 415 1-1.

**A) Two-dimensional GRW simulations of transport**

A1) Two-dimensional GRW simulations (performed on the Jump supercomputer at Research Center Jülich) aiming at obtaining ensembles of realizations for transport in unbounded domains, with different initial conditions and for the following fixed parameters: hydraulic conductivity $K$ with variance $\sigma^2_{\log K} = 0.1$, exponential and Gaussian shape of $\log K$, correlation length $\lambda_{\log K} = 1$ m, mean flow velocity $U = 1$ m/day, and isotropic local dispersion coefficient $D = 0.01$ m$^2$/day.

A2) Detailed investigations on the accuracy of the simulations for travel times exceeding $1000\lambda_{\log K}$ conducted in the following two directions.

A2.1) Computation of the theoretical up-scaled coefficients from the correlations of the Kraichnan velocities; Computation of the cross-correlations between initial positions $x_0$ and velocity fluctuations along paths starting from $x_0$; Assessment of GRW reliability as function of the number of periodic modes in Kraichnan routine [Kraichnan, 1970] and the number of random velocity realizations.

A2.2) Simulations for 20 000 time steps (travel distances of $10 000 \lambda_{\log K}$) and larger number of particles (for instance, as large as the number of solute molecules injected in groundwater during a field test).

A3) Investigations on the pre-asymptotic transport regime and the approach to the up-scaled Gaussian behavior based on analyses of the concentration fields and of the effective coefficients.

A3.1) The study of the dependence of the transport on the transverse dimension of the initial plume by statistical processing of the simulations obtained at (A1).

A3.2) Investigations on the role of the local dispersion by statistical processing of the ensembles of realizations for the same hydraulic conductivity, point instantaneous sources, and Péclet numbers of 100, 1000, and 10 000 (computed between 11.2002 - 02.2003 on the Cray T3E-1200 system at Research Center Jülich).

Step (A) aimed at answering the following questions:

a) Are the simulated concentration fields convergent to the theoretical solution and how accurate are the numerical computations?

b) What is the explanation of the loss in accuracy after thousands of heterogeneity scales?

c) To what extent are the predictions of the stochastic model relevant for the cases of correlation structures, plume extensions, and Péclet numbers which are investigated?

**RESULTS:**

A1) Ensembles of GRW simulations containing between 512 and 1024 realizations have been obtained for the scheduled transport parameters and a fixed number of periodic modes in Kraichnan procedure of $N_p=6400$. Each GRW simulation was done for a different realization of the velocity and used a number of $N=10^{10}$ particles. For point instantaneous source as an initial condition, the particles were released at the origin of the grid. For extended sources, the particles were uniformly distributed in transverse slabs, ($1\lambda_{\log K}$,$L\lambda_{\log K}$), longitudinal slabs, ($L\lambda_{\log K}$,1 $\lambda_{\log K}$), or squares, ($L\lambda_{\log K}$,$L\lambda_{\log K}$), for $L=10$, 50 and 100.

The results for point and transverse extended sources have been used in [Suciu et al., 2006a]. Results for point source and extended sources with $L=100$ are used in [Suciu et al., 2006c] and a tableau with conclusions drawn from all the simulated initial conditions will be included in a technical note scheduled to be submitted for publication in Water Resources Research.

A2.1) The theoretical up-scaled dispersion coefficients computed from the correlations of the numerically generated Kraichnan velocities are shown in Figure B7 and commented in paragraphs 43 and 65 of [Suciu et al., 2006a]. It was found that the confidence intervals of these coefficients grow with the scale of the simulation domain, even for large transverse plumes and
large Np in Kraichnan routine. Therefore, more useful to assess the accuracy of GRW simulations were the analytically derived asymptotic coefficients. The comparisons shown in Figure 9 of [Suciu et al., 2006a] show that GRW approximates the up-scaled coefficients in a range one order of magnitude smaller than the local dispersion coefficient, as required for reliable simulations. This test, together with the validation of the GRW algorithm against a deterministic solution [Vamoș et al., 2003] and against a numerical method for transport in random fields which is free of overshooting errors [Suciu et al., 2005a], indicates that the conclusions concerning the pre-asymptotic behavior and ergodicity are not vitiated by numerical errors.

Cross-correlations between the initial positions x₀ and velocity fluctuations along straight lines perpendicular at x₀ to the initial slab source were found to be negligible (in agreement to what is expected to be obtained in first order approximations). But the correlations initial positions - velocity along the paths of the advection-diffusion process (during GRW simulations) are significant and are responsible for the pre-asymptotic behavior of the process [Suciu et al., 2006a,c].

The accuracy of the GRW simulations was mainly affected by the quality of the Kraichnan velocity fields. Preliminary investigations have shown that Np=6400 periodic modes and R=256 were enough to obtain the desired precision for simulations over thousands of dimensional times. There were no significant differences between simulations for exponential and Gaussian shaped logK correlations (with the exception of somewhat larger fluctuations at early times for the case of Gaussian correlations). A receipt to guide similar simulations is to consider R of the order of the number of realizations and Np of the order of the total simulation time [Suciu et al., 2006a, Appendix B2]. These results were confirmed and completed by a more detailed investigation on the performance of Kraichnan routine, based on approximate solutions of transport by a "Langevin iteration method" [Eberhard et al., 2006]. In this paper the inefficiency of the Karachinan method for small Np and large simulation times has been explained by a logarithmic increase of fluctuations at large times, which however can be postponed by increasing Np.

