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Abstract

We describe methods for the numerical solution of nonlinear problems with stochastic uncertainties in the operator, boundary conditions, and right hand side. First, we compute statistics of the solution directly as high-dimensional integrals and compare their evaluation by sparse (Smolyak) quadrature and Monte Carlo integration. Subsequently, we employ a Galerkin method to obtain an expansion of the solution in a stochastic ansatz-space. This requires the numerical evaluation of the residual, which is again a high-dimensional integral, and we show that sparse quadrature may be an efficient technique for this. The large nonlinear system resulting from the Galerkin conditions is solved by quasi-Newton methods. Finally, we alternatively compute the expansion of the solution by direct orthogonal projection onto stochastic ansatz-functions. We apply the methods to a prototype nonlinear groundwater-flow situation (pressure equation).

1 Introduction

Oftentimes, numerical simulations of real-world systems are required even though not all parameters are exactly known. For example, in the simulation of groundwater flow exact knowledge about the conductivity of the soil, the magnitude of source terms, or about the in- and out-flows is usually not available. The uncertainties inherent in the model result in uncertainties in the results of numerical simulations, a fact which is often ignored in common practice. Clearly, it is desirable to quantify the uncertainties in the solution depending on the model's uncertainties.

Stochastic models are one way to quantify uncertainties. Uncertain parameters are modelled by random variables, uncertain time-dependent functions by stochastic processes, and uncertain spatial properties by random fields [1, 52, 8]. If the physical system is described by a partial differential equation (PDE), then the combination with the stochastic model results in a stochastic PDE (SPDE). The solution of the SPDE is a random field describing both the expected system-response and its quantitative uncertainty.

SPDEs can be interpreted mathematically in several ways. We are concerned with randomness in space, and the SPDEs considered here are different from stochastic differential equations (SDEs) or PDEs describing a time evolution driven by white noise, e.g. [27]. A theory of SPDEs where products between random fields are interpreted as Wick products was developed in [18]. This allows the use of highly irregular random fields as coefficients and obtain the solution as a stochastic distribution. Its main shortcoming is that—e.g. for linear problems—higher statistical moments of system parameters do not influence the mean of the answer, a contradiction to the results of homogenisation theory. Also the required existence of strong solutions in [18] results in considerable restrictions on the boundary conditions and source terms. These may be relaxed by a variational formulation [30, 50], but nonetheless the Wick product seems not to be the right model for the problems that we aim at. If products are instead interpreted in the usual sense, stronger regularity is required for the random fields [6]. The stochastic regularity of the solution determines the convergence rate of numerical approximations, and a variational theory for this was earlier devised in [5]. Further investigations with partly stronger constraints on the stochastic parameters can be found in [3, 4, 46].

The ultimate goal in the solution of SPDEs is usually the computation of response statistics. Monte Carlo methods may be utilised for this, but they require a high computational effort. We show that sparse (Smolyak) quadrature methods may be an efficient alternative. These have first been described in [47] and have found increasing attention in recent years, e.g. [35, 41, 11].

Some alternatives to Monte Carlo methods have been developed in the field of stochastic mechanics, for example perturbation methods, e.g. [26], methods based on the Neumann series, e.g. [15, 3], or the spectral stochastic finite element method (SSFEM) [15]. The latter method expands the stochastic fields in eigenfunctions of their covariance kernels and obtains the solution by a Galerkin method in a space of stochastic ansatz-functions. More information, references and reviews on stochastic finite elements can be found in [29, 45, 49, 20].

Following [15], stochastic Galerkin methods have been applied to various linear problems, e.g. [12, 13, 39, 31, 24, 23]. Recently, nonlinear problems with stochastic source terms have been tackled, e.g. [55], but publications on Galerkin methods for nonlinear stochastic operators are scarce. In section 6.1 we describe a stochastic Galerkin method for general nonlinear boundary value problems with stochastic uncertainties in the operator and in the source terms. As ansatz-functions we use tensor products of spatial finite elements and stochastic functions. Application of the Galerkin conditions yields a large system of nonlinear equations. We show that the numerical evaluation of the residual may be performed efficiently by quadrature techniques and solve the resulting large nonlinear system by a preconditioned BFGS scheme, e.g. [33].

Alternatively, we obtain the solution by projecting orthogonally onto the stochastic ansatz-space, where the projections are evaluated by Smolyak quadrature. This requires the solution of many smaller but uncoupled nonlinear systems instead of one large coupled system.

2 Model Problem

The numerical methods presented below can be used to solve arbitrary nonlinear problems with stochastic uncertainties, and are applied here to a prototypical model of stationary nonlinear groundwater flow.

2.1 Physical Description

A simple model for stationary groundwater flow in a region $R \subset \mathbb{R}^d$, where the flow depends nonlinearly on the hydraulic head u, is the PDE

$$-\nabla \cdot (\hat{\kappa}(x,u)\nabla u(x)) = f(x), \qquad x \in R \tag{1}$$

with appropriate boundary conditions. The solution u is the hydraulic head, and f are the sinks and source terms. The hydraulic conductivity $\hat{\kappa}$ depends on the hydraulic head and on soil properties which we describe by another field $\kappa(x), x \in R$. We use the model $\hat{\kappa}(x,u) = \kappa(x) + cu(x)^2$, $c > 0$.

The stochastic uncertainty in the soil-properties is quantified by defining $\kappa(x)$ for each $x \in R$ as a random variable $\kappa(x) : \Omega \to \mathbb{R}$ on a suitable probability space $(\Omega, \mathcal{B}, \Gamma)$. Here Ω is the set of elementary events, $\mathcal{B}$ a σ-algebra and Γ a measure. As a consequence, $\kappa : R \times \Omega \to \mathbb{R}$ is a random field [1, 52, 8], and one may identify Ω with the set of “all possible soil properties”, i.e. with the space of all realisations $\kappa(\cdot,\omega) : R \to \mathbb{R}$, $\omega \in \Omega$, cf. Fig. 1. As this space is usually infinite dimensional, the probability space is in some sense infinite dimensional as well.

The probability space can be defined by the joint statistic of all possible combinations $\kappa(x_1), \dots, \kappa(x_m)$, $m \in \mathbb{N}$, $x_1, \dots, x_m \in R$ (all finite dimensional distributions), see e.g. [1] for details. Often, only second order statistics (mean and covariance) and marginal distributions are known from measurements. These may be prescribed by a point-wise transformation

$$\kappa(x,\omega) = \phi(x, \gamma(x,\omega)), \qquad x \in R, \omega \in \Omega, \tag{2}$$

of a Gaussian random field $\gamma(x,\omega)$ defined by its mean $\mu_\gamma(x)$ and its covariance $\mathrm{cov}_\gamma(x,y)$. Without loss of generality we choose $\mu_\gamma(x) = 0$ and $\mathrm{var}_\gamma(x) = \mathrm{cov}_\gamma(x,x) = 1$.

