Numerical modeling of boundary value problems for differential equations with random coefficients

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Abstract. This paper deals with the numerical modeling of differential equations with coefficients in the form of random fields. Using the Karhunen-Loève expansion, we approximate these coefficients as a sum of independent random variables and real functions. This allows us to use the computational probabilistic analysis. In particular, we apply the technique of probabilistic extensions to construct the probability density functions of the processes under study. As a result, we present a comparison of our approach with Monte Carlo method in terms of the number of operations and demonstrate the results of numerical experiments for boundary value problems for differential equations of the elliptic type.

1. Introduction

Numerical modeling is a tool widely used to predict the behavior of complex systems, as well as to assess risks and make decisions. Such predictions are obtained by using mathematical models whose solutions describe a phenomenon of interest.

Uncertainty in the input data of the model [1] is the main reason for possible discrepancies between observations and approximate solutions. Input uncertainties of the model manifest in coefficients, forcing terms, boundary and initial condition data, geometry, etc. The solution of such problems is discussed in Stochastic Finite element methods [2].

In this paper, we focus on problems with random coefficients. For these purposes, we use Computational Probabilistic Analysis (CPA) [3]. The basis of the CPA is the numerical computation of the distribution laws for functions with random arguments and numerical operations on probability density functions. When sufficient data are available, we can aggregate them into probability distributions.

One approach to accounting for the random nature of the input data is Monte Carlo method [4]. With all its positive qualities, this method has a number of disadvantages. One of the most significant drawbacks is the low convergence rate.

It is important that many practical tasks with random inputs require faster methods. Among the methods for solving differential equations with random coefficients, it is necessary to distinguish the stochastic collocation method [2, 5], which in some cases can significantly reduce the number of solutions to the original problem as compared to Monte Carlo method.

In [6], a numerical approximation to the exact solution is sought for space of the tensor product of a finite element space and the span of the tensor product of polynomials of degree at most \( p \). In [7], the stochastic collocations method and the polynomial chaos expansion in the
probabilistic space of the input data is used to construct a numerical solution. The complexity of such algorithms is determined by the order of the polynomials and the number of harmonics in the Karhunen-Loève expansion.

Currently, the computational probabilistic analysis is used for problems under stochastic uncertainty [8]. For solving differential equations with random coefficients, such an analysis has a comparable number of operations with the stochastic collocation method, in addition, it allows one to construct the probability density functions of numerical solutions.

In the computational probabilistic analysis, piecewise polynomial functions to represent various probability density functions are used. Piecewise polynomial functions are determined by grids of dimension \( m \) and the values of the functions at the grid nodes. Histograms, frequency polygons, splines, etc. are examples of such functions [3].

The probability density functions of random variables \( x, y, z \) will be denoted by the bold type of \( x, y, z \). Let us identify through \( R \) a set of all probability density functions.

2. The probabilistic extension

Let \((x_1, x_2, \ldots, x_n)\) be a system of continuous random variables with the joint probability density function \( p(x_1, x_2, \ldots, x_n) \). Let a random variable \( z \) be the function

\[ z = f(x_1, x_2, \ldots, x_n), \]

where \( f : \mathbb{R}^n \to \mathbb{R} \).

**Definition 1** We say that the random function \( f : \mathbb{R}^n \to \mathbb{R} \) is a probabilistic continuation of the deterministic function \( f : \mathbb{R}^n \to \mathbb{R} \) on the set \( D \subset \mathbb{R}^n \), if \( f(x) = f(x) \) for all arguments \( x \in D \).

**Definition 2** The random function \( f : \mathbb{R}^n \to \mathbb{R} \) is called the probabilistic extension of the deterministic function \( f : \mathbb{R}^n \to \mathbb{R} \) on the set \( D \subset \mathbb{R}^n \), if

(i) it is probabilistic continuation of \( f \) on \( D \),

(ii) the probability density function \( f \) coincides with the probability density function \( z \) of the random variable \( z = f(x_1, x_2, \ldots, x_n) \), where \( (x_1, x_2, \ldots, x_n) \) is a system of continuous random variables with the joint probability density function \( p(x_1, x_2, \ldots, x_n) \).