A2.2) Simulations for 20000 time steps (travel distances of 10000 λlogK) and N=10^27 particles have shown that, for the transport problem considered here, the effective dispersion coefficients level off after the plume originating from a point source has traveled between 8000 and 10000 λlogK (data available on cluster “agro001” at Research Center Jülich). Since the focus was mainly on extended sources, which reach the asymptotic regime for the mean dispersion coefficients much faster, the investigations on ergodicity used only simulations over scales up to 4000 λlogK.

For the relevant parameters σ^2 logK = 0.1 and Pé=100, the increase of N from 10^10 to 10^27 has no influence on the simulations for cross-section concentrations and dispersion coefficients, as already indicated in [Suciu et al., 2004a]. Larger σ^2 logK and/or Pé could require larger N and some tests suggest considering in GRW procedure a number of particles as large as the number of solute molecules injected in groundwater during field tests (see item (C1) below).

A3.1) The dependence of the transport on the transverse dimension of the initial plume has been analyzed by statistical processing of the simulations obtained at (A1) and the results have been published in Water Resources Research [Suciu et al., 2006a].

A3.2) Investigations on the role of the local dispersion, for hydraulic conductivity of variance σ^2 logK = 0.1 and point instantaneous sources, have revealed that for larger Pé the dispersion coefficients reach the asymptotic regime later. But it was also found that the increase of Pé could result in numerical artifacts which manifest by asymmetric plumes (contrary to the expected Gaussian shape of the plumes for small σ^2 logK). Therefore it was concluded that the accuracy of the 2-dimensional simulations based on Kraichnan generator and particles methods is not guaranteed for larger σ^2 logK and/or Pé [Suciu et al., 2006a, Appendix B1].

Most of the results obtained in this part of the project were published in [Suciu et al., 2006a].
This paper is a new version, with major changes, of the manuscript [Suciu et al., 2004b] which was rejected from publication in Water Resources Research. The published paper includes, at the express request of the reviewers, the content of the technical note scheduled as a supplement of the rejected manuscript.

The investigations on ergodicity presented in [Suciu et al., 2006a] are based on a newly introduced definition. This definition quantifies the departure from the ergodic behavior of the transport by the root mean square deviation of an observable from the corresponding theoretical prediction. In practice, the “ergodicity range” is estimated by the deviation of the ensemble mean of the observable from the theoretical value and by its standard deviation around the mean. Specific meanings of the term “ergodicity” as used by different authors are recoverable as particular cases of this definition of ergodicity in a large sense.

The main results of the paper are as follows.

- The simulations based on GRW and Kraichnan routine fulfilled the required accuracy criteria.
- A numerical evidence of the asymptotic ergodicity (with respect to the macrodispersion model) was provided for transport in velocity fields with finite correlation lengths.
- For the rather ideal transport process considered, an initial source extending over $100\lambda_{\log K}$ across the mean flow, and at timescales of practical interest (hundreds of days), the uncertainty of the stochastic prediction is of about 90% for the longitudinal dispersion coefficient and the cross-section concentration, and tens of times larger for the transverse coefficient.
- Large initial plumes, commonly called “ergodic plumes” have a nonergodic behavior in the sense that the ergodicity range does not decrease monotonously and uniformly in time with increasing plume dimension (result in agreement with [Naff et al., 1998] and recently reinforced by numerical findings of Janković et al. [2006]).
- Vanishing centroid variance, $R_{ij} \approx 0$, is not a sufficient condition for ergodic behavior of the dispersion because even if this condition is fulfilled the standard deviations of the dispersion quantities can still be very large.
- Clear evidence has been obtained that the expressions (3) and (4) (given above) for the ensemble average of the second moments of the plume are not unconditionally equivalent, not even for statistically homogeneous velocity fields with finite correlation lengths. This result confirms the doubts formulated by Sposito and Dagan [1994].

During the review process some basic issues such as the meaning and the definition of the dispersion coefficients, the notions of self-averaging and ergodicity have been discussed and their understanding improved.

**B) Investigations on the time behavior of the effective coefficients**

(This item was initially not included into the DFG Project SU 415 1-1)

**B1** A minimal theory aiming at improving the understanding of some concepts often used in the hydrological literature. The focus was on the computation of the various dispersion coefficients by the two equivalent approaches of Itô and Fokker-Planck equations.

**B2** The analysis of the variance of the plume center of mass $R_{ij}$ (or equivalently of the “center of mass” dispersion coefficient) and of the cross-correlations initial positions-velocity fluctuations was scheduled to assess their influence on the pre-asymptotic behavior.

**B3** Investigations on first order approximations were also scheduled, for the purpose of evaluations and in the attempt to clarify the consistency issue.

**RESULTS:**

**B1** A minimal theoretical frame to compute dispersion quantities (second moments or equivalent dispersion coefficients) has been presented for both Itô formalism [Suciu et al., 2006c] and the approach based on Fokker-Planck equation [Suciu et al., 2005b].