It is a well-known fact that a standard distributed Gaussian random variable $\mathcal{N}(0,1)$ can be mapped to a random variable with distribution function F_κ by the transformation $F_\kappa^{-1}(\mathrm{erf}(\mathcal{N}(0,1)))$, where erf is the Gaussian distribution function. Thus, $\kappa(x,\omega)$ can be given any marginal distribution by choosing ϕ in Eq. (2) appropriately. Additionally, the combination of ϕ and $\mathrm{cov}_\gamma(x,y)$ may be chosen such that $\kappa(x,\omega)$ satisfies given second order statistics $\mu_\kappa(x)$ and $\mathrm{cov}_\kappa(x,y)$, cf. [43].

For a physically and mathematically well-defined model, the soil properties should be bounded from above and below,

$$0 < \hat{\kappa}_- \leq \kappa_-(x) \leq \kappa(x,\omega) \leq \kappa_+(x) \leq \hat{\kappa}_+ < \infty, \qquad x \in R. \tag{3}$$

In our model this is guaranteed by a suitable choice of ϕ in Eq. (2), assigning to $\kappa(x)$ a $\beta(1/2,1/2)$-distribution (the probability distribution has the shape of half sinus-wave). The transformation is

$$\kappa(x,\omega) = c_1(x) + c_2(x)\arccos(\mathrm{erf}(\gamma(x,\omega))). \tag{4}$$

Uncertainties in the other parameters may be modelled similarly, and a combination with Eq. (1) yields the stochastic PDE

$$-\nabla\cdot(\kappa(x,u,\omega)\nabla u(x,\omega)) = f(x,\omega), \qquad x \in R, \tag{5}$$

$$\frac{\partial}{\partial n}(\kappa(x,u,\omega))\nabla u(x,\omega) = f_N(x,\omega), \qquad x \in \Gamma_N, \quad \Gamma_N \cup \Gamma_D = \partial R \tag{6}$$

$$u(x,\omega) = f_D(x,\omega), \qquad x \in \Gamma_D, \tag{7}$$

for Γ-almost all $\omega \in \Omega$. The hydraulic head $u(x,\omega)$ as the solution of Eqs. (5–7) is now also a random field. Our goal is to compute response statistics, e.g. the mean $\mu_u(x) = \mathbf{E}(u(x))$, the covariance $\mathrm{cov}_u(x,y) = \mathbf{E}((u(x)-\mu_u(x))(u(y)-\mu_u(y)))$, or the probability that the hydraulic head exceeds some threshold, $p_u(x) = \mathrm{P}\{u(x) > u_0\} = \mathbf{E}\left(\chi_{(u_0,\infty)}(u(x))\right)$, where χ_A is the characteristic function of the set A. All these statistics $s_u(x)$ are integrals with respect to the measure $d\Gamma(\omega)$,

$$s_u(x) = \mathbf{E}(s(u(x))) = \int_\Omega s(u(x,\omega))\, d\Gamma(\omega). \tag{8}$$

The numerical evaluation of such statistics requires a discretisation of Eqs. (5–7) in space and in the stochastic dimension, and both discretisations may be performed independently of each other. Almost any technique may be used for the spatial discretisation, and we use finite elements in section 3.

Once the problem is discretised in space, numerical methods may be applied in the stochastic dimension, e.g. Monte Carlo simulations. But before numerical simulations can be performed, it is necessary to approximate Eqs. (5–7) in a finite number of independent random variables. This will be done in section 4.

2.2 Mathematical Formulation

Let us now briefly sketch the mathematical framework in which we want to set this problem. Assuming for a moment that there is no stochastic dependence, then we choose for the possible solutions the space

$$W = \{u \in W_p^1(R) | u \, \text{satisfies essential boundary conditions}\}, \tag{9}$$

and allow for the right-hand-side $f \in W^*$, which for $W = \overset{\circ}{W}{}_p^1(R)$ would be $W_q^{-1}(R)$, where $1/p + 1/q = 1$. For the coefficient $\kappa(x)$ we assume $\kappa \in L_\infty(R)$ satisfying Eq. (3), and this way the Nemicky operator

$$N : u \mapsto (\kappa + cu^2)\nabla u \tag{10}$$

is a continuous map from W into $L_q(R)$ for $p = 4$ because of the type of nonlinearity.

This makes the semilinear (linear in v) form

$$a(u,v) := \int_R \nabla v(x) \cdot N(u)(x) \, dx \tag{11}$$

hemicontinuous in u and continuous in v, and defines a hemicontinuous (nonlinear) operator $A : W \to W^*$ such that

$$\forall u, v \in W : \quad a(u,v) = \langle A(u), v \rangle_W, \tag{12}$$

where $\langle \cdot, \cdot \rangle_W$ is the duality pairing between W and its dual W^*.

This operator is strictly monotone and coercive. Standard arguments on monotone operators e.g. [19, 38] allow us then to conclude that the problem to find $u \in W$ such that

$$\forall v \in W : \quad a(u,v) = \langle A(u), v \rangle_W = \langle f, v \rangle_W \tag{13}$$

has a unique solution. In the linear case this reduces to the Lax-Milgram lemma.

We want to extend this to the stochastic situation, cf. [5, 3, 4, 46] for the linear case. We look for a solution in a space which comes from completing the space of linear combinations of products of basis functions $\{u_k\}$ in W and $\{\phi_l\}$ in (S)

$$\sum_{k,l} u_k(x)\phi_l(\omega), \tag{14}$$

i.e. the tensor product $W \otimes (S)$, where (S) is an appropriate space of stochastic functions (random variables). In our case the simplest choice is $(S) = L_p(\Omega)$ with $p = 4$ because of the type of nonlinearity. This tensor product is isomorphic to

$L_p(\Omega, W)$, i.e. a space of W-valued random variables. It is certainly possible to use more refined and general spaces for (S), as was done in [5] for the linear Hilbert space case.

Letting ∇_ω act on a typical term $u_k(x)\phi_l(\omega)$ as

(15) $$\nabla_\omega(u_k(x)\phi_l(\omega)) := (\nabla u_k(x))\phi_l(\omega),$$

we can extend this by linearity and continuity to $W \otimes (S)$, and obtain a continuous operator $\nabla \otimes Id : W \otimes (S) \to L_p(R) \otimes (S)$.

