Probabilistic collocation and Lagrangian sampling for tracer transport in randomly heterogeneous porous media

F. Müller, D.W. Meyer* and P. Jenny* $\,$

Research Report No. 2011-34 May 2011

Seminar für Angewandte Mathematik Eidgenössische Technische Hochschule CH-8092 Zürich Switzerland

^{*}Institute of Fluid Dynamics, ETH Zurich, Switzerland

Probabilistic Collocation and Lagrangian Sampling for Tracer Transport in Randomly Heterogeneous Porous Media

Florian Müller^{*}, Daniel W. Meyer, Patrick Jenny Institute of Fluid Dynamics, ETH Zurich, Switzerland

Abstract

The Karhunen–Loeve (KL) decomposition and the polynomial chaos (PC) expansion are elegant and efficient tools for uncertainty propagation in porous media. Over recent years, KL/PC-based frameworks have successfully been applied in several contributions for the flow problem in the subsurface context. It was also shown, however, that the accurate solution of the transport problem with KL/PC techniques is more challenging. We propose a framework that utilizes KL/PC in combination with sparse Smolyak quadrature for the flow problem only. In a subsequent step, a Lagrangian Monte Carlo sampling technique is used for transport, where the flow field samples are calculated very efficiently based on the solutions at relatively few quadrature points. To increase the computational efficiency of the PC-based flow field sampling, a new reduction method is applied. Compared to a conventional full MC method that includes both flow and transport, the proposed PC/MC method (PCMCM) for flow/transport, respectively, saves on the computational cost of the flow problem. The applicability of PCMCM is demonstrated for transport simulations in multivariate Gaussian log-conductivity fields that are unconditional and conditional on conductivity measurements.

Keywords: Probabilistic collocation, Karhunen-Loeve expansion, Polynomial chaos, Smolyak sparse grid, Heterogeneous porous media, Tracer transport

Preprint submitted to Advances in Water Resources

April 21, 2011

^{*}Tel.: +41 44 633 9249; fax: +41 44 632 1104. E-mail address: florian.mueller@sam.math.ethz.ch.

1. Introduction

Predictions of flow and transport in the subsurface are plagued by uncertainty. Corresponding predictive tools are required for groundwater management or more specifically for the design of contamination prevention measures and remediation actions. Soil parameters that determine flow and transport, e.g., the hydraulic log-conductivity $Y(\mathbf{x})$, are typically heterogeneous in space \mathbf{x} [1]. However, measurements of some of these parameters and most importantly of $Y(\mathbf{x})$ are only available at points (in a two-dimensional setting). The resulting uncertainty in the log-conductivity field is quantified by geostatistical models [2]. A standard model is based on the assumption that $Y(\mathbf{x}) = Y(\mathbf{x}) + Y'(\mathbf{x})$ can be represented by a multivariate Gaussian random field, which is characterized by a mean distribution $\overline{Y}(\mathbf{x})$ and a zeromean fluctuation $Y'(\mathbf{x})$. Latter is joint normally distributed at all points in space and is determined by the covariance function $C_Y(\mathbf{x}, \mathbf{y})$ given at two spatial locations \mathbf{x} and \mathbf{y} . In many application examples, the unconditional (without any measurements) log-conductivity field $Y(\mathbf{x})$ is assumed to have a constant variance $Y'(\mathbf{x})^2 = \sigma_Y^2$ and correlation length vector $\boldsymbol{\eta}$.

With the uncertainty in the transport parameters quantified, it remains to be determined how the parameter uncertainty propagates through the flow and transport model and what uncertainty will eventually result in the hydraulic head, flow field, or concentrations of transported substances. An obvious approach is to sample realizations of $Y(\mathbf{x})$ from the geostatistical model and to use a deterministic simulation framework for flow and transport [3, 4]. From the resulting concentration distributions or flow-field realizations, statistics can be compiled that quantify the uncertainty in the dependent quantities. This so-called Monte Carlo (MC) approach—even though conceptually simple—is computationally expensive. A large number of simulations have to be performed to reduce the statistical error to an acceptable level. Each simulation involves the solution of an elliptic flow problem followed by a hyperbolic or parabolic transport problem.

Unlike MC, stochastic moment equation (SME) methods approach the uncertainty propagation problem by analytical means. Low-order approximations with respect to a small parameter Y' are introduced into the flow and transport equations [5, 6]. The resulting concentration mean and variances are typically verified with MC or experimental data for two-dimensional contamination scenarios with point-like contaminant injections, e.g., [7, 4, 8]. Two-dimensional domains are frequently considered to represent shallow confined aquifers with large horizontal extensions [7]. SME predictions are limited to small log-conductivity variances σ_Y^2 or in other words aquifers with small heterogeneity levels [9].

Ghanem [10, 11, 12] initiated a different class of methods called probabilistic spectral Galerkin. It utilizes Karhunen-Loeve (KL) and polynomial chaos (PC) expansions. For sufficiently large correlation lengthscales of multivariate Gaussian fields, KL expansions have advantageous convergence properties. More precisely, only a low number of expansion terms have to be included and accordingly the Y-probability space can be approximated by a low N-dimensional space whose coordinates ξ_n with $n = 1 \dots N$ are standard normal random variables ([13] and [14] sections 4.2.1 and 2.1, respectively). In Ghanem's work, the dependent variables hydraulic head [12, 11] and concentration [11] were expressed as PC expansions in terms of P N-dimensional Hermite polynomials $\Psi_1(\boldsymbol{\xi}^N), \ldots, \Psi_P(\boldsymbol{\xi}^N)$ with $\boldsymbol{\xi}^N = [\xi_n]_{n=1}^N$. The *P* chaos expansion coefficients that determine the statistics of the dependent variables were finally calculated with a Galerkin projection method. In both contributions [11, 12] the structure of chaos expansion coefficients was analyzed. No validation of the outlined PC method with MC was provided, however. Compared to MC, Ghanem's spectral Galerkin method is intrusive in the sense that the KL/PC expansions with subsequent Galerkin projection lead to a new system of equations for the P PC coefficients that is no longer solvable with computer codes commonly applied in MC simulations.

Zhang and Lu [15] proposed a KL-based moment equation (KLME) method, where a KL expansion for $Y(\mathbf{x})$ was combined with a low-order approximation with respect to Y' for the hydraulic head. Mean and variances of the hydraulic head were successfully validated with MC data for σ_Y^2 up to 2. A generalization of [15] was provided in [16], where KLME simulations that included conductivity measurements were validated and also flow field statistics were verified. Lu and Zhang [17] performed three-dimensional time-dependent flow simulations with a KLME-based method and discussed the relation between PC-based techniques and the KLME approach. Liu, Lu, and Zhang [18] validated the KLME approach for transport simulations of a passive tracer successfully with MC data for σ_V^2 up to 0.5. For larger log-conductivity variances, i.e., $\sigma_Y^2 = 1$, the KLME method starts to produce noticeable errors compared to MC. Compared to the previously discussed Galerkin-projection-based methods, the KLME approach is nonintrusive meaning that codes from an existing MC simulation framework are applicable. KLME is, however, by construction limited to rather small σ_Y^2

similar to conventional SME-based approaches.