Consequently, we can write down

\[ z = f(x_1, \ldots, x_n). \]

If at some point \( \xi \) it is necessary to directly indicate the value of the probability density function \( f \), we will use the notation

\[ z(\xi) = f(x_1, \ldots, x_n)(\xi). \]

**Theorem 2.1** ([8]) Let \( x_1, x_2, \ldots, x_n \) be random variables, \( f(x_1, x_2, \ldots, x_n) \) be a probabilistic extension of a function \( f(x_1, x_2, \ldots, x_n) \) and for all real \( t \) a function \( f(t, x_2, \ldots, x_n) \) be a probabilistic extension of the function \( f(t, x_2, \ldots, x_n) \). Then

\[ f(x_1, x_2, \ldots, x_n)(\xi) = \int_{\text{supp}(x_1)} x_1(t) f(t, x_2, \ldots, x_n)(\xi) dt. \] (1)

**Corollary 1** ([8]) Theorem 2.1 implies the possibility of recursive computations for the general form of probability extensions and, eventually, reduction to the calculation of the one-dimensional case.
The numerical calculation of integral (1) is represented as a quadrature
\[
\int x_1(t) f(t, x_2, \ldots, x_n)(\xi) dt \approx \sum_{l=1}^{m} \gamma_l x_1(t_l) f(t_l, x_2, \ldots, x_n)(\xi).
\]

Further, to calculate \( f(t_l, x_2, \ldots, x_n)(\xi) \), we will also use numerical quadratures, etc.

Let \( f(x_1, x_2, \ldots, x_n) \) be a rational function. We can obtain the probabilistic extension \( f \) by replacing (i) the real variables \( x_1, x_2, \ldots, x_n \) with the probability density functions \( x_1, x_2, \ldots, x_n \) and (ii) the real arithmetic operations with corresponding probabilistic operations. The result \( f \) is called a natural probabilistic extension [8].

**Theorem 2.2 ([8])** Let \( x_1, \ldots, x_n \) be independent random variables. If \( f(t_1, \ldots, t_n) \) is a rational expression where each variable \( t_i \) does not occur more often than once, then the natural probabilistic extension approximates a probabilistic extension.

Assuming \( f(x_1, x_2) = x_1 \ast x_2 \), where \( \ast \in \{+, -, \cdot, /\} \), we can obtain analytic formulas for determining the probability densities of the arithmetic operation results for random variables.

For example, to find the probability density \( x_1 + x_2 \) of the sum of two random variables \( x_1 + x_2 \), the following relation is used:
\[
(x_1 + x_2)(\xi) = \int_{-\infty}^{\infty} p(\xi - v, v) dv = \int_{-\infty}^{\infty} p(v, \xi - v) dv. \tag{2}
\]

To find the probability density of \( x_1/x_2 \) the following formula is used
\[
(x_1/x_2)(\xi) = \int_{0}^{\infty} v p(\xi v, v) dv - \int_{-\infty}^{0} v p(v, \xi v) dv. \tag{3}
\]

The probability density function for the product \( x_1 x_2 \) of two random variables \( x_1, x_2 \) is determined by the relation
\[
(x_1 x_2)(\xi) = \int_{0}^{\infty} (1/v) p(\xi/v, v) dv - \int_{-\infty}^{0} (1/v) p(v, \xi/v) dv. \tag{4}
\]

The commutativity and associativity of arithmetic operations of addition and multiplication directly follow from these formulas.

Consider an example
\[
z = a_1 x_1 + a_2 x_2 + \ldots + a_n x_n. \tag{5}
\]

If the random variables are independent, we can calculate the value of (5) using numerical probabilistic arithmetic sequentially calculating piecewise polynomial approximations. To calculate one addition, we need \( Cm^2 \) polynomial calculations. Accordingly, the total number of calculations will be equal to \( Cnm^2 \).