**B2** Some results on the behavior of the dispersion coefficients for large transverse plumes...
have been published in [Suciu et al., 2006a]. The theoretical issues raised in this paper were developed in the manuscripts [Suciu et al., 2005b; 2006c].

**B3)** An evaluation of first order approximations by Eulerian perturbation methods (EPM) and the Langevin iteration method (LIM) has been done in a paper accepted for publication in Water Resources Research [Suciu et al., 2006b]. The consistency issue has been formulated shortly for the non-dimensional form of the Langevin equation. (The Itô representation has not been used explicitly because for constant diffusion coefficient the Itô and the Stratonovich forms of the Langevin equation coincide. Moreover, the solution of the first iteration of the Langevin equation trivially verifies the properties of the Itô integral, even for variable diffusion coefficients.) It has been shown that, for the advection dominated problem considered in the paper, the EPM and LIM approximations yield inconsistent first order approximations, since the zero-th order terms contain contributions of the first order in the small parameter of the problem. The inconsistency is in fact an advantage for all the approximations of this kind, i.e. obtained by iterations around the un-perturbed problem consisting of a diffusion process in the mean velocity field. By considering in zero-th order contributions from higher orders, these methods avoid higher order approximations required by consistent expansions if one wants to obtain non-trivial results. The evaluation was done by comparisons, for the same ensemble of Kraichnan fields, with GRW simulations which were previously validated by the BGRW method [Suciu et al., 2005a; Suciu et Vamoş, 2006]. The results show that LIM and EPM yield equivalent asymptotic expansions and are affected by acceptable small errors after one dispersion timescale. The evaluation of the LIM approximation was further used for a detailed investigation on the performance of the Kraichnan routine with respect to self-averaging simulations for large scale problems of transport in Gaussian fields [Eberhard et al., 2006]. The evaluation of LIM and EPM approximations also lead to useful recommendations concerning the use of theoretical dispersion coefficients for parameter identification from field data [Suciu et al., 2006b, paragraph 21]. (The Editor assigned to oversee the peer-review process appreciated that we have done “an excellent job in addressing the issues of applicability of the approach”.)

The Reviewers’ comments helped us to clarify some technical details concerning the concept of “consistent asymptotic expansions” and the actual meaning of the dispersion coefficients for the pre-asymptotic regime.

**C) Numerical simulations of the Krauthausen field experiments**

**C1)** Test runs of the two-dimensional GRW codes in order to assess the discretization parameters, the necessary memory and the cpu time.

**C2)** Ensembles of realizations, simulated on the Jump supercomputer, based on the geo-statistical parameters which characterize the Krauthausen site.

**RESULTS:**

**C1)** The Krauthausen experimental field, near the Research center Jülich, has the horizontal dimensions of about 200 m along the mean flow direction and 50 m on the transverse direction. The log-hydraulic conductivity can be characterized by a horizontal correlation length \( \lambda_{\log K} \approx 6.7 \) m and a variance \( \sigma^2_{\log K} \approx 1.3 \), as determined from grain size data from different layers of the aquifer [Vereecken et al., 2000]. The transverse local scale dispersivity is expected to belong to a range of 1 mm - 100 mm and a typical value of the mean flow velocity is \( U = 0.5 \) m/d [Vanderborght and Vereecken, 2002]. Therefore, for simulations, the (isotropic) local dispersion coefficient was chosen to be \( D = 0.01 \) m\(^2\)/d. For this reference set of parameters, GRW simulations were executed on a 2-dimensional grid of 400 m \( \times \) 160 m with a time step of 1 d and a space step of 0.1 m. The latter ensures a very fine discretization of the velocity of 67 velocity values per log-hydraulic conductivity correlation length. Even if a coarser grid can be used to save memory and computing time, it was not necessary since all the simulation tests lasted less
than 4 min. The velocity field was simulated with the Kraichnan routine, which yields an approximation of the first order in $\sigma^2_{\log K}$ of the Darcy velocity [Suciu et al., 2006a]. The total number of particles in a given GRW simulation was fixed at $N=135.9 \times 10^{27}$, corresponding to the number of molecules contained in the 135.9 Kg of NaBr injected during a tracer test at the Krauthausen field [Vanderborght and Vereecken, 2001]. The initial condition was a uniform concentration in a rectangle of $1 \times 20$ m, which approximates the injection conditions of the Bromide tracer test. Simulated breakthrough curves (BTC) were computed by summing up the numbers of particles contained in slices of $1 \times 160$ m at different downstream locations and by normalization with the initial concentration.

**C2)** A comparison between GRW simulations and the measured cross-section averaged BTC, at the reference plane located at 55 m, during the Bromide tracer test at Krauthausen are shown in Figure 1. (The thin red lines in Figure 1 represent the range of two standard deviations around the ensemble mean concentration, $C(t; 55 \text{ m}) \pm \sigma C$.) The average BRC over $R=10$ realizations overestimates the central region of the measured BTC and underestimates the tail. After about 120 days, the measured BTC is underestimated with more than one standard deviation of the simulated concentrations.