Xiu and Hesthaven [19] have introduced a probabilistic collocation method (PCM) as a non-intrusive alternative to the spectral Galerkin-projection method of Ghanem [10]. They used a collocation grid in the parameter probability space (spanned by $\boldsymbol{\xi}_N$) in combination with a deterministic simulation framework also applicable for MC to determine the solutions of the dependent variables at the collocation points. Based on the results at the collocation points, the overall probabilistic solution can be estimated by using Lagrange polynomials for interpolation in random space. As an alternative to interpolation, however, statistical means of the dependent variables can be estimated with a quadrature formula if the collocation points are chosen accordingly (equation 3.12 in [19]). For the selection of the collocation points, full tensor products of one-dimensional nodal sets and Smolyak sparse grids were discussed. Full tensor products have the disadvantage that the number of points grows exponentially with N, i.e., the dimensionality of the parameter probability space. Li and Zhang [20] applied a KL/PC/PCM method for uncertainty quantification of the hydraulic head. The KL expansion was used to represent the parameter uncertainty of the log-conductivity. A Hermite PC expansion was applied to approximate the hydraulic head in terms of the independent KL variables $\boldsymbol{\xi}^{N}$. To determine the *P* coefficients of the PC expansion, it is postulated that the PC expansion at P given points is equivalent to the solution at these points which leads to a PCM. The collocation points were sequentially selected from a full tensor product. Li and Zhang mention that their outlined point selection procedure can become computationally demanding for increasing N. Recently, Lin and Tartakovsky [21] have applied a KL/PCM-based method for passive tracer transport. For the log-conductivity $Y(\mathbf{x})$, a KL expansion with the random variable vector $\boldsymbol{\xi}^N$ and N = 4 was applied. To numerically evaluate concentration moments, which involves integration over the $\boldsymbol{\xi}^N$ -probability-space, Gauss quadrature was used in combination with a Smolyak sparse grid to keep the number of quadrature points at an acceptable level. In the work of Lin and Tartakovsky, however, it is questionable whether four terms in the KL expansion are sufficient for their three-dimensional domain with Y-correlation lengths being one third of the domain or smaller. For the largest heterogeneity level considered, a large number of quadrature points were required (one fourth of the number of MC runs) to obtain acceptable agreement with the MC reference. Together with the KLME results reported in [18] this indicates that the accurate probabilistic solution of the transport problem seems to pose an

additional challenge besides the flow problem.

In the present study, the KL expansion is used to parametrize the logconductivity process by scalar random variables ξ_n . The generally infinite number of random variables involved is truncated, leading to an approximated log-conductivity process based on a finite, N-dimensional vector $\boldsymbol{\xi}^{N}$ of random variables (section 3). The dependence of the hydraulic head on the log-conductivity is represented by a Hermite PC expansion in terms of $\boldsymbol{\xi}^N$ (section 5.1). After exploiting the orthonormality of the Hermite basis functions, the resulting N-dimensional integral over the $\boldsymbol{\xi}^N$ -probability space is numerically approximated with Smolyak quadrature (section 5.3). This approach is computationally more efficient compared to the tensor-productbased PCM used in the work of Li and Zhang [20]. Moreover, no intrinsic limitation with respect to σ_Y^2 (like in KLME-based methods) is involved. With the PC expansion determined, moments of the hydraulic head field are readily available and sampling the hydraulic head or the flow field is computationally inexpensive. To further increase the sampling efficiency, we outline in section 5.5 a new reduction technique for the PC expansion. For a classical point-injection transport scenario (section 6) without pore-scale dispersion (PSD), we present an accurate Lagrangian solution method, which is computationally efficient (section 7) and less error-prone compared to the previously discussed transport approaches. For validation of the new method with MC, a spatially two-dimensional setting is considered. Results of both unconditional and conditional simulations including conductivity measurements are reported in section 8.

2. Problem Formulation

In this work, we focus on a two-dimensional confined aquifer with uncertain hydraulic conductivity distribution. For incompressible steady state flow in a saturated porous medium, the elliptic partial differential equation (PDE)

$$-\nabla \cdot (K(\mathbf{x},\omega)\nabla h(\mathbf{x},\omega)) = 0 \tag{1}$$

determines together with suitably chosen boundary conditions the hydraulic head $h(\mathbf{x}, \omega)$. $K(\mathbf{x}, \omega)$ represents the hydraulic conductivity and ω is a random event coordinate that reflects the randomness of K and of variables that depend on K like h. \mathbf{x} is a spatial coordinate vector with components x_1 and x_2 . The average pore velocity is given by Darcy's law, i.e.

$$\mathbf{v}(\mathbf{x},\omega) = -\frac{1}{\phi} K(\mathbf{x},\omega) \nabla h(\mathbf{x},\omega), \qquad (2)$$

where ϕ is the porosity which is assumed to be constant.

The transport of a passive tracer in the absence of PSD is described by the Eulerian advection equation, i.e.,

$$\frac{\partial c(\mathbf{x},\omega)}{\partial t} + \mathbf{v}(\mathbf{x},\omega) \cdot \nabla c(\mathbf{x},\omega) = 0, \qquad (3)$$

where $c(\mathbf{x}, \omega)$ is the tracer concentration. With PSD neglected, it was for example shown by Meyer and Tchelepi [22] (section 2) that the Eulerian description (3) is equivalent to a particle-based Lagrangian formulation, which reads

$$\mathbf{X}(\mathbf{X}_0, t, \omega) = \mathbf{X}_0 + \int_{t_0}^t \mathbf{v}(\mathbf{X}(\mathbf{X}_0, s, \omega), \omega) ds,$$
(4)

and where $\mathbf{X}(\mathbf{X}_0, t, \omega)$ is the tracer particle position at time t dependent on the injection point \mathbf{X}_0 at $t = t_0$.

3. Karhunen-Loeve (KL) Expansion

To parametrize the log-conductivity $Y(\mathbf{x}, \omega) = \ln[K(\mathbf{x}, \omega)]$ in terms of scalar random variables, we apply Karhunen-Loeve (KL) expansions. In the next two sections, KL expansions for unconditional and conditional logconductivity fields without and with measurements, respectively, are outlined.