The Nemicky operator $N_\omega : W \otimes (S) \to L_q(R) \otimes (S)^*$ is then defined by

(16) $$N_\omega(u(x,\omega)) := (\kappa(x,\omega) + cu(x,\omega)^2)\nabla_\omega u(x,\omega), \qquad u \in W \otimes (S).$$

For the stochastic field $\kappa(x,\omega)$ we shall assume similarly to Eq. (3) that it is bounded from below and above for Γ-almost all ω.

As before, with these ingredients we obtain a semilinear form

(17) $$\hat{a}(u,v) := \int_\Omega \int_R \nabla_\omega v \cdot N_\omega(u)\, dx\, d\Gamma(\omega), \qquad u,v \in W \otimes (S).$$

The SPDE Eq. (5) may now be cast in a variational form, requiring us to find a solution $u \in W \otimes (S)$ such that

(18) $$\forall v \in W \otimes (S) : \quad \mathbf{E}\left(\langle \hat{A}(u), v\rangle_W\right) = \hat{a}(u,v) = \mathbf{E}\left(\langle f(\omega), v(\omega)\rangle_W\right).$$

Again this defines a nonlinear, strictly monotone, hemicontinuous, coercive operator $\hat{A}$ from $W \otimes (S)$ into its dual. The same arguments as in the deterministic case may be used to ascertain the existence and uniqueness of a solution $u \in W \otimes (S)$.

3 Discretisation in Space

Almost any technique may be used for the spatial discretisation, e.g. finite differences or finite elements, and we use a finite element discretisation of the region $R \subset \mathbb{R}^d$ with a vector of ansatz-functions $\mathbf{N}(x) = (N_1(x), \ldots, N_n(x))$, e.g. [48, 56]. An ansatz for the solution in $\mathbf{N}(x)$ yields a semi-discretisation of Eqs. (5–7). Similarly to the method of lines for instationary boundary value problems where the coefficients would be time-dependent, we obtain an expansion

(19) $$u^{semi}(x,\omega) = \sum_{i=1}^{n} u_i(\omega) N_i(x) = \mathbf{N}(x)\mathbf{u}(\omega),$$

where the degrees of freedom are random variables $\mathbf{u}(\omega) = (u_1(\omega), \ldots, u_n(\omega))^T$.

By inserting the ansatz into the SPDE Eq. (5) and applying Galerkin conditions, a system of nonlinear stochastic equations results,

(20) $$\mathbf{f}(\mathbf{u}(\omega), \omega) = 0 \qquad \text{for } \Gamma\text{-almost all } \omega \in \Omega.$$

4 Discretisation of the Probability Space

In order to solve Eq. (20) numerically, an approximation in a finite number of independent random variables is necessary. This is obtained by representing each random field in a countable number of independent random variables, and subsequently keeping only the most important terms. We show this exemplary for the soil-parameter $\kappa(x,\omega) = \phi(x,\gamma(x,\omega))$ defined in Eq. (2).

We apply the Karhunen–Loève expansion (KL-expansion), e.g. cf. [51, 1], which represents a random field in a countable number of uncorrelated random variables. The KL-expansion of the underlying Gaussian field γ with $\mathbf{E}(\gamma(x)) = 0$ is

$$(21) \qquad \gamma(x,\omega) = \lim_{m\to\infty} \gamma_m(x,\omega), \qquad \gamma_m(x,\omega) = \sum_{i=1}^{m} \sqrt{\lambda_i}\, g_i(x)\, \omega_i, \qquad x \in R,$$

where $\omega = (\omega_1, \omega_2, \ldots)$ are uncorrelated and hence independent Gaussian random variables with $\mathbf{E}(\omega_i) = 0$ and $\mathbf{E}\left(\omega_i\,\omega_j\right) = \delta_{ij}$ for $i, j \in \mathbb{N}$. The $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_i \geq \cdots \geq 0$ and $g_i \in L_2(R)$ are the eigenvalues and eigenfunctions of the symmetric and positive semidefinite Fredholm operator

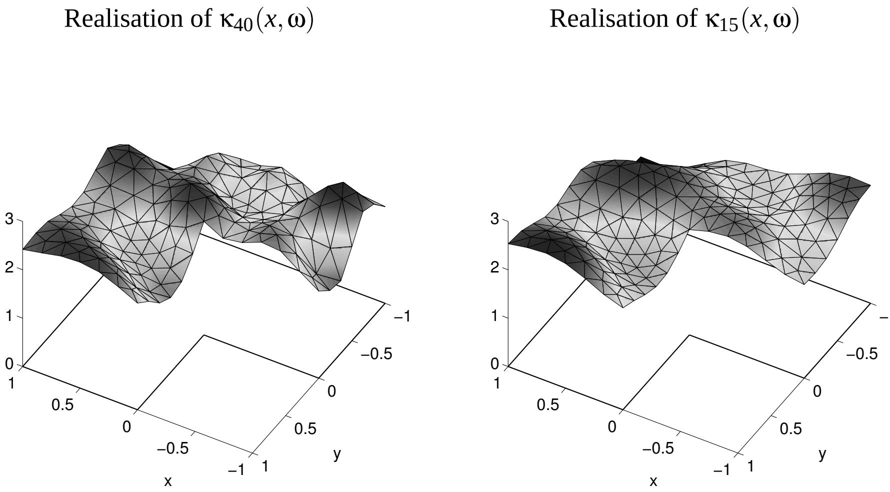
$$(22) \qquad (C_\gamma g)(x) = \int_R \operatorname{cov}_\gamma(x,y) g(y)\, dy = \lambda_i g_i(x).$$

Analytical solutions of the eigenvalue problem are usually unknown, but they may be computed numerically by standard techniques, e.g. [2]. The KL-expansion is optimal in the sense that it has the smallest L_2-error $\|\gamma(x,\omega) - \gamma_m(x,\omega)\|_{L_2(R\times\Omega)}$ among all approximations of γ in m uncorrelated random variables, e.g. cf. [15].

For the numerical treatment, the KL-expansion is truncated after a finite number of terms, and the soil-parameter is approximated as $\kappa_m(x,\omega) = \phi(x,\gamma_m(x,\omega))$, where now $\omega = (\omega_1, \ldots, \omega_m)$. Alternatively, an approximation with the same marginal distribution as κ may be obtained as $\hat{\kappa}_m(x,\omega) = \phi(x, s_m(x)\gamma_m(x,\omega))$ with a scaling factor $s_m(x) = \operatorname{var}(\gamma_m(x))^{-1/2}$. The price for this is a larger error $\|\hat{\kappa}_m - \kappa\|_{L_2(R\times\Omega)}$ and a larger error in the spatial correlation than for κ_m.