The results improve a little bit by increasing $\sigma^2_{\log K}$ to 4.0, which roughly corresponds to the maximum variance of $\log K$ at Krauthausen (e.g. [Englert, 2002, Table A9, layer 4]). The large
values of the measured BTC are better approximated now and the tail is captured until about 160 days (Figure 2). The difference between the two sets of simulations can be explained by the larger plume extensions in simulations for $\sigma_{\log K}^2 = 4.0$, as shown in Figures 3 and 4.

The time behavior of the second moment of the ensemble averaged concentration, $\Sigma_{ii}$, of the ensemble average of the second moment of the actual concentration, $S_{ii}$, and of the variance of the center of mass, $R_{ii}$, $i=1,2$, is shown in Figures 5 and 6, for the larger simulated variance of the logK field. (The thin lines in Figures 5 and 6 represent standard deviations of the corresponding moments divided by $\sqrt{(R-1)} = 3$.) One notices that only the transverse dispersion reaches the asymptotic regime (constant dispersion coefficients) until the end of the simulation period. As for the longitudinal dispersion, $S_{11}/(2t) < \Sigma_{11}/(2t)$ and both are far from the theoretical (first-order) value of $D + U\sigma_{\log K}^2 \lambda_{\log K} = 13.41 \text{ m}^2/\text{d}$. The effect of the initial transverse plume on the early times behavior of the transverse dispersion is similar to that found in numerical simulations for smaller $\sigma_{\log K}^2$ [Suciu et al., 2006a]: small variability of $R_{22}$, and large fluctuations for $S_{22}$ and $\Sigma_{22}$. The negative values of the coefficients $S_{22}/(2t)$ and $\Sigma_{22}/(2t)$ are explained by the removal of the initial variance $S_{22}(0)$.

The results presented above illustrate the possible utility of the 2-dimensional GRW simulations for interpretations of field data. However a comparison with Krauthausen field data presented in [Vereecken et al., 2000; Vanderborght and Vereecken, 2001] or an identification of the properties of the aquifer is still premature. Firstly, the large value $\sigma_{\log K}^2 = 4.0$ is not representative for the Bromide tracer test since the plume did not reach the profound layer 4 of the Krauthausen aquifer [Vereecken et al., 2000]. Secondly, the large plume asymmetry, as shown in Figures 3 and 4, can also be caused by partial trapping of the computational particles in 2-dimensional simulations using Kraichnan velocity fields [Dentz et al, 2003; Suciu et al, 2006a]. To distinguish between this numerical artifact and enhanced spreading caused by increased $\sigma_{\log K}^2$, the 2-dimensional GRW simulations should be compared with 3-dimensional simulations, not affected by such artifacts. The very likely sinking of the plume caused by a density of the injected solute higher than water density [Vereecken et al., 2000] also requires a modified numerical algorithm of transport simulations.

**D) The elaboration of the three-dimensional GRW codes**

**D1)** The three-dimensional C++ code for transport in heterogeneous aquifers will be developed in two variants: one in which the velocity field will be generated during the GRW simulation of the transport by the Kraichnan routine, and one where the velocity field is an input, already computed by a different code (for instance, the TRACE finite element code developed at
D2) Tests by comparisons with other verified methods for advection-dominated problems, simulations for Darcy velocity fields computed by TRACE code, comparisons with the TRACE - ParTrace method (developed at Research Center Jülich), and some tests for linear reactions.

RESULTS:

D1) The recently developed 3-dimensional GRW C++ code (UGRW3D.cpp) uses the following algorithm. The spreading of the particles lying at the grid site \((i_x, i_y, i_z)\) at the time step \(k\) is described by

\[
\begin{align*}
n(i_x, i_y, i_z, k) &= \delta n(j_x, j_y, j_z | i_x, i_y, i_z, k) + \\
& \quad \delta n(j_x - d_x, j_y, j_z | j_x, j_y, j_z, k) + \\
& \quad \delta n(j_x, j_y - d_y, j_z | j_x, j_y, j_z, k) + \\
& \quad \delta n(j_x, j_y, j_z - d_z | j_x, j_y, j_z, k),
\end{align*}
\]

where \(\delta n(j_x, j_y, j_z | i_x, i_y, i_z, k)\) is the number of particles which after an advection step remain at the new position \((j_x, j_y, j_z) = (i_x + v_x, i_y + v_y, i_z + v_z)\), and the following three lines account for the particles undergoing diffusion jumps on the \(x\), \(y\) and \(z\) directions, respectively. The discrete advection displacements \((v_x, v_y, v_z)\) are given by

\[
\begin{align*}
v_x &= V_x(x) \delta t / \delta x, \\
v_y &= V_y(x) \delta t / \delta y, \\
v_z &= V_z(x) \delta t / \delta z,
\end{align*}
\]

where \(V_x, V_y, V_z\) are the components of the velocity field, \(V(x)\), \(\delta x, \delta y, \delta z\) are the space steps and \(\delta t\) is the time step. The amplitudes of the diffusion jumps, \(d_x, d_y\), and \(d_z\), are defined by

\[
\begin{align*}
r_x &= 2D_x \delta t / (d_x^2), \\
r_y &= 2D_y \delta t / (d_y^2), \\
r_z &= 2D_z \delta t / (d_z^2),
\end{align*}
\]

where \(D_x, D_y\) and \(D_z\) are the components of a diagonal diffusion tensor \(D(x)\) and the parameters \(r_x, r_y\), and \(r_z\), related by \(r_x + r_y + r_z \leq 1\), describe the fractions of the number of particles \(n\) which undergo diffusion jumps on the three space directions.