3.1. Unconditional KL Expansion

Like in most contributions discussed in the introduction, we assume that the log-conductivity $Y(\mathbf{x}, \omega) = \ln[K(\mathbf{x}, \omega)]$ is a Gaussian process with given mean $\overline{Y}(\mathbf{x})$ and bounded, symmetric, positive-definite covariance function $C_Y(\mathbf{x}, \mathbf{x}')$ ([10] equation (2.7)). Such a process can be represented with the KL expansion as

$$Y(\mathbf{x},\omega) = \overline{Y}(\mathbf{x}) + Y'(\mathbf{x},\omega) = \overline{Y}(\mathbf{x}) + \sum_{n=1}^{\infty} \sqrt{\lambda_n} f_n(\mathbf{x}) \xi_n,$$
 (5)

where the logarithmic conductivity $Y(\mathbf{x}, \omega)$ is split into a mean $\overline{Y}(\mathbf{x})$ and a fluctuation $Y'(\mathbf{x}, \omega)$ with $\overline{Y'} = 0$. $Y'(\mathbf{x}, \omega)$ is then replaced by an infinite sum, which represents the actual KL expansion [10, 14, 13]. ξ_n are $n = 1...\infty$ independently distributed standard normal random variables. The eigenvalues λ_n and eigenfunctions $f_n(\mathbf{x})$ are obtained from solving the following Fredholm equation of the covariance function $C_Y(\mathbf{x}, \mathbf{x'})$:

$$\int_{D} C_{Y}(\mathbf{x}, \mathbf{x}') f(\mathbf{x}) d\mathbf{x} = \lambda f(\mathbf{x}'), \qquad (6)$$

where D is the aquifer domain. The Fredholm equation admits infinitely many eigenpairs $(\lambda_n, f_n(\mathbf{x}))$. After normalizing the orthogonal eigenfunctions such that

$$\int_D f_m(\mathbf{x}) f_n(\mathbf{x}) d\mathbf{x} = \delta_{mn} \text{ with } n = 1 \dots \infty \text{ and } m = 1 \dots \infty,$$

the eigenpairs can be sorted in a non-increasing order, i.e.

$$\lambda_1 \ge \lambda_2 \ge \dots \ge \lambda_\infty \ge 0. \tag{7}$$

In general, the Fredholm equation (6) has to be solved numerically (see [10], p. 43). Specifically for a space stationary covariance function, the fast multipole method proposed by Schwab and Todor [23] can be applied. For certain cases, however, solutions are available in analytical form. In this work, the separable covariance function

$$C_Y(\mathbf{x}, \mathbf{x}') = \sigma_Y^2 \exp\left(-\frac{|x_1 - x_1'|}{\eta_1} - \frac{|x_2 - x_2'|}{\eta_2}\right)$$
(8)

is used, where σ_Y^2 is the variance of the Gaussian log-conductivity process and η_1 and η_2 are the correlation lengths in the two spatial directions x_1 and x_2 , respectively. The covariance function (8) depends only on the separation vector between the two points \mathbf{x} and \mathbf{x}' , i.e., $C_Y(\mathbf{x}, \mathbf{x}') = C_Y(|\mathbf{x} - \mathbf{x}'|)$, and therefore is spatially independent. For this choice of covariance function, the Fredholm equation (6) has an analytical solution [24]. The analytical eigenvalues and eigenfunctions for the two-dimensional case are based on the solution of the Fredholm equation with the spatially one-dimensional covariance function

$$C_Y(x_1, x_1') = \sigma_Y^2 \exp\left(-\frac{|x_1 - x_1'|}{\eta_1}\right).$$

The corresponding eigenvalues and eigenfunctions for the one-dimensional case are given by

$$\lambda_n = \frac{2\eta_1 \sigma_Y^2}{\eta_1^2 w_n^2 + 1} \text{ and} f_n(x_1) = \frac{\eta_1 w_n (\cos(w_n x_1) + \sin(w_n x_1))}{\sqrt{(\eta_1^2 w_n^2 + 1)L_1/2 + \eta_1}},$$

where L_1 is the one-dimensional domain size $(0 \le x_1 \le L_1)$ and w_n are the positive roots of the characteristic equation

$$(\eta_1^2 w^2 - 1)\sin(wL_1) - 2\eta_1 w\cos(wL_1) = 0.$$

Sorting the infinitely many positive roots w_n in an increasing order yields a decreasing series of eigenvalues λ_n .

The analytical eigenvalues and eigenfunctions for the two dimensional covariance function (8) on a rectangular domain $(0 \le x_1 \le L_1, 0 \le x_2 \le L_2)$ are then constructed from the one-dimensional solutions:

$$\lambda_n = \frac{4\eta_1\eta_2\sigma_Y^2}{(\eta_1^2w_{n_1}^2 + 1)(\eta_2^2w_{n_2}^2 + 1)}$$

$$f_n(\mathbf{x}) = f_{n_1}(x_1)f_{n_2}(x_2).$$

The eigenvalues λ_n can be sorted to be non-increasing as in equation (7).

If the eigenvalues λ_n decay sufficiently fast to zero for increasing n, one can truncate the KL expansion (5) after N terms. This makes the KL expansion computationally accessible and reduces the dimensionality of the Y-probability space while still accurately approximating the infinite expansion. An upper limit for the sum of all eigenvalues can be derived as follows: squaring both sides of the KL expansion, i.e. of

$$Y'(\mathbf{x},\omega) = \sum_{n=1}^{\infty} \sqrt{\lambda_n} f_n(\mathbf{x}) \xi_n,$$

multiplying with the joint normal probability density function of all ξ_n , and integrating over stochastic and physical space leads to an expression for the sum of all eigenvalues

$$|D|\sigma_Y^2 = \sum_{n=1}^{\infty} \lambda_n,\tag{9}$$



Figure 1: Eigenvalue decay (a) and accumulated eigenvalue convergence (b) dependent on the correlation length $\eta = \eta_1 = \eta_2$ for a quadratic physical domain with side length $L = L_1 = L_2 = 1$.

where |D| is the size of the spatial domain D (length in 1d, area in 2d, volume in 3d) and σ_Y^2 is the log-conductivity variance that is assumed to be independent of \mathbf{x} . This expression provides an easily calculable limit for the sum of all eigenvalues and therefore proves to be useful for investigating the effect of truncating the KL expansion. Moreover, since equation (9) is resulting from the square of the KL expansion of $Y'(\mathbf{x}, \omega)$, $|D|\sigma_Y^2$ can be viewed as a total energy and the λ_n as energy fractions.

With the choice of covariance function (8), the eigenvalue decay is strongly linked to the correlation lengths η_1 and η_2 . Figure 1 illustrates how the eigenvalues decay for different correlation lengths $\eta = \eta_1 = \eta_2$ and how the cumulative sum of eigenvalues converges to the limit given by equation (9). In this example, a quadratic physical domain was used with side length L = $L_1 = L_2 = 1$. A short correlation length η implies a slow convergence and therefore requires more terms to be retained in the KL expansion for an accurate reproduction of the underlying Gaussian process.