As more and more eigenfunctions are used in the truncated KL-series, finer scales of spatial fluctuations are resolved by the approximation. This is demonstrated in Fig. 1 by showing realisations of $\kappa_m(x,\omega)$ for 40 and 15 KL-terms.

The other random fields—e.g. the right hand side—in the SPDE Eq. (5) are approximated similarly. If in toto m independent Gaussian random variables are kept, the problem may be described in a probability space $(\Omega^{(m)}, \mathcal{B}_m, \Gamma_m)$, where the space of elementary events $\Omega^{(m)} = \mathbb{R}^m$ and Γ_m is the Gaussian measure with $d\Gamma_m(\omega) = (2\pi)^{-m/2} \exp\left(-\sum_{i=1}^{m} \omega_i^2/2\right) d\omega$, and $d\omega$ is the usual Lebesgue measure on $\mathbb{R}^m$. Inserting this into Eq. (20), we obtain a set of n nonlinear equations



Realisation of $\kappa_{40}(x,\omega)$

Realisation of $\kappa_{15}(x,\omega)$

Figure 1: Realisations of $\kappa_m(x,\omega)$ on an L-shaped region for different numbers of KL-terms.

depending on m Gaussian random variables,

$$\mathbf{f}(\mathbf{u}(\omega),\omega) = 0 \qquad \text{for } \omega = (\omega_1,\dots,\omega_m) \in \Omega^{(m)}. \tag{23}$$

5 Integrals in High Dimensions

Having found a computationally tractable representation such as Eq. (23), we may now compute statistics like Eq. (8). For a fixed $x \in R$, every statistics can be written as the expectation of a function $\psi : \Omega^{(m)} \to \mathbb{R}$, and we discuss techniques for the numerical evaluation of

$$s := \mathbf{E}\left(\psi(\omega)\right) \;=\; \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \psi(\omega_1,\dots,\omega_m)\, d\Gamma_1(\omega_1)\cdots d\Gamma_1(\omega_m), \tag{24}$$

where $d\Gamma_1(\omega_i)$ is the one-dimensional Gaussian measure.

Several methods may be used for this, and their efficiency depends on the dimension m and on the properties of the integrand $\psi(\omega) = s(\mathbf{N}(x)\mathbf{u}(\omega))$, where $\mathbf{u}(\omega)$ is a solution of Eq. (23). In reliability investigations such integrals arise in the computation of failure probabilities, and often FORM- or SORM-methods (first/second order reliability methods) are used there, e.g. cf. [17]. We shall briefly sketch Monte Carlo methods, e.g. [7], Quasi Monte Carlo methods, e.g. [7, 34], full tensor-quadrature, and we shall expand somewhat on sparse (Smolyak) tensor-quadrature [47]. Each of these methods obtains an approximation s_Z

of Eq. (24) by evaluating the integrand in Z integration points $\omega^{(1)},\ldots,\omega^{(Z)} \in \Omega^{(m)}$, and then linearly combining the results with weights $w_1,\ldots,w_Z \in \mathbb{R}$,

$$s_Z = \sum_{i=1}^{Z} w_i \psi(\omega^{(i)}).$$

Monte Carlo methods (MC-methods) obtain the integration points as Z independent realisations of $\omega \in \Omega^{(m)}$ distributed according to the probability-measure Γ_m, and use constant weights $w_i = Z^{-1}$. MC-methods are probabilistic as the integration points are chosen randomly, and therefore the approximation s_Z and the error $s - s_Z$ are random variables. For large Z, the error is approximately $\sigma_\psi Z^{-1/2}\mathcal{N}(0,1)$, where $\mathcal{N}(0,1)$ is a standard-distributed Gaussian random variable and σ_ψ the standard deviation of the integrand. Due to the $O(\sigma_\psi Z^{-1/2})$ behaviour of the error, MC-methods converge slowly—for instance, the error is reduced by one order of magnitude if the number of evaluations is increased by two orders. They are well suited for integrands with small variance and low accuracy requirements. In applications, their efficiency is usually increased somewhat by variance reduction and importance sampling, cf. e.g. [7, 45, 44] and the references therein. The significant advantage of MC-methods is that their convergence rate is independent of the dimension, while the efficiency of the other methods discussed here decreases with increasing dimension.

Quasi-Monte Carlo methods (QMC-methods) are an alternative to Monte Carlo methods, e.g. [34, 7]. Informally speaking, they choose the sequence of integration points such that “for any number of points Z the integral $\mathbf{E}(1)$ is approximated well by the sequence”. Such sequences are called quasi-random numbers or low discrepancy sequences [34]. The most commonly used QMC-methods have an error of $O\big(\|\psi\|_{BV} Z^{-1}(\log Z)^m\big)$, where $\|\psi\|_{BV}$ denotes the bounded variation norm. If the dimension is not too large and the integrand is smooth, the term Z^{-1} dominates the error and QMC-methods may be more efficient than MC-methods, e.g. cf. [7] and the references therein.

The efficiency of MC-methods depends on the standard deviation σ_ψ, and the efficiency of QMC-methods depends on the first partial derivatives of the integrand, higher-order smoothness is not exploited. In contrast to this, the efficiency of usual quadrature formulas depends strongly on the smoothness of the integrand.

Quadrature formulas for the high-dimensional integral Eq. (24) can be constructed as tensor products of one-dimensional quadrature formulas. We use here tensor products of Gauss-Hermite-formulas Q_z with $z \in \mathbb{N}$ integration points $\omega^{(z,i)} \in \mathbb{R}$ and weights $w_{z,i}$, $i = 1,\ldots,z$. As is well-known, they integrate polynomials of degree less than $2z$ exactly and yield an error of order $O(z^{-(2r-1)})$ for r-times continuously differentiable integrands.

The evaluation of Eq. (24) can be performed by the “full” tensor product of the one-dimensional formulas

$$(25)\quad Q_z^m\psi := (Q_z^1 \otimes \cdots \otimes Q_z^1)\psi = \sum_{i_1=1}^{z} \cdots \sum_{i_m=1}^{z} w_{z,i_1} \cdots w_{z,i_m} \psi(\omega^{(z,i_1)}, \ldots, \omega^{(z,i_m)}).$$

This “full” tensor-quadrature evaluates the integrand on a regular mesh of $Z = z^m$ points, and the approximation-error has order $O(Z^{-(2r-1)/m})$. Due to the exponential growth of the effort with increasing dimension, the application of full tensor-quadrature is impractical for high stochastic dimensions, which has been termed the “curse of dimension”, e.g. cf. [36].