The main difference with respect to the 2-dimensional GRW codes used in [Suciu at al., 2004a, 2006a] consists in the fact that the algorithm described above no longer is a superposition of 1-dimensional procedures and is therefore more adequate for problems with space-variable diffusion coefficients. A similar procedure was successfully used for \(V(x) = 0\) and 2-dimensional non-homogeneous and non-isotropic diffusion [Vamoş et al., 2004]. However, in the form described above, the UGRW3D code is applicable only for small space variations of the diffusion coefficients. For exact computations, the drift coefficient \(V\) has to be corrected by a term proportional to the divergence of the rows of the diffusion tensor [Suciu and Vamoş, 2006].

D2) A first test of the 3-dimensional code was done by comparisons with the results given by the two-dimensional code, for small variance \(\sigma_{\log K}^2 = 0.1\), Kraichnan approximation of the velocity and point source. Comparisons between cross-section averaged concentrations in 2- and 3-dimensional simulations (Figure 7) show a good agreement, as anticipated by previous theoretical and numerical results [see e.g. Suciu et al., 2006, Section 1]. The cross-section concentrations are still close for larger variance (Figure 8) but the behavior of the dispersion coefficients is different even for small \(\sigma_{\log K}^2\). As seen in Figures 9 and 10, in the 3-dimensional case the approach to the Fickian behavior is faster. One can also remark that the pre-asymptotic longitudinal dispersion coefficients in the 3-dimensional case are larger than in the 2-dimensional one, as also indicated by recent comparisons between 2- and 3-dimensional first-order approximations [Eberhard et al., 2006].

Further validation of the 3-dimensional code can be done by comparisons with the newly elaborated biased global random walk code [Suciu et al, 2005a]. Unlike in the biased GRW
procedure, as used in UGRW3D.cpp, the biased algorithm (BGRW) simulates advective displacements by a bias in the mean number of jumps: \( n(r_x + v_x) \) particles jump in the positive x-direction, \( n(r_x - v_x) \) in the opposite direction, and similarly for y- and z-directions. The procedure was successfully used to evaluate 2-dimensional GRW codes and first order approximations of transport in spatially heterogeneous media [Suciu and Vamoş, 2006; Suciu et al., 2006b].

![Figure 7. Comparison between 2- and 3-dim cross-section concentrations (\( \sigma_{\text{log}K}=0.1 \)).](image1.png)

![Figure 8. Comparison between 2- and 3-dim cross-section concentrations (\( \sigma_{\text{log}K}=1.0 \)).](image2.png)

![Figure 9. Longitudinal dispersion coefficients; 2- and 3-dim GRW simulations for \( \sigma_{\text{log}K}=0.1 \).](image3.png)

![Figure 10. Transverse dispersion coefficients; 2- and 3-dim GRW simulations for \( \sigma_{\text{log}K}=0.1 \).](image4.png)

Results obtained in the first 14 months of the DFG Project SU 415 1-1 were presented in:
- 8 manuscripts, of which 2 are published, 2 accepted for publication, 1 submitted, and 3 in work;
- 3 international conferences (ASIM-2005, Erlangen, September 12-15, 2005; EGU General Assembly, Vienna, April 2-7, 2006; Academic Days - “T. Popoviciu Centenary”, Cluj-Napoca, Romania, June 29-30, 2006);
- 3 Seminar-talks at Institute of Applied Mathematics (AM1) of Friedrich Alexander University Erlangen-Nürnebrg (http://www1.am.uni-erlangen.de/~suciu/presentations.html).
Objectives of the DFG Project SU 415 1-2

A) **GRW simulations and stochastic analyses of the pre-asymptotic transport**, for advection-dispersion as basic mechanism of transport, with focus on:
   A1) *Memory effects* due to persistent influence of the initial conditions on the dispersion in velocity fields with finite correlation range;
   A2) *Dependence of memory effects on the velocity correlation range.*

The topic of this part of the project proposal is also of great importance in physics, whenever the transport process cannot be approximated by a Brownian motion (i.e. the parameters of the system are characterized by non-vanishing correlation lengths).

B) **Further development of the GRW stochastic simulations method**, with the following specific objectives:
   B1) Developing an efficient method for *ergodic GRW simulations*, using single velocity realizations;
   B2) *Investigations on some technical issues*, (different versions of the GRW algorithm, number of particles and boundary conditions for real life applications);
   B3) *Compatibility between GRW and other codes.*

As far as no interactions between particles have to be accounted for, the GRW stochastic simulations method is applicable to a variety of diffusion problems in technology, environmental and life sciences.