3.2. Measurement-Based Conditional KL Expansion

In cases where conductivity measurements are available, the covariance function $C_Y^{(c)}(\mathbf{x}, \mathbf{x}')$ conditional on measurements becomes spatially dependent, i.e., $C_Y^{(c)}(\mathbf{x}, \mathbf{x}') \neq C_Y^{(c)}(|\mathbf{x} - \mathbf{x}'|)$. Lu and Zhang [16] have outlined a procedure where the eigenpairs $(\lambda_n^{(c)}, f_n^{(c)}(\mathbf{x}))$ of the conditional KL expan-

sion

$$Y^{(c)}(\mathbf{x},\omega) = \overline{Y}^{(c)}(\mathbf{x}) + \sum_{n=1}^{\infty} \sqrt{\lambda_n^{(c)}} f_n^{(c)}(\mathbf{x}) \xi_n$$
(10)

are determined based on the unconditional ones. Here, ξ_n are—like in the unconditional expansion—independently distributed standard normal random variables. Details about the calculation of $\overline{Y}^{(c)}(\mathbf{x})$ and the conditional eigenpairs are provided in section 3.2 of [16].

4. Monte Carlo (MC) Simulation

As suggested by Zhang and Lu [15] (top of p.777), the KL expansion provides an elegant method to produce multivariate Gaussian log-conductivity fields that may include measurements. Accordingly, we will use this method not only for our PC-based technique, but also apply it in the MC framework to produce reference data. The MC simulation loop therefore involves the following steps:

- Generate a realization of the standard normal random vector $\boldsymbol{\xi}^N$ and calculate the hydraulic conductivity $Y^N(\mathbf{x}, \boldsymbol{\xi}^N)$ or $Y^{(c)N}(\mathbf{x}, \boldsymbol{\xi}^N)$ based on the truncated versions of equations (5) or (10), respectively, with N terms included.
- Solve the flow problem consisting of the elliptic PDE (1) for the hydraulic head and equation (2) for the flow field.
- Perform particle tracking with equation (4) to solve the transport problem.

This MC simulation loop is repeated until the statistical error has converged to an acceptably low level.

5. PC/PCM Methodology

To sample the hydraulic head probability space more efficiently and to reduce the number of required elliptic problem solutions, a polynomial chaos (PC) expansion for the hydraulic head is introduced in the next section. The expansion coefficients are determined with a probabilistic collocation method (PCM) as outlined in section 5.2.

5.1. Polynomial Chaos (PC) Expansion

The PC representation provides a direct connection between the random variables $\boldsymbol{\xi}^N$ in the KL expansion and the dependent hydraulic head distributions. Generally, the PC expansion of a spatially random field $h(\mathbf{x}, \omega)$ has the following form:

$$h(\mathbf{x},\omega) = \tilde{h}_{0}(\mathbf{x}) + \sum_{i_{1}=1}^{\infty} \tilde{h}_{i_{1}}(\mathbf{x}) \tilde{\Psi}_{1}(\xi_{i_{1}}) + \sum_{i_{1}=1}^{\infty} \sum_{i_{2}=1}^{i_{1}} \tilde{h}_{i_{1},i_{2}}(\mathbf{x}) \tilde{\Psi}_{2}(\xi_{i_{1}},\xi_{i_{2}}) + \sum_{i_{1}=1}^{\infty} \sum_{i_{2}=1}^{i_{1}} \sum_{i_{3}=1}^{i_{2}} \tilde{h}_{i_{1},i_{2},i_{3}}(\mathbf{x}) \tilde{\Psi}_{3}(\xi_{i_{1}},\xi_{i_{2}},\xi_{i_{3}}) + \dots, \qquad (11)$$

where the $\tilde{h}_{i_1,\ldots,i_d}(\mathbf{x})$ are deterministic functions that reflect the spatial dependence of $h(\mathbf{x},\omega)$, and $\tilde{\Psi}_d(\xi_{i_1},\ldots,\xi_{i_d})$ are orthogonal polynomials of order d with respect to the random variables $\xi_{i_1},\ldots,\xi_{i_d}$ [10, 14, 13, 25]. Here, $h(\mathbf{x},\omega)$ is the hydraulic head. Equation (11) can be written more compactly as

$$h^{N}(\mathbf{x},\omega) = \sum_{p=1}^{\infty} h_{p}(\mathbf{x})\Psi_{p}(\boldsymbol{\xi}).$$
(12)

The $\Psi_p(\boldsymbol{\xi})$ are still orthonormal polynomials, but the indexing is different. There is a one-to-one correspondence between the summands in equations (11) and (12). In practice, the PC expansion (11) has to be truncated in terms of the number of random variables N:

$$h^{N}(\mathbf{x}, \boldsymbol{\xi}^{N}) = \sum_{p=1}^{\infty} h_{p}(\mathbf{x}) \Psi_{p}(\boldsymbol{\xi}^{N}), \qquad (13)$$

as well as in terms of polynomial order d:

$$h^{N,P}(\mathbf{x},\boldsymbol{\xi}^N) = \sum_{p=1}^P h_p(\mathbf{x})\Psi_p(\boldsymbol{\xi}^N).$$
(14)

If we allow for a maximum polynomial order of d and limit the number of random variables to N, equation (14) consists of $P = \frac{(N+d)!}{N!d!}$ terms. For this

work, where standard normal random variables are used in the KL expansion of the conductivity, normalized Hermite polynomials (see AppendixB) are best suited for the PC expansion ([25] section 4). Hermite polynomials satisfy an orthonormality property with respect to the joint standard normal probability measure $d\mu(\boldsymbol{\xi}^N)$, i.e.,

$$\int_{\Omega} \Psi_p(\boldsymbol{\xi}^N) \Psi_{p'}(\boldsymbol{\xi}^N) d\mu(\boldsymbol{\xi}^N) = \delta_{pp'}, \qquad (15)$$

where Ω denotes the probability space spanned by $\boldsymbol{\xi}^{N}$.

5.2. Probabilistic Collocation Method (PCM)

To determine the PC expansion coefficients $h_p(\mathbf{x})$, we multiply both sides of the N-truncated PC expansion (13) by the polynomial basis $\Psi_{p'}$, integrate with the corresponding probability measure over the space Ω , and apply the orthonormality property (15), which eventually leads to

$$h_{p'}(\mathbf{x}) = \int_{\Omega} h^N(\mathbf{x}, \boldsymbol{\xi}^N) \Psi_{p'}(\boldsymbol{\xi}^N) d\mu(\boldsymbol{\xi}^N).$$
(16)

Here, the integral on the right hand side involves the solution of the PDE (1) at every point in Ω . To resolve this, we approximate this integral by using quadrature in Ω : in the integrand of equation (16), $h^N(\mathbf{x}, \boldsymbol{\xi}^N)$ is evaluated only at few quadrature or collocation points in Ω . An approximation of the integral can then be calculated with a multidimensional quadrature formula. In [13], this approach is referred to as probabilistic collocation with discrete projection.