Smolyak quadrature or “sparse” quadrature [47] can be applied in much higher dimensions—for recent works cf. e.g. [35, 37, 41] and the references therein. A software package is available at [40].

Like full tensor-quadrature, Smolyak quadrature formulas are constructed from tensor products of one-dimensional quadrature formulas, but these are combined so that in only some dimensions quadrature formulas of high order are used while formulas of lower order are used in the other dimensions. For a multi-index $\mathbf{z} \in \mathbb{N}^m$ with $|\mathbf{z}| = \sum_i z_i$ and $z \in \mathbb{N}$ the Smolyak quadrature formula is

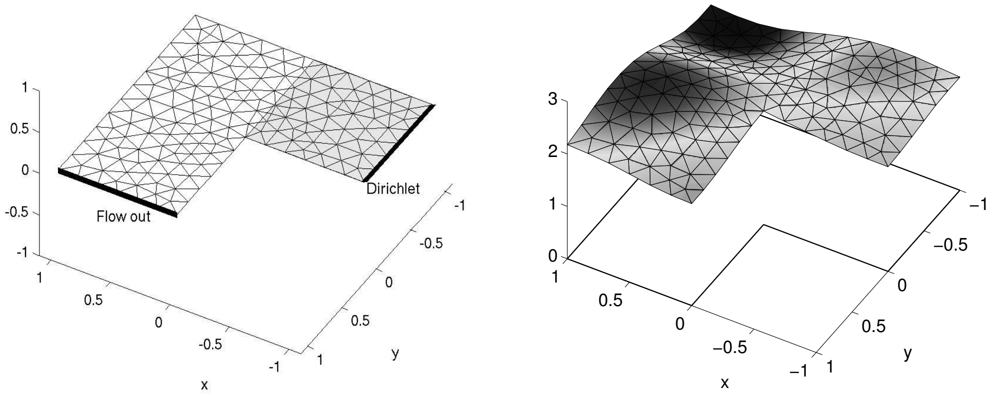
$$S_z^m := \sum_{z \leq |\mathbf{z}| \leq z+m-1} (-1)^{z+m-1-|\mathbf{z}|} \binom{z-1}{|\mathbf{z}|-z} \cdot Q_{z_1} \otimes \cdots \otimes Q_{z_m}.$$

For a fixed z the number of evaluations grows significantly slower in the number of dimensions than for full quadrature. The price is a larger error: full quadrature Q_z^m integrates polynomials $\omega_1^{k_1} \cdots \omega_N^{k_m}$ exactly if their partial polynomial degree $\max_i k_i$ does not exceed $2z-1$. Smolyak formulas S_z^m integrate multivariate polynomials exactly only if their total polynomial degree $\sum_{i=1}^m k_i$ is at most $2z-1$.

As in [37], we will use one-dimensional Gauss-Hermite formulas for the Smolyak construction. Their advantage is a high exactness for smooth integrands, but usually nested integration formulas are used instead in the literature, i.e. formulas where the integration points of the lower-order formulas are subsets of the integration points of the higher-order formulas. When such formulas—e.g. Clenshaw-Curtis formulas—are used, the integration points form a sparse grid, and the number of integration points grows more slowly in the number of dimensions, e.g. cf. [42]. Developments are currently under way to use nested quadrature formulas for SPDEs.

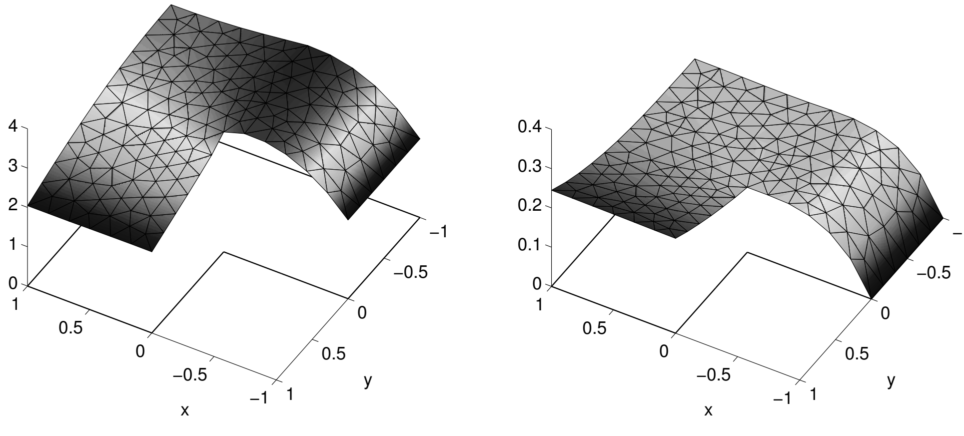
5.1 Numerical Experiments: Computation of Statistics

We compute the mean and standard deviation for the nonlinear groundwater flow problem with geometry and boundary conditions shown in Fig. 2 by naive Monte



Gray area: sources, unlabeled bd.: no flow

A realisation of the soil parameter $\kappa_6(x,\omega)$



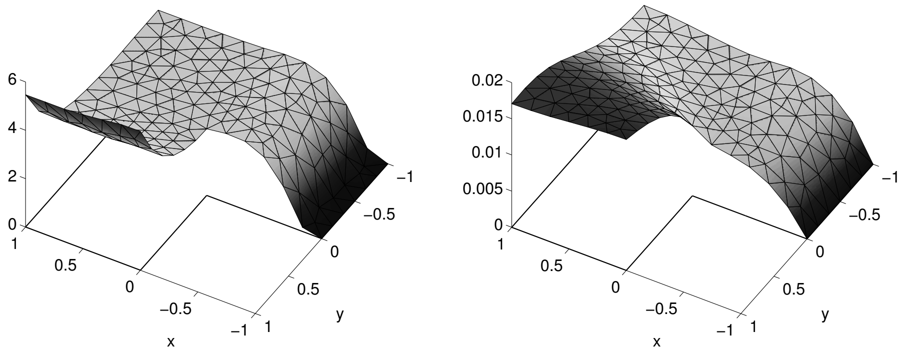
Reference solution, mean

Reference solution, standard deviation

Figure 2: Geometry and Realisation of the Material

Error $\cdot 10^4$ of mean for S_4^6 ($Z = 455$ integration points).

Error in mean for Monte Carlo ($Z = 500$).



Error $\cdot 10^3$ of std-dev. for S_4^6 ($Z = 455$).

Error in std-dev. for Monte Carlo ($Z = 500$).