Work schedule

Time durations relative to the beginning of the project

<table>
<thead>
<tr>
<th>Goals</th>
<th>Time in months</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>01 02 03 04 05 06 07 08 09 10 11 12 13 14 15 16 17 18</td>
</tr>
<tr>
<td>A1</td>
<td></td>
</tr>
<tr>
<td>A2</td>
<td></td>
</tr>
<tr>
<td>B1</td>
<td></td>
</tr>
<tr>
<td>B2</td>
<td></td>
</tr>
<tr>
<td>B3</td>
<td></td>
</tr>
</tbody>
</table>
A) GRW simulations and stochastic analyses of the pre-asymptotic transport

A1) Memory effects

The “local dispersion” process in advection-dispersion approaches to transport in spatially heterogeneous systems is modeled by a Wiener process. The diffusion coefficient is defined by the rate of increase of dispersion, \( D = \frac{s(t)}{(2t)} \), or equivalently, with a Green-Kubo relation, by the time integral of the velocity autocorrelation function of the diffusing particle. For the Wiener process, this correlation is a white noise with zero correlation time, i.e. a Dirac-delta function. In this case the diffusion coefficient is constant in time and the process “has no memory”. Consequently, the trajectories of the Wiener process are fractal sets: a new process starting at an arbitrary space point on a trajectory reproduces the whole pattern of trajectories of the Wiener process and it obviously has the same dispersion \( s(t) \) [Gardiner, 1985]. More realistic for diffusive movements of particles which interact with the background medium (atoms, molecules or “Brownian particles”) are models of short-range memory. In such a case, the velocity is modeled by the solutions of a Langevin equation, its correlation decays exponentially in time, and the Green-Kubo formula gives a constant coefficient after the integration of the velocity correlation over a rather short time interval [Suciu, 2001]. In physical literature “memory effects” generically denote the departure from these ideal situations (as for instance when velocity verifies a generalized non-Markovian Langevin equation). Such effects manifest in many fields (polymers, plasma, semiconductors, surface diffusion, turbulent flows), are related to the anomalous diffusion, but the role of memory effects is not completely clear, not even for the case of normal diffusion [Klages, 1996; Yulmetyev et al., 2003; Mokshin et al., 2005].

For diffusion in space random velocity fields, the issue of memory effects has two additional levels of difficulty. The first one is a consequence of the space dependence of the velocity. This implies that advection-dispersion processes starting from different initial space points very probably have different second moments (or dispersions) \( s(t) \). This is the main difference with respect to the micro-physics problems mentioned above, where the velocity is usually function of time only and an advection dispersion process with such a velocity would have the same dispersion \( s(t) \) for all possible starting points. The second difficulty comes from the fact that velocity is known only in a statistical sense (mean, variance, correlations). Therefore, if one aims at descriptions for actual physical systems, the model of diffusion in random fields has to predict not only the ensemble mean dispersion \( S(t) = <s(t)> \) but also its variance. The implications are serious mainly for initial concentration distributions with large spatial support (or “large sources”). The superposition of many plumes originating from spatially distributed point-like sources is not equivalent with the plume evolving from a large source with the same spatial dimensions. The result of spatially integrated (averaged) dispersions of the former is instead close to the average over the ensemble of velocity realizations \( S(t) \) of the dispersion for a point like injection [Suciu et al., 2006d] (see also item “ergodic simulations”, (B1) below). Since the dispersions for point and large sources behave quite differently [Suciu et al., 2006a] a helpful computational tool is forbidden: ensemble averages cannot be performed before space averages with respect to initial concentration distributions.

The relation (3), discussed above at “State of the art”, is often used to compute the moment of the ensemble averaged concentration \( \sum_{ii} \) by adding to the ensemble averaged dispersion \( S_{ii} \) the variance of the center of mass \( R_{ii} \) [Zhang and Seo, 2004]. Approaches based on various hypotheses, as for instance the permutation of space and ensemble averages discussed above, attempt to identify the ensemble moment \( \sum_{ij} \) (diminished by the moment of the initial plume), with an ergodic moment \( X_{ij}(t) = \sum_{ii}(t) - S_{ij}(0) = S_{ii}(t) - S_{ii}(0) + R_{ii}(t) \), [see e.g. Dagan, 1990; Sposito and Dagan, 1994; Suciu et al., 2006a]. The ergodic moment should not normally depend on the shape and dimension of the initial plume. Therefore, it could be used as a free-of-memory characteristic of transport which only depends on the parameters of the aquifer (variance,
correlation length, shape of the correlation function of the logK field, and local dispersion coefficient).

The numerical results from Figure 11 show that an ergodic moment $\sum_i(t) - S_i(0)$ cannot be defined by relation (3) in general, but only for slab sources perpendicular to i-axis.

These new results complete those published in [Suciu et al., 2006a] and motivate further investigations on memory effects shown by the behavior of the ensemble quantity $\sum_i$. As Figure 11 suggests, longitudinal ergodic moments can be defined by $X_{11}(t) = \sum_{11}(t) - S_{11}(0)$ for large transverse slabs sources, and transverse ergodic moments can be defined similarly for longitudinal slabs. As shown in Figure 12, the moments derived in this way are close to a true ergodic behavior: not only is the mean close to a reference value (that of point source) but the standard deviation also decreases with increasing dimension of the initial plume.

Figure 11. Time behavior of the second moment of the ensemble averaged concentration $\sum_i(t)$ strongly depends on the shape and dimension of the initial plume. (2-dimensional GRW simulations as described in [Suciu et al., 2006a].)