5.3. Smolyak Quadrature

There are different ways to construct a multidimensional quadrature formula. A straight forward multidimensional quadrature rule is obtained from building the tensor product of one-dimensional rules. One-dimensional quadrature rules of the form

$$Q_I^1 u \equiv \sum_{i=1}^I w_i u(\Xi_i) \approx \int_{\Omega} u(\xi) \, d\xi$$

are used to approximately integrate a function $u(\xi)$ for $\xi \in \Omega$. It is based on the function values at points $\Xi_i \in \Omega$ and weights w_i , both with $i = 1 \dots I$. In Q_I^1 , the superscript 1 reflects the dimensionality of the quadrature rule and the subscript I specifies the number of quadrature points. The full tensor rule for integrating an N-dimensional function $u(\xi_1, \ldots, \xi_N)$ is defined as:

$$(Q_I^1 \otimes \cdots \otimes Q_I^1)u \equiv \sum_{i_1=1}^I \cdots \sum_{i_N=1}^I w_{i_1} \dots w_{i_N} u(\Xi_{i_1}, \dots, \Xi_{i_N}).$$

Clearly, the number of full tensor quadrature points is I^N . In general, the stochastic dimensionality N, i.e. the number of terms in the truncated KL expansion, is numerous. Hence, a quadrature formula for the integration over a high dimensional space constructed in a tensor product manner suffers from an unfavorable growth of quadrature points with every additional random dimension.

To avoid this so-called 'curse of dimensionality', we resort to Smolyak's quadrature [26]. Let $Q_{I_n}^1$ with $n = 1 \dots N$ denote N one-dimensional quadrature rules with rule n, i.e., $Q_{I_n}^1$, having I_n quadrature points and weights. Smolyak's rule then reads:

$$Q_q^N u \equiv \sum_{q-N+1 \le |\mathbf{I}| \le q} (-1)^{q-|I|} \cdot \binom{N-1}{q-|\mathbf{I}|} \cdot (Q_{I_1}^1 \otimes \dots \otimes Q_{I_N}^1) u.$$
(17)

Every summand of the Smolyak quadrature represents a weighted full tensor rule, for which the number of coordinate points in the different dimensions are given by $\mathbf{I} = \{I_1, \ldots, I_N\}$. q specifies the sparseness of the quadrature rule, since it limits the total number of coordinate points in all dimensions $|\mathbf{I}| = I_1 + \cdots + I_N$. Stacking different grids, for which the total number of coordinate points is fixed, on top of each other leads to a sparse grid structure.

Note that the full tensor and the Smolyak quadrature allow for different orders of multidimensional polynomials that can be integrated exactly. Assuming the one-dimensional integration rule consists of I quadrature points and weights to integrate a polynomial up to degree 2I - 1 exactly. The full tensor quadrature rule then integrates products of one-dimensional polynomials with each degree at most 2I - 1 exactly. On the other hand, the Smolyak quadrature limits the total polynomial exactness: an integral over a multidimensional polynomial of total degree 2(q - N + 1) - 1 or less is computed exactly. Therefore, Smolyak's quadrature limits the polynomial exactness in a more suitable way in the sense that it avoids an exponential growth of quadrature points with respect to the dimensionality N.



Figure 2: Full tensor Gauss-Hermite grid with I = 6 one-dimensional coordinates (a) and a comparable Smolyak grid with sparseness parameter q = 7 (b).

A comparison of a two-dimensional (N = 2) full tensor quadrature grid with $I = I_1 = I_2 = 6$ and a Smolyak sparse grid with the sparseness parameter q = 7 is provided in figure 2. Relating the full tensor parameter I and the sparseness parameter q for a comparison with I = (q - N + 1) is motivated by the discussion in the previous paragraph. As a building block for the multidimensional rules, the one-dimensional Gauss-Hermite quadrature (see AppendixA) is used. Since Gauss-Hermite quadrature points are not nested, the sparseness of Smolyak's grid does not pay off at low dimensions, but eventually, as the dimensionality is increased, the number of quadrature points are dramatically reduced. Further information on Smolyak quadrature and sparse grids can be found in [27, 19, 21].

5.4. Transport

The PC representation (14) provides a direct formal connection between the random number vector $\boldsymbol{\xi}^N$ —that determines the conductivity field $Y^N(\mathbf{x}, \boldsymbol{\xi}^N)$ or $Y^{(c)N}(\mathbf{x}, \boldsymbol{\xi}^N)$ by means of the KL expansions (5) or (10), respectively and the hydraulic head $h^{N,P}(\mathbf{x}, \boldsymbol{\xi}^N)$. With the hydraulic conductivity and the hydraulic head, the associated velocity field can be calculated based on equation (2). Consequently, once the PC and KL expansion coefficients $h_p(\mathbf{x})$ with $p = 1 \dots P$ and $\sqrt{\lambda_n} f_n(\mathbf{x})$ with $n = 1 \dots N$, respectively, are determined, flow field realizations can be generated or sampled very efficiently based on the random number vector $\boldsymbol{\xi}^{N}$. Unlike in the MC method outlined in section 4, no elliptic flow problems have to be solved. In the absence of PSD, the streamline method (4) is subsequently applicable to solve the transport problem. This strategy is computationally efficient and circumvents limitations (KLME [18]) and inaccuracies discussed (KL/PC/PCM [20]) in the introduction. In the following, we refer to the new method outlined in this section as probabilistic collocation MC method (PCMCM).

5.5. PC Reduction

For the previously outlined sampling technique, the number of polynomial basis functions P present in the PC expansion influences directly the computational cost. After having calculated—based on equations (16) and (17) the PC expansion with P terms, the number of PC terms is reduced in view of an efficient sampling of transport statistics. To this end, the velocity field described by equations (2), (5) and (14), i.e.,

$$\mathbf{v}^{N,P}(\mathbf{x},\boldsymbol{\xi}^{N}) = -\frac{1}{\phi} \exp(\overline{Y}(\mathbf{x}) + \sum_{n=1}^{N} \sqrt{\lambda_{n}} f_{n}(\mathbf{x}) \xi_{n}) \sum_{p=1}^{P} \nabla h_{p}(\mathbf{x}) \Psi_{p}(\boldsymbol{\xi}^{N}),$$

is relevant. To verify the importance of different terms in the second sum with summation index p, the energy norm $(\int_D \nabla h_p(\mathbf{x})^2 \mathbf{dx})^{1/2}$ of the coefficients $h_p(\mathbf{x})$ is considered. Terms with a norm being below a certain threshold are discarded from the PC expansion. This reduction step leads to a more compact and computationally efficient PC representation involving $P_{red} < P$ terms.

6. Test Cases

To investigate the performance of the PCMCM method, a quadratic confined aquifer with side length $L = L_1 = L_2$ was considered similar to the test cases used in [20] and [21]. The boundary conditions for the flow problem (1) are specified as illustrated in figure 3. Dirichlet type boundaries were applied at the left and right sides of the domain, i.e.,

$$h(\mathbf{x}, \omega) = h_{in}$$
 and h_{out} at $x_1 = 0$ and L_1 , respectively,

and Neumann type no-flow boundaries are prescribed at the top and bottom domain sides, i.e.,

$$\frac{\partial h(\mathbf{x},\omega)}{\partial x_2} = 0 \text{ at } x_2 = 0 \text{ and } L_2.$$



Figure 3: Computational domain with boundary conditions of the confined aquifer considered. The thick black line represents an exemplary tracer particle trajectory.