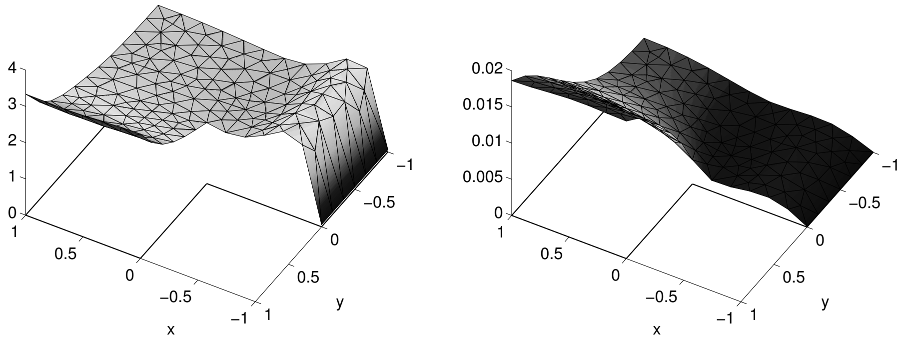


Figure 3: Errors for the Solution by direct integration

Carlo integration and by Smolyak quadrature. The soil parameter $\kappa(x,\omega)$ is chosen beta-distributed with mean $\mu_\kappa(x) = 2$ and standard deviation $\sigma_\kappa(x) = 0.43$, and six KL-terms of the underlying Gaussian field are kept, see Fig. 2 for a realisation. The mean and standard deviation of the reference solution were computed by Smolyak-quadrature S_6^6 in altogether $Z = 6,188$ integration points, and are shown in the bottom row of Fig. 2.

We have then used Smolyak quadrature S_4^6 with 451 integration points and Monte Carlo simulation with 500 integration points. The resulting errors in mean and standard deviation with respect to the reference solution are shown in Fig. 3. The errors from the naive Monte Carlo simulation are larger than the error from the Smolyak integration—about forty times larger for the mean and six times larger for the standard deviation. Thus, a naive Monte Carlo simulation would require an approximately $1,600$ times higher effort to obtain the same accuracy.

6 Expansion in Stochastic Functions

Above, statistics have been computed directly by integration in the high-dimensional probability space. Alternatively, we now obtain the solution by an expansion in tensor products of the FEM ansatz-functions and stochastic ansatz-functions [15]. The resulting approximation yields a functional representation in $\omega = (\omega_1,\dots,\omega_m)$ and may therefore be called a response surface [25].

For the stochastic ansatz we choose linearly independent $H_\alpha \in (S)$, where the multi-indices α are from a finite set $\mathcal{I}$, and where (S) is the space of admissible stochastic functions discussed in section 2.2. We expand the solution of Eq. (23) as

$$\mathbf{u}_{\mathcal{I}}(\omega) = \sum_{\alpha\in\mathcal{I}} \mathbf{u}^{(\alpha)} H_\alpha(\omega). \tag{26}$$

Each vector $\mathbf{u}^{(\alpha)} = \left(u_1^{(\alpha)},\dots,u_n^{(\alpha)}\right)^T$ belongs to a stochastic ansatz-function and contains one coefficient for each spatial degree of freedom. The vector of all unknowns is the block-vector $\mathbf{u} = (\dots,\mathbf{u}^{(\alpha)},\dots)^T$. Altogether with Eq. (19) we have an expansion in tensor products of FEM ansatz-functions and stochastic functions

$$u^{disc}(x,\omega) = \sum_{i=1}^{n} \sum_{\alpha\in\mathcal{I}} N_i(x) H_\alpha(\omega) u_i^{(\alpha)}. \tag{27}$$

Once the block-vector $\mathbf{u}$ is found, statistics can be computed either analytically or by the methods of section 5. Realisations of $u^{disc}(x,\omega)$ can be generated at almost negligible costs (it is a response surface) and hence the numerical evaluation of statistics is cheap.

In principle, any set of linearly independent functions $\{H_\alpha\}_{\alpha\in\mathcal{I}} \subset (S)$ may be used for the ansatz. Ghanem and Spanos [15] and many later works have used multivariate Hermite polynomials which are orthogonal with respect to Gaussian measure and which are also known as Wiener's polynomial chaos [53]. SPDEs are sometimes defined in probability spaces with a non-Gaussian measure, and the orthogonal multivariate polynomials there are called generalised polynomial chaos, cf. [54]. For the case that all random variables have bounded range, piecewise polynomials were used in [9]. For the same case, an *hp*-method with piecewise polynomials was proposed in [4]. One way to realise piecewise polynomials in high dimensions may be sparse ansatz-spaces constructed by the same principle as the Smolyak quadrature formulas discussed above. Applications of sparse ansatz-spaces to (non-stochastic) PDEs can be found e.g. in [46, 16].

We assume the solution $u(x,\omega)$ to be smooth in ω, and hence global polynomials seem to be an appropriate ansatz in the stochastic dimension. We use multivariate Hermite polynomials (polynomial chaos), which are defined for multi-indices $\alpha = (\alpha_1,\dots,\alpha_m) \in \mathbb{N}_0^m$ by

$$H_\alpha(\omega) = \prod_{i=1}^{m} h_{\alpha_i}(\omega_i), \qquad \omega = (\omega_1,\dots,\omega_m) \in \boldsymbol{\Omega}^{(m)},$$

where h_j denotes the Hermite polynomial of degree j scaled so that $\mathbf{E}\left(H_\alpha H_\beta\right) = \delta_{\alpha\beta}$. As suggested in [15], we use as ansatz-space the so-called polynomial chaos of order p which contains all multivariate Hermite polynomials with a total degree of at most p, i.e. $\mathcal{I} = \left\{\alpha \mid |\alpha| = \sum_{i=1}^{m} \alpha_i \le p\right\}$. This choice is similar to the Smolyak construction, and hence $\{H_\alpha\}_{\alpha\in\mathcal{I}}$ may be viewed as a sparse ansatz.

For the computation of **u** we present two possibilities: the Galerkin method and a direct orthogonal projection onto the stochastic ansatz-space.

6.1 Stochastic Galerkin Method

Just as in finite element methods, we can apply Galerkin conditions in the stochastic dimension to obtain the solution. By inserting the ansatz Eq. (26) into the semi-discretised problem Eq. (23) and projecting the residual onto $\{H_\beta\}_{\beta\in\mathcal{I}}$, a large nonlinear system with $n\cdot|\mathcal{I}|$ coupled equations results. The coefficients $\mathbf{u}^{(\alpha)}$ are found by imposing the Galerkin conditions

$$\mathbf{E}\left(\mathbf{f}\big(\omega, \sum_{\alpha\in\mathcal{I}} \mathbf{u}^{(\alpha)} H_\alpha(\omega)\big) H_\beta(\omega)\right) = 0, \qquad \forall\beta\in\mathcal{I}. \tag{28}$$

Evaluating the Residual: In order to solve Eq. (28), we need to evaluate it. This requires the computation of high-dimensional integrals.