3. The partial differential equations with random coefficients
Let us consider the Dirichlet problem:
\[
Lu = f, \quad x \in D, \tag{6}
\]
\[
u(x) = 0, \quad x \in \partial D, \tag{7}
\]
where \( D \) is a bounded open domain in \( R^2 \), with the piecewise smooth boundary \( \partial D \),
\[
Lu = - \sum_{i=1}^{2} \frac{\partial}{\partial x_i} (a_i \frac{\partial}{\partial x_i} u).
\]
We assume that the coefficients $a_i \in C^1(D)$, $f \in C(D)$ and that 

$$a_i \geq c > 0, \forall x \in D.$$ 

The operator $L$ has the coefficients $a_i(x, \omega_a)$ with $x \in D$ and $\omega \in \Omega_a$, where $(\Omega_a, F_a, \mathbb{P}_a)$ denotes a complete probability space and $(\Omega_f, F_f, \mathbb{P}_f)$, $f(x, \omega_f)$, respectively.

### 4. The parametrization of random inputs

Next, we will use the Karhunen–Loève expansions to the approximated random field using the independent random variables [6, 7]. In [2], it is shown that, given the covariance function $\text{Cov}_a(x, x')$, the random field $a(x, \omega)$ can be expressed as an infinite sum

$$a(x, \omega) = \sum_{n=1}^{\infty} \sqrt{\lambda_n} A_n(x) a_n(\omega),$$

where $\{\lambda_n, A_n(x)\}_{n=1}^{\infty}$ denote a pairs of eigenvalues and functions of a given covariance function and $a_n(\omega)_{n=1}^{\infty}$ are independent random variables with zero mean and unit variance. Decomposition (8) is well known as the Karhunen–Loève (KL) expansions of the random field [2]. The KL expansions is also known as the proper orthogonal decomposition (POD) and the principal component analysis (PCA).

The truncated KL expansions make it possible to approximate random fields

$$a(x, \omega) \approx a(x, \omega)_N = \sum_{n=1}^{N} \sqrt{\lambda_n} A_n(x) a_n(\omega).$$

Moreover, the error monotonically decreases with an increase in the number of terms in the expansion.

### 5. The Galerkin approach

We will use the Galerkin approach to solve boundary value problems. Let $\mathcal{T}_h$ be a partition of $D$ comprised of elements $T$ and

$$\mathcal{D} = \cup_i T_i,$$

and $T_i \cap T_j = \emptyset$, or share a common edge, or share a common corner if $i \neq j$, where $\Omega_h = \{x_i\}_{i=1}^{N}$ are nodes of the partition, and $u_i^h = u_i^h(x_i), i = 1, \ldots, N$, are the values of some numerical solutions of problem (6)–(7).

If $\mathcal{T}_h$ is a triangulation, then the finite element space $S^h$ is defined by introducing a piecewise-polynomial basis on $\mathcal{T}_h$:

$$S^h = \{s(x)|s \in H^1(D) \cap H^1_0(D), s|_T \in \mathcal{P}^n, T \in \mathcal{T}_h\},$$

where $\mathcal{P}^n$ is a set of polynomials of degree $n$. In case of $\mathcal{T}_h$ being a rectangular partition, the subspace $S^n$ is defined by the piecewise Hermite polynomials of degree $n$ [9].