A constant mean flow in x_1 -direction is resulting from the prescribed constant hydraulic head boundaries at $x_1 = 0$ and $x_1 = L_1$. The porosity for the calculation of the flow velocity with Darcy's law (2) was set to $\phi = 1$. At position $\mathbf{x} = (0.0446L_1, L_2/2)^T$, a passive tracer was injected to study transport in the absence of PSD. An exemplary tracer particle trajectory is depicted in figure 3.

Both unconditional (first case) and conditional (second case) simulations were performed. In the conditional case, the set of conductivity measurements depicted in figure 4 was used. These measurements locally reduce uncertainty of the log-conductivity. An exemplary conductivity realization calculated from the conditional KL expansion (10) with N = 100 terms is depicted in figure 4.

The mean and variance of the unconditional logarithmic conductivity were set to $\overline{Y} = 0$ and $\sigma_Y^2 = 1$. The correlation length in the two spacial directions were set to $\eta_1 = \eta_2 = 0.4$ for an aquifer domain of size $L = L_1 =$ $L_2 = 1$. Together with the covariance function given by equation (8), this determines the unconditional Gaussian log-conductivity process completely. The characterization of the conditional process involves in addition to the previously outlined parameters the log-conductivity measurements depicted in figure 4.



Figure 4: Logarithmic conductivity measurements and exemplary realization from the conditional KL expansion (10) with N = 100 terms.

7. Numerical Method

In this section, details of the numerics and the implementation of the outlined PCMCM are provided.

7.1. KL Expansion

As illustrated in section 3, the number of terms retained in the KL expansion in order to maintain a certain accuracy depends on the decay of the eigenvalues λ_n . With the choice of $\eta_1 = \eta_2 = 0.4$ for a domain of size $L_1 = 1$ by $L_2 = 1$, N = 20 terms are kept in the KL expansion in order to preserve around 80% of the total energy (9). Compared to the works [20] and [21], this energy content seems rather high. Li and Zhang [20] retain seven KL terms in a two dimensional setting with the same normalized correlation lengths of $\eta_1/L_1 = \eta_2/L_2 = 0.4$. Lin and Tartakovsky [21] worked with four KL modes in a three-dimensional setting with $L_1 = 6$, $L_2 = L_3 = 3$, and $\eta_1 = \eta_2 = \eta_3 = 1$, which leads to a very low residual energy content. We observed in our setting that N = 20 KL expansion terms are necessary in order to obtain sufficiently accurate results.

7.2. Smolyak Quadrature

With N = 20 terms in the KL expansion and the sparseness parameter q = 22, a Smolyak grid with 861 quadrature points is resulting in the *N*-dimensional space spanned by $\boldsymbol{\xi}^{N}$. Consequently, to obtain the hydraulic head values $h^{N}(\mathbf{x}, \boldsymbol{\Xi}^{N})$ at the quadrature points $\boldsymbol{\Xi}^{N}$, the same number of

flow problems (1) must be solved. For efficiency reasons it is important that this number is much smaller compared to the number of MC samples required for PCMCM.

As explained in section 5.3, the Smolyak quadrature relies on one-dimensional quadrature rules. Since the integration to be approximated is with respect to a joint Gaussian measure (see equation (16)), the one-dimensional quadrature rule is given by the Gauss-Hermite quadrature (see AppendixA). This provides a one-dimensional integration accuracy of polynomial degree 2I - 1 for I quadrature coordinates. Based on the one-dimensional integration accuracy, the Smolyak quadrature with N = 20 dimensions can exactly integrate multidimensional polynomials of degree 2(q - N + 1) - 1 = 5 or smaller.

7.3. PC Expansion

As discussed in section 5.1, normalized Hermite polynomials (see AppendixB) are best suited in connection with standard normal random variables. It is not clear a priori though, where to truncate the PC representation of the hydraulic head field, i.e., for which polynomial basis functions the projection in equation (16) should be computed. Usually, Hermite polynomial basis functions of low order and basis functions associated with random variables corresponding to large KL eigenvalues are of major importance. In this work and in the contribution of Li and Zhang [20], polynomials up to order d=2were applied. The order 2 restriction for the PC basis functions is also motivated by the Smolyak quadrature accuracy of order 5. If the actual hydraulic head solution was indeed not featuring any PC basis functions of order above 2, the Smolyak quadrature for the projections (16) would be exact, since at most polynomials of order 4 would appear in the integral. In the reduction step described in section 5.5, around 70% of the P = 231 PC terms were eliminated leading to $P_{red} = 66$ remaining terms for the unconditional case. A similar fraction of PC terms was discarded in the conditional case.

7.4. Flow and Streamline Solvers

For the solution of the deterministic flow problem (1) at the quadrature points with the boundary conditions outlined in section 6, the flow solver by Meyer and Tchelepi [22] was applied. The aquifer domain was discretized with 101×101 equi-sized grid cells. For tracer transport, the semi-analytical streamline tracking algorithm outlined by Pollock [28] was used. To sample transport statistics, $5 \cdot 10^5$ sample trajectories were generated.



Figure 5: Exemplary tracer trajectories: MC with N = 100 random dimensions (a) and PCMCM with N = 20 random dimensions (b).

8. Results

The PCMCM results are compared with two different MC data sets. The first MC simulation was produced with the same number of KL terms as in the PCMCM, i.e., N = 20, whereas in the second MC simulation—to which we refer to as reference MC solution—100 KL terms were used. By comparing the PCMCM solution to the MC solution with the same number of terms, i.e., N = 20, deviations can directly be related to limitations of the PC expansion and the Smolyak quadrature. Differences between the MC with only 20 KL terms and the reference MC with N = 100, on the other hand, can be attributed to truncation errors of the KL expansion.

In figure 5, the first 100 tracer trajectory realizations from both PCMCM and MC method are depicted. In these results, no conductivity measurements were taken into account. The PCMCM does not guarantee a divergence free velocity field, which gives rise to non-physical tracer trajectories like the PCMCM trajectory that impacts at the upper no-flow boundary. Overall, in the PCMCM, around 1% of the sampled trajectories in both the conditional and unconditional cases violated mass conservation, i.e., got trapped inside the domain or impacted at no-flow boundaries. These trajectories were not taken into account for output statistics.

In figures 6 and 7, tracer particle position histograms are provided for

the unconditional case and two different travel times t = 0.2 and 0.5, respectively. There is very good agreement with the reference MC for both times. Neither the PCMCM nor the MC with 20 KL terms introduce major statistical error. The preparatory step in the PCMCM simulation to identify the PC representation for the hydraulic head took 130 sec. Moreover, 120 sec were required to perform the subsequent hydraulic head and transport sampling in the PCMCM. On the other hand, the MC approach with N = 20random variables took 1070 sec for the same amount of samples and with N = 100 around 1380 sec.