In [21] we have done this analytically by using the fact that the projection of a smooth function $\psi : \Omega^{(m)} \to \mathbb{R}$ onto a multivariate Hermite polynomial of unit norm may be computed as $\mathbf{E}\left(\psi(\omega)H_\alpha(\omega)\right) = (\alpha!)^{-1/2}\mathbf{E}\left(D^\alpha\psi(\omega)\right)$, where $\alpha! = \prod_{i=1}^m \alpha_i!$ and D^α is the partial derivative corresponding to the multi-index α, e.g. cf. [28]. But the analytic evaluation is difficult for general nonlinear problems and hence numerical techniques are required.

Any of the techniques from section 5 may be used, and as a representative example we evaluate the residual Eq. (28) for a simple case with only one spatial degree of freedom. It models a spring where the reaction force depends nonlinearly on the displacement $u \in \mathbb{R}$ and is given by the equation

$$f(u) = 0, \qquad f(u) := \kappa(u)u - 1, \quad u \in \mathbb{R}. \tag{29}$$

We choose $\kappa(u) = a + bu^2$, with two independent random variables a and b given as nonlinear transformations $a = a(\omega_1)$, $b = b(\omega_2)$ of independent standard Gaussian random variables ω_1, ω_2. By selecting the transformations analogous to Eq. (4), both a and b have $\beta(1/2, 1/2)$-distributions. The displacement $u = u(\omega)$ is now a random variable satisfying

$$0 = f(u,\omega) = \kappa(u(\omega),\omega)u(\omega) - 1. \tag{30}$$

The stochastic discretisation is performed by a polynomial chaos expansion of total degree 4 in ω_1 and ω_2, Galerkin conditions are applied, and the residual Eq. (28) is evaluated for a typical coefficient vector $\mathbf{u}$ by Monte Carlo integration and by quadrature.

Total polynomial Degree $\lvert\beta\rvert$ of H_β	Standard-deviation σ of $r_\beta(\omega)$	Monte Carlo $Z = 10^6$ Error $\cdot 10^3$	Quadrature $Z = 36$ Error $\cdot 10^3$
0	0.26	0.5	≈ 0
1	0.27	0.2	0.008
2	0.61	1.2	≈ 0
3	0.77	1.5	0.07
4	2.29	4.5	≈ 0

Table 1: Evaluation of the residual for the nonlinear stochastic spring. We show the standard deviation of the residual $r_\beta(\omega) = f(\omega, \sum_\alpha u^\alpha H_\alpha(\omega))H_\beta(\omega)$ for selected β and the absolute errors for $\mathbf{E}\left(r_\beta\right)$ when using Monte Carlo integration and full Gauss-Hermite quadrature with partial polynomial exactness of order 11.

The standard deviation of the residual $r_\beta(\omega) := f(\omega, \sum_\alpha u^\alpha H_\alpha(\omega))H_\beta(\omega)$ grows with increasing $\lvert\beta\rvert$ as Table 6.1 shows. A reason for this may be that the orthogonal polynomials H_β oscillate strongly for large $\lvert\beta\rvert$, so that the nonlinear transformation of the oscillating ansatz $f(\omega, \sum_\alpha u^{(\alpha)} H_\alpha(\omega))$ combined with the multiplication by an oscillating function H_β results in a high variance of the integrand. As a consequence, even when a million Monte Carlo evaluations are used, a significant error for $\mathbf{E}\left(r_\beta(\omega)\right)$ remains in this example. In order to reduce the error in the fourth row below $1 \cdot 10^{-3}$, approximately 20 million evaluations would be required. The same qualitative behaviour arises in the numerical solution of the groundwater flow problem and of other SPDEs. This "naive" Monte Carlo method may of course be enhanced, e.g. by variance reduction techniques, but the principal problem remains the same.

For this two-dimensional example the errors obtained by quadrature are negligible for few evaluations—the residual is smooth in ω and hence well-suited for evaluation by quadrature. In higher stochastic dimensions and in the computations presented below we therefore evaluate the residual by Smolyak quadrature.

For the SPDE, the numerical evaluation of Eq. (28) in Z integration points requires Z evaluations of $\mathbf{r}(\omega) = \mathbf{f}\big(\omega, \sum_{\alpha \in \mathcal{I}} \mathbf{u}^{(\alpha)} H_\alpha(\omega)\big)$, and already existing FEM-software for the solution of the spatial problem may be utilised for this in a black-box fashion. Usually, each evaluation of $\mathbf{r}(\omega)$ for a given ω requires a numerical integration over the spatial region $R \subset \mathbb{R}^d$ of the SPDE.

The Coupled System: We solve the nonlinear system Eq. (28) by the BFGS method with line-searches, e.g. cf. [33, 10]. In every iteration a correction of the current block-vector iterate $\mathbf{u}_k$ is computed as

$$\begin{aligned} \mathbf{u}_{k+1} - \mathbf{u}_k &= -\mathbf{H}_k \mathbf{f}(\mathbf{u}_k), \\ \mathbf{H}_k &= \mathbf{H}_0 + \sum_{j=1}^{k} (r_j \mathbf{p}_j \mathbf{p}_j^T + s_j \mathbf{q}_j \mathbf{q}_j^T). \end{aligned}$$

The block-vectors $\mathbf{p}_j, \mathbf{q}_j$ and the scalars r_j, s_j are results of the previous iterations of the BFGS method, cf. [33, 10]. A preconditioner or initial $\mathbf{H}_0$ is necessary in order to obtain good convergence. We use a block-diagonal preconditioner, where each block in the diagonal is the Jacobian of the deterministic system obtained by replacing the stochastic fields by their mean values.

6.2 Direct Projection

The orthonormality of the H_α can be exploited to compute the solution by direct orthogonal projection. It may be observed that the coefficient $\mathbf{u}^{(\alpha)}$ can be expressed as

$$\mathbf{u}^{(\alpha)} = \mathbf{E}\left(\mathbf{u}(\omega) H_\alpha(\omega)\right), \tag{31}$$

which may evaluated directly by the methods from section 5. The numerical evaluation of the expectation is a sum over Z integration points, and at each integration point a different realisation of the system $\mathbf{f}(\omega, \mathbf{u}(\omega)) = 0$ has to be solved. The block vector $\mathbf{u}$ is hence obtained by solving many uncoupled problems. This method is sometimes called “non-intrusive SFEM” [14]; it is similar to the original Monte Carlo ideas, but in contrast to these, a response surface is obtained directly.