Figure 12. $\sum_i(t)$ for $i \perp L$ show an “ergodic” behavior: the mean is almost the same as for point sources (but slightly different from 1st order approximation estimation) and the standard deviation (represented by thin lines) is small for large dimensions L of the slab source.
The ergodic moments can further be used to quantify the memory effects. To do that, one notes that the single realization counterparts of the quantities $S_{ii}$, $\sum_{ii}$, $X_{ii}$, and $R_{ii}$, obtained by ensemble averaging, are related by

\begin{equation}
S_{ii}(t) = S_{ii}(0) + x_{ii}(t) + m_{ii}(t) - r_{ii}(t) \tag{5}
\end{equation}

The term $m_{ii}$ in (5) has been called “memory term”, since its ensemble average quantifies the memory effect $(\sum_{ii} - S_{ii}(0) - X_{ii})$ shown by the ensemble moment $\sum_{ii}$ in most of the cases presented in Figure 11. If the local dispersion is neglected, $m_{ii}$ reduces to the supplementary term of the second moment which Sposito and Dagan [1994] derived for deterministic advective transport. Using the Itô formalism, the memory term appears to be the result of the correlations between initial positions and velocity fluctuations along the paths of the advection-dispersion process [Suciu et al., 2006c]. The corresponding memory coefficients $d_{\text{mem}} = m_{ii}/(2t)$ are presented in Figure 13. (Computations based on (5) and $x_{ii}$ estimated for L=100 in Figure 12.)

![Figure 13. Memory dispersion coefficients for different shapes of a large source (also compared with coefficients of purely advective transport in the case of large transverse slab source). Thin lines represent standard deviations divided by the square root of the number of velocity realizations.](image)

![Figure 14. For initial plumes with large dimensions $L \geq 50$, the standard deviation of the numerically estimated $\sum_{ii}(t)$ practically coincides with that of the estimated ensemble averaged dispersion $S_{ii}(t)$ (represented by thin lines).](image)
One observes that memory effects quantified by \( \mu_{\text{mem}} \) are significant not only in the mean (i.e. as difference between \( \Sigma_{ii} \) and \( X_{ii} \)) but especially because they show important sample-to-sample fluctuations. Since the fluctuations of the ergodic coefficients are negligible, the standard deviations of the memory coefficients practically coincide with those of the ensemble moments \( \Sigma_{ii} \). As indicated by Figure 14, for large plumes the fluctuations of the dispersions \( s_{ii} \) are practically caused by memory effects, which are very probably responsible for recently found non-ergodic behavior of large plumes in pre-asymptotic transport regime [Suciu et al., 2006a].

**A2) Dependence of Memory effects on the velocity correlation range**

In micro-physics applications memory effects are mainly due to non-Markovian evolution of velocity autocorrelation functions and characterize the persistence of the pre-asymptotic regime [Harayama et al., 2002]. For the advection-dispersion model of transport in systems with space variable properties (and for memory-free local dispersion), memory effects are induced by dependence on initial conditions. The similarity with micro-physics consists in the determinant role of the velocity correlation (temporal in the former, spatial in the latter case). This is clearly indicated by the extreme cases of uncorrelated velocities and the case of infinite correlation range as described by Matheron and de Marsily [1980] (which shows both normal dispersion \( \sim t \) and super-diffusive \( t^{3/2} \) time behavior). In the first case, short-range memory effects are expected [Vamoş et al., 2001]. In the second case one expects that memory terms could have an infinite relaxation time. That’s why the dependence on the spatial correlation range of the velocity field should be investigated first, and afterwards the role of the other parameters (variance of logK field, its correlation model, Pe number).

The existing results of 2-dimensional GRW simulations will be compared with analyzes of memory effects for white noise velocity, for the model of Matheron and de Marsily [1980], as well as with simulations for larger finite correlation ranges.

These investigations will use both stochastic analysis and GRW stochastic simulations. The manuscript [Suciu et al., 2006d] presents a derivation of the structure of the terms in (5) based on Kolmogorov’s definition of diffusion. This approach, which can be generalized to include jump processes and reactions, could be more appropriate for theoretical investigations. Another advantage could be the use of the Markov semigroup of evolution operators to investigate the consequences of considering strong ergodic properties of the local dispersion and velocity field (such as “mixing” and “exactness”). The manuscript [Suciu et al., 2006d] will be improved to give an even shorter and clearer derivation of the theoretical result and to include analyses on the role of correlation range. Since the memory effects are proved for arbitrary space and time variable drift and diffusion coefficients of the Fokker-Planck equation, with applications in various physical problems, the manuscript will be submitted to a journal of physics.

**B) Further development of the GRW stochastic simulations method.**

**B1) Ergodic GRW simulations.**

Even if transport originating from large solute sources is not ergodic in the commonly used sense of this term (i.e. the larger the source, the smaller the difference between realizations and ensemble averages, not only asymptotically but at all times) [Suciu et al., 2006a], the ergodicity of the space random velocity field with finite correlation range [Chilès and Delfiner, 1999] implies a useful “ergodic” property of the numerical simulations. Namely, when single realization simulations are done for changing origin of the coordinate system, distributed over a large area included into the support of a given realization of the velocity, the spatial average over the locations of the origin is close to the ensemble average (for a fixed origin of the coordinate system) over the realizations of the velocity field [Suciu et al., 2006d]. This property has already been indicated by simulations in Kraichnan fields. The efficiency of the “ergodic simulations”
method could be improved by replacing the Kraichnan generator with the improved “Fourier-wavelet” generator recently developed by the group lead by Prof. Karl Sabelfeld from Weierstraß Institut - Berlin [Kramer et al., 2006; Kurbanmuradov and Sabelfeld, 2005].