As is seen in figure 7a, a significant fraction of particles, i.e. 14.3%, has left the computational domain at time t = 0.5. These particles were excluded from the histograms. Especially in the x_2 particle position histogram, this leads to a certain bias.

Particle histograms at time t = 0.5 for the conditional case with measurements are provided in figure 8. In general, the choice of measurements causes the conductivity to be higher in the upper part of the aquifer domain and this region is therefore subject to more tracer discharge, which is confirmed by inspection of figure 8. When comparing the PCMCM results to the MC reference simulations, one can conclude that the PCMCM works accurately. Truncating the conditional KL expansion after N = 20 terms, however, leads to slight deviations as is observable from a comparison of the two MC simulations. Similar or better agreement was found at time t = 0.2.

Since the MC simulations with N = 20 and N = 100 random dimensions exhibit significant differences in the conditional case, it needs to be verified that N = 100 is still sufficient as a reference. In figure 9, we check the convergence of the MC results for N = 100, 200, and 400, which indicates that at N = 100, the MC results have converged and no additional KL terms are required also in the conditional case.

9. Discussion and Conclusions

In this work, a new framework for the propagation of uncertainty from the hydraulic conductivity field to advective tracer transport is outlined. For the description of the uncertain conductivity field, a Karhunen-Loeve (KL) expansion was applied. This expansion can accommodate for measurement values at different spatial locations. A Hermite-polynomial-based polynomial chaos (PC) expansion was used to describe the uncertainty resulting in the



Figure 6: Normalized position histograms of the tracer particle ensemble at t = 0.2: (a) x_1 position; (b) x_2 position; (c) MC, **x** position, N = 20 random dimensions; (d) MC, **x** position, N = 100 random dimensions; (e) PCMCM, **x** position, N = 20 random dimensions.



Figure 7: Normalized position histograms of the tracer particle ensemble at t = 0.5: (a) x_1 position; (b) x_2 position; (c) MC, **x** position, N = 20 random dimensions; (d) MC, **x** position, N = 100 random dimensions; (e) PCMCM, **x** position, N = 20 random dimensions.



Figure 8: Normalized position histograms of the tracer particle ensemble at t = 0.5, conditional on logarithmic conductivity measurements: (a) x_1 position; (b) x_2 position; (c) MC, x position, N = 20 random dimensions; (d) MC, x position, N = 100 random dimensions; (e) PCMCM, \mathbf{x} position, N = 20 random dimensions; (f) mean of logarithmic conductivity, conditional on measurements.



Figure 9: Normalized position histograms of the tracer particle ensemble at t = 0.5, conditional on logarithmic conductivity measurements: x_1 position. MC simulations with different numbers of terms in the KL expansion, i.e., N = 100, 200, and 400, are reported.

hydraulic conductivity and the flow field. To fully determine the PC expansion, Smolyak quadrature was employed and deterministic flow problems at relatively few quadrature points were solved. For an increasing number of terms in the KL expansion and order of the PC expansion, the number of quadrature points grows. With the PC expansion determined, hydraulic head and transport realizations can be generated at relatively low computational costs compared to Monte Carlo (MC) simulations. For the transport part, a convectional streamline approach was used, which avoids inaccuracies resulting from corresponding PC expansions as reported in previous contributions. To reduce the computational cost associated with the PC expansion, a new reduction technique was outlined leading to a more compact PC expansion.

The resulting PC/MC method (PCMCM) was validated with MC reference data for a quadratic confined aquifer with a multivariate Gaussian logconductivity field. The correlation length of the log-conductivity field was set to 40% of the aquifer side length and the log-conductivity variance to $\sigma_Y^2 = 1$. Both unconditional and conditional simulations with log-conductivity measurements were performed. For the investigated test cases, the PCMCM provided very accurate transport statistics at considerably lower computational cost compared to the MC method.

For shorter log-conductivity correlation lengths, more terms in the KL expansion have to be included, which increases the number of terms in the PC expansion and eventually can lead to large numbers of quadrature points of similar order as samples in the MC method. Similarly, for large σ_Y^2 , the order

of the PC expansion has to be increased, which also leads to a larger number of quadrature points. To treat shorter correlation lengths and higher σ_Y^2 in the future, adaptive procedures are needed to compute the PC expansion of the hydraulic head. The significance of different terms in the KL expansion is quantified by their individual eigenvalues. Adaptive methodologies could benefit from this fact to increase the manageable random dimensionality. The current approach, however, does not distribute the number of quadrature points in an adaptive manner (i.e., placing more quadrature points in dimensions representing random variables of greater importance), but discards unimportant PC expansion terms. For more information on adaptive probabilistic schemes the reader is referred to [14, 29].

10. Acknowledgment

This work is performed as part of the ETH interdisciplinary research grant CH1-03 10-1. Florian Müller wishes to thank Siddhartha Mishra and Christoph Schwab for their advise and he is also grateful to Andrea Barth and Claude J. Gittelson for their help in familiarizing with uncertainty quantification.

AppendixA. Gauss-Hermite Quadrature

The Gauss-Hermite quadrature is tailored for integration with respect to the standard Gaussian measure $1/\sqrt{2\pi} \exp(-\xi^2/2)$. The *I* quadrature points Ξ_i , i = 1...I, are the roots of the *I*'th order normalized Hermite polynomial $\Psi^I(\xi)$ as defined by the recurrence relation (B.1). (The roots of the 'Physicist's' Hermite polynomials are listed in [30], table 25.10. In order to obtain the roots of the normalized Hermite polynomials for the Gaussian measure, the tabulated roots need to be rescaled by a factor of $\sqrt{2}$.) The corresponding weights can then be calculated as

$$w_i = \frac{1}{I\Psi^{I-1}(\Xi_i)}.$$

AppendixB. Hermite Polynomials

The one-dimensional Hermite polynomials are constructed from the following recurrence relation:

$$\Psi^{-1} = 0, \ \Psi^{0} = 1 \text{ and } \Psi^{d+1}(\xi) = \frac{1}{\sqrt{d+1}} (\xi \Psi^{d}(\xi) - \sqrt{d} \Psi^{d-1}(\xi)), \quad (B.1)$$

where d indicates the order of a polynomial and ξ is the standard normal random variable. The one-dimensional Hermite polynomials serve as building blocks for the N-dimensional case:

$$\Psi_p(\boldsymbol{\xi}^N) = \prod_{n=1}^N \Psi^{d_n}(\xi_n),$$

where every distinct one-dimensional index set $[d_n]_{n=1}^N$ is associated with a unique index p. The order of a multidimensional Hermite polynomial is $\sum_{n=1}^N d_n$.