Below, we perform the integration by Smolyak quadrature—a comparison between Monte Carlo methods and Smolyak quadrature for evaluating Eq. (31) will be published elsewhere.

6.3 Numerical Experiments

For the groundwater-flow problem the solution was obtained by the Galerkin scheme discussed in section 6.1, and we choose a polynomial chaos of degree 2 in 6 independent Gaussian variables as ansatz (28 stochastic functions). A spatial discretisation in 170 degrees of freedom was performed, totalling $4,760$ nonlinear equations. The BFGS solver required 19 iterations, and as the first iterations required line-searches, the residual had to be evaluated 24 times. The residual was integrated by the 5-stage Smolyak quadrature S_5^6 in $Z = 1,820$ integration points. As the evaluation in each integration point requires one integration in the spatial dimension, $43,680$ spatial integrations were performed.

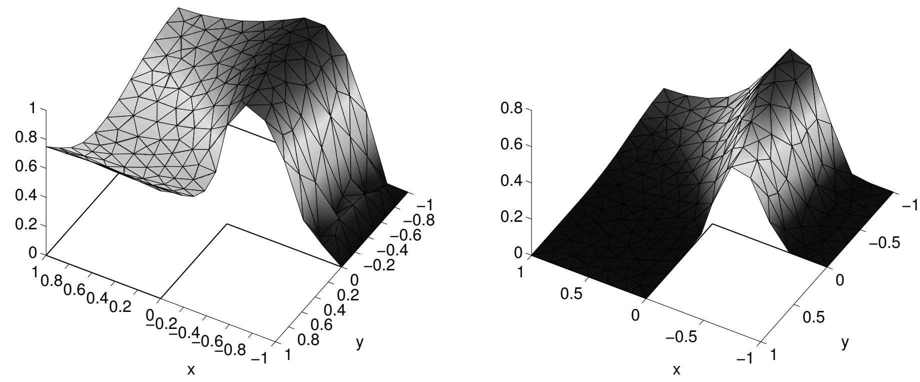
To assess the validity of the results, we compare the mean of the solution obtained by the Galerkin scheme to the results computed in section 6.3 by direct integration. The error is shown Fig. 4, and it is small in the “eye-ball” norm.

Additionally, a reference solution for the block-vector $\mathbf{u}$ was computed by orthogonal projection as discussed in section 6.2. The projection was evaluated by a 6-stage Smolyak-quadrature S_6^6 requiring $6,188$ integration points, and in each integration point the deterministic problem was solved for the material parameters associated with that point. In Fig. 4 we show one component of the reference solution and the error of the Galerkin approximation with respect to this component. Again, the error is small, and the same is true for the errors in the components not shown here.

Finally, the response surface obtained by the Galerkin method was used to compute the probability $p_{u_0}(x) = \text{Prob}\{u(x) > 3.25\}$. For this we used a naive Monte Carlo simulation with $100,000$ samples—realisations for the solution can be computed directly from the response surface $u_{galerk}(x, \omega)$, and hence this computation is much cheaper than a direct application of Monte Carlo-techniques. The result is shown in Fig. 4.

Error $\cdot 10^4$ of mean computed by the Galerkin scheme.

Prob$\{u(x) > 3.25\}$ from MC-simulation of response surface



$u_{direct}^{(\alpha)} = \mathbf{E}\,(u(\omega)H_\alpha)$ for $\alpha = (0,0,0,1,0,0)$.

Error $\cdot 10^4$ in $u_{galerk}^{(\alpha)}$ for the Galerkin scheme.

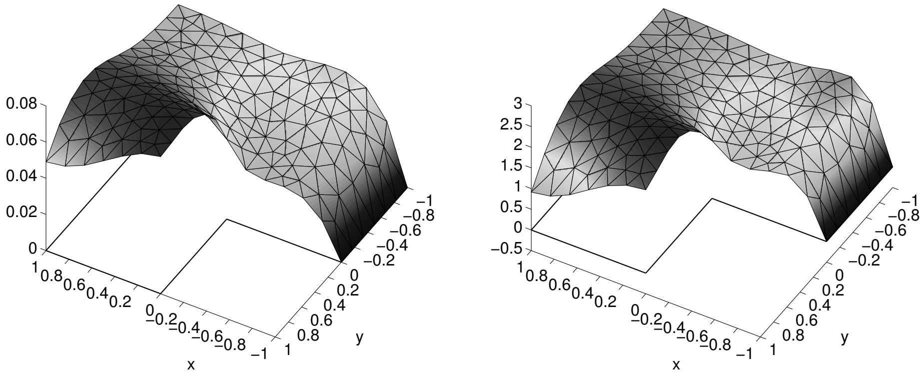


Figure 4: Solutions and errors obtained by the direct projection and by the Galerkin method

7 Conclusions

We have focused here on aspects of high-dimensional integration. In previous work we discuss the nonlinear solver [21, 22], aspects of non-Gaussian random fields, and the linear solvers used for preconditioning in more detail [32].

The first steps in solving stochastic problems are the spatial discretisation and an approximation in a finite number of independent random variables which may be interpreted as an approximation in a finite-dimensional probability space. Each of the numerical methods requires the computation of expectations. These are integrals in the probability space, and an important challenge is the efficient evaluation of such integrals for moderate to high stochastic dimensions.

We have computed the integrals by Monte Carlo methods and quadrature. Full quadrature is practical only for small stochastic dimensions. Smolyak quadrature can be used in higher dimensions, for example it has been applied to problems from finance in 360 stochastic dimensions in [41]. Monte Carlo methods are applicable independently of the number of dimensions, but their effort is high if a high accuracy is required or if the integrand has large variance.

We have solved stochastic boundary value problems by three different methods, each of which requires high-dimensional integration:

1. Computation of response statistics directly by integration (the original MC-method).
2. By a Galerkin method in a stochastic ansatz-space, solving the resulting large system of nonlinear equations by a quasi-Newton method.
3. Computation of the expansion by direct orthogonal projection.

More experiments and comparisons are necessary to appreciate which of these three methods is the most efficient in order to compute response statistics of SPDEs. These are under way and will be published elsewhere.

The experiments performed in the present work indicate that Smolyak quadrature may be an efficient alternative to Monte Carlo methods in stochastic mechanics, even though we have only compared them to naive Monte Carlo methods without variance reduction. Sparse quadrature certainly merits more attention, especially as it can be easily integrated in existing Monte Carlo codes and as software for sparse quadrature is available, e.g. cf. [40].

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