“Ergodic simulations” will be implemented for the problems formulated at item (A) above. After a validation of the method by comparisons with the stochastic simulations method based on ensemble averages, the “ergodic simulations” method will be tried whenever possible. By avoiding the computation of large ensembles of velocity fields, it is expected that this approach can considerably reduce the computational costs for the scheduled stochastic simulations.

The development of the method is scheduled for the months 7-18 of the Project.

**B2) Investigations on some technical issues.**

The “reduced fluctuations” procedure currently used in U- and B-GRW codes, based on eq. 2.6 of Vamoș et al. [2003], is completely deterministic. Therefore it cannot simulate single particles trajectories, which could be necessary in direct computations of “ergodic” and “memory” parts of the second spatial moments of the plume (defined at item (A) above). However, the advantage of this procedure is that it does not use random numbers generators. To keep the computational costs at low levels, the “reduced fluctuations” procedure will be modified by using a minimal number of calls of the random numbers generator. Another possibility to be investigated is the use of an “erf-function” distribution to approximate the Bernoulli distributed numbers of GRW jumps [Vamoș et al., 2003]. (This erf-GRW version has already been implemented in an older code, “grw.f90”, made available for the colleagues from Research Center Jülich since 2001.)

The issue of the total number of particles to be used in GRW simulations will be analyzed in greater detail. For small variance $\sigma^2_{\log K} \approx 0.1$ of the log-hydraulic conductivity a number of $N=10^{10}$ particles was shown to be large enough to ensure statistically convergent simulations for given velocity realizations [Suciu et al., 2004a, 2006a]. But the preliminary simulations of the Krauthausen field tracer experiments indicate that the number of particles should be considerably increased for $\sigma^2_{\log K}$ larger than 1 and for simulation times larger than hundreds of $\lambda_{\log K}/U$. The assessment of optimal values of $N$ will use the procedure described below.

Simulations for recordings of the cross-section concentration at reference planes (BTC’s) will be implemented on computational domains smaller than the actual plume extension. To do that, one can use “transmission boundary conditions” [Kinzelbach, 1992] (see also [Vamoș et al., 2003] for an application to simulations for Gaussian concentration distributions using small dimension grids). Another possible procedure is to impose an “absorbing boundary condition” [Vamoș et al., 2003] at a distance of a few standard deviations of the velocity downstream from the BTC reference plane.

This task is scheduled for the months 7-10 of the Project.

**B3) Compatibility between GRW and other codes.**

The 3-dimensional UGRW3D.cpp code will be adapted to use the output velocity field generated by UG Software, a flexible toolbox for solving partial differential equations developed by the group “Technische Simulation” from Heidelberg University. Darcy velocity fields will be generated by the UG version implemented at the Institute for Applied Mathematics (Institute I lead by Prof. Peter Knabner) of Erlangen-Nürnberg University.

UGRW3D.cpp will also be made compatible with TRACE finite element code developed at Research Center Jülich. In view of possible comparisons, the GRW procedure for variable local-dispersion coefficients (proportional to advection velocity) will use the same interpolation of the velocity field and computation of dispesivity tensor coefficients as the “ParTrace” code developed at Research Center Jülich.
Cooperation with other scientists

Objective (A) will be coordinated by Professor Harry Vereecken from Research Center Jülich, Institute of Chemistry and Dynamic of the Geosphere, Institute IV: Agrosphere and Professor Karl Sabelfeld form Weierstraß Institut - Berlin, research group Stochastic Algorithms and Nonparametric Statistics.

Objective (B) will be coordinated by Professor Peter Knabner from the Friedrich Alexander University Erlangen-Nürnberg, Institute for Applied Mathematics I.

Foreign cooperations

Objectives (A) and (B) will be achieved in cooperation with Dr. Călin Vamoș, Dr. Călin Ioan Gheorghiu, and Prof. Ion Păvăloiu, from “Tiberiu Popoviciu” Institute of Numerical Analysis, in the frame of the Fundamental Program of the Romanian Academy called “Interdisciplinary Program for the Prevention of Major Risk Phenomena at National Level”.

Computing resources

The following computing facilities will be available during the execution of the project: the 17 processors cluster at Institute of Applied Mathematics I of Friedrich-Alexander University Erlangen-Nürnberg, the Jump supercomputer at Research Center Jülich, and the IA32 cluster at Regionales Rechenzentrum Erlangen (RRZE).
REFERENCES:
Bakalis, E., C. Vlahos, and M. Kosmas (2006), Diffusion in the presence of a plume: From the continuous Gaussian to a discrete lattice model, Physica A, 360, 1--16.


Suciu N., C. Vamoș, and K. Sabelfeld (2005b), When do diffusing particles forget their initial position? (manuscript in work).


Suciu N., C. Vamoș, and K. Sabelfeld (2006d), Ergodic simulations of diffusion in random velocity field (manuscript in work to be submitted for *MCQMC06., Ulm, August 14-18, 2006*).