- L. W. Gelhar, Stochastic subsurface hydrology from theory to applications, Water Resour. Res. 22 (1986) S135–S145.
- [2] A. G. Journel, C. Huijbregts, Mining geostatistics, Academic Press, London a.o., 1978.
- [3] R. A. Freeze, A stochastic-conceptual analysis of one-dimensional groundwater flow in nonuniform homogeneous media, Water Resour. Res. 11 (1975) 725–741.
- [4] P. Salandin, V. Fiorotto, Solute transport in highly heterogeneous aquifers, Water Resour. Res. 34 (1998) 949–961.
- [5] G. Dagan, Solute transport in heterogeneous porous formations, J. Fluid Mech. 145 (1984) 151–177.
- [6] A. Fiori, G. Dagan, Concentration fluctuations in aquifer transport: A rigorous first-order solution and applications, J. Contam. Hydrol. 45 (2000) 139–163.
- [7] D. L. Freyberg, A natural gradient experiment on solute transport in a sand aquifer. 2. spatial moments and the advection and dispersion of nonreactive tracers, Water Resour. Res. 22 (1986) 2031–2046.
- [8] V. Fiorotto, E. Caroni, Solute concentration statistics in heterogeneous aquifers for finite peclet values, Transport Porous Med. 48 (2002) 331– 351.
- [9] E. Caroni, V. Fiorotto, Analysis of concentration as sampled in natural aquifers, Transport Porous Med. 59 (2005) 19–45.

- [10] R. G. Ghanem, P. D. Spanos, Stochastic finite elements: a spectral approach, Springer, New York [etc.], 1991.
- [11] R. Ghanem, Probabilistic characterization of transport in heterogeneous media, Comput. Method. Appl. M. 158 (1998) 199–220.
- [12] R. Ghanem, Scales of fluctuation and the propagation of uncertainty in random porous media, Water Resour. Res. 34 (1998) 2123–2136.
- [13] D. B. Xiu, Numerical methods for stochastic computations a spectral method approach, Princeton University Press, Princeton, N.J., 2010.
- [14] O. P. Le Maitre, O. M. Knio, Spectral methods for uncertainty quantification with applications to computational fluid dynamics, Scientific computation, Springer, Dordrecht, 2010.
- [15] Y. K. Zhang, D. Zhang, Forum: The state of stochastic hydrology, Stoch. Env. Res. Risk. A. 18 (2004) 265–265.
- [16] Z. M. Lu, D. X. Zhang, Conditional simulations of flow in randomly heterogeneous porous media using a kl-based moment-equation approach, Adv. Water. Resour. 27 (2004) 859–874.
- [17] Z. M. Lu, D. X. Zhang, Accurate, efficient quantification of uncertainty for flow in heterogeneous reservoirs using the klme approach, SPE J. 11 (2006) 239–247.
- [18] G. S. Liu, Z. M. Lu, D. X. Zhang, Stochastic uncertainty analysis for solute transport in randomly heterogeneous media using a karhunenloeve-based moment equation approach, Water Resour. Res. 43 (2007).
- [19] D. B. Xiu, J. S. Hesthaven, High-order collocation methods for differential equations with random inputs, SIAM J. Sci. Comput. 27 (2005) 1118–1139.
- [20] H. Li, D. X. Zhang, Probabilistic collocation method for flow in porous media: Comparisons with other stochastic methods, Water Resour. Res. 43 (2007).
- [21] G. Lin, A. M. Tartakovsky, An efficient, high-order probabilistic collocation method on sparse grids for three-dimensional flow and solute

transport in randomly heterogeneous porous media, Adv. Water. Resour. 32 (2009) 712–722.

- [22] D. W. Meyer, H. A. Tchelepi, Particle-based transport model with markovian velocity processes for tracer dispersion in highly heterogeneous porous media, Water Resour. Res. 46 (2010) W11552.
- [23] C. Schwab, R. A. Todor, Karhunen-Loève approximation of random fields by generalized fast multipole methods., J. Comput. Phys. 217 (2006) 100–122.
- [24] D. X. Zhang, Z. M. Lu, An efficient, high-order perturbation approach for flow in random porous media via karhunen-loeve and polynomial expansions, J. Comput. Phys. 194 (2004) 773–794.
- [25] D. B. Xiu, G. E. Karniadakis, The wiener-askey polynomial chaos for stochastic differential equations, SIAM J. Sci. Comput. 24 (2002) 619– 644.
- [26] S. Smolyak, Quadrature and interpolation formulas for tensor products of certain classes of functions, Dokl. Akad. Nauk SSSR 4 (1963).
- [27] T. Gerstner, M. Griebel, Numerical integration using sparse grids, Numer. Algorithms 18 (1998) 209–232.
- [28] D. W. Pollock, Semianalytical computation of path lines for finitedifference models, Ground Water 26 (1988) 743–750.
- [29] F. Nobile, R. Tempone, C. G. Webster, An anisotropic sparse grid stochastic collocation method for partial differential equations with random input data., SIAM J. Numer. Aanal. 46 (2008) 2411–2442.
- [30] M. Abramowitz, Handbook of mathematical functions with formulas, graphs, and mathematical tables, Dover Publications, New York, 9th edition, 1972.

Research Reports

No. Authors/Title

11-34	F. Müller, D.W. Meyer and P. Jenny Probabilistic collocation and Lagrangian sampling for tracer transport in randomly heterogeneous porous media
11-33	<i>R. Bourquin, V. Gradinaru and G.A. Hagedorn</i> Non-adiabatic transitions near avoided crossings: theory and numerics
11-32	J. Šukys, S. Mishra and Ch. Schwab Static load balancing for multi-level Monte Carlo finite volume solvers
11-31	C.J. Gittelson, J. Könnö, Ch. Schwab and R. Stenberg The multi-level Monte Carlo Finite Element Method for a stochastic Brinkman problem
11-30	A. Barth, A. Lang and Ch. Schwab Multi-level Monte Carlo Finite Element method for parabolic stochastic partial differential equations
11-29	M. Hansen and Ch. Schwab Analytic regularity and nonlinear approximation of a class of parametric semilinear elliptic PDEs
11-28	R. Hiptmair and S. Mao Stable multilevel splittings of boundary edge element spaces
11-27	Ph. Grohs Shearlets and microlocal analysis
11-26	<i>H. Kumar</i> Implicit-explicit Runge-Kutta methods for the two-fluid MHD equations
11-25	H. Papasaika, E. Kokiopoulou, E. Baltsavias, K. Schindler and D. Kressner Sparsity-seeking fusion of digital elevation models
11-24	H. Harbrecht and J. Li A fast deterministic method for stochastic elliptic interface problems based on low-rank approximation
11-23	P. Corti and S. Mishra Stable finite difference schemes for the magnetic induction equation with Hall effect
11-22	H. Kumar and S. Mishra Entropy stable numerical schemes for two-fluid MHD equations
11-21	H. Heumann, R. Hiptmair, K. Li and J. Xu Semi-Lagrangian methods for advection of differential forms