Following the Galerkin method, we will seek a solution in the weak formulation [9]

$$(Lu, v) = (f, v), \forall v \in H^1.$$ 

where

$$(u, v) = \int_D u(x)v(x)dx,$$
and $$||u||_{L^2} = \sqrt{\langle u, u \rangle}.$$ 

Let $$S^h \subset H^1$$ be a finite-dimensional space with the basis $$\varphi_i(x), i = 1, ..., N$$, the numerical solution $$u^h \in S^h$$ will be sought for $$N$$ in the form

$$u^h(x) = \sum_{i=1}^{N} u_i \varphi_i(x), \quad x \in D.$$ 

Then following the Galerkin approach

$$(Lu^h, v^h) = (f, v^h), \forall v^h \in S^h.$$  \hspace{1cm} (10)

Note that the accuracy of the numerical solution

$$||u - u^h||_{L^2} \leq Kh^{n+1}||u||_{W^{n+1}_2},$$

where $$K$$ is a constant independent of $$h$$, $$n$$ is the degree of polynomials.

6. General methods

Our objective is to construct the probability density function of the numerical solution $$u^h$$. Note that the solution $$u^h$$ of the problem (10) depends on the sets of random variables $$\{a_i, i = 1, \ldots, N_a\}, \{f_i, i = 1, \ldots, N_f\}, u^h = u^h(x, a_1, ..., a_{N_a}, f_1, ..., f_{N_f})$$. In what follows, we will assume that we know the probability density function $$\{a_i, i = 1, \ldots, N_a\}, \{f_i, i = 1, \ldots, N_f\}$$.

We start with a special case when the operator $$L$$ is linear and does not depend on the random coefficients We fix the set $$a^* = \{a_1, ..., a_{N_a}\}$$

$$L(a^*)u = \sum_{i=1}^{N_f} f_i F_i(x).$$

We numerically solve particular problems

$$L(a^*)u^i = F_i(x)$$

or

$$u^{hi} = (L^h(a^*))^{-1}F^{hi}.$$ 

Then, due to the construction of probabilistic extensions, the numerical solution will be the sum of particular solutions

$$u^h(x, a_1, ..., a_{N_a}, f_1, ..., f_{N_f}) = \sum_{i=1}^{N_f} f_i u^{hi}(x).$$

Thus, in the case of independent random constants $$f_i$$, we fall within the scope of the natural probabilistic extension to find $$u^h(x)$$, we can use probabilistic arithmetic.

Consider the case when the differential operator depends on the random constants $$a_i$$

$$L(a)u = f.$$ 

Let it be necessary to find a probabilistic extension of a numerical solution at some point $$u^h(x) = u^h(x, a_1, ..., a_{N_a})$$. For definiteness, assume that $$a_1, ..., a_k$$ are given by piecewise polynomial functions on the grids $$\omega_i = \{x_{i0}, x_{i1}, ..., x_{im}\}$$ of the dimension $$m$$, $$a_{ij} = a_i(x_j)$$. Then,
following the general approach for constructing probabilistic extensions, we solve $m^k$ for all the sets $a_{1,j}, a_{2,j}, ..., a_{k,j}$. Next, following Corollary 1, we construct the probabilistic extension $u^h(x, a_1, ..., a_k)$.

The final probabilistic extension can be represented as

$$u^h(x) = \int \int a_1(t_1) ... a_{N_a}(t_{N_a}) u^h(x, t_1, ..., t_{N_a}, f_1, ..., f_{N_f}) dt_1 ... dt_{N_a}. \quad (11)$$

Integral (11) will be calculated using numerical quadratures. The number of calculation operations (11) is proportional to $m^{N_a}$, the accuracy depends on the degree of piecewise polynomial functions and the orders $\alpha$ of convergence of quadrature formulas.

Let us estimate the number of operations required to achieve the accuracy $\varepsilon$. To achieve the precision $\varepsilon$ to Monte Carlo method needs the number of solutions to problem (10)

$$N_{MC} \sim \varepsilon^{-2}.$$ 

In the case of probability extensions, the accuracy is $\varepsilon \sim h^\alpha$, where $h$ is the grid step when using quadratures, $\alpha$ is the order of convergence of the quadrature formula. Thus, the number $m \sim 1/h$ is the number of nodes in the grid. The number of solutions to problem (10)

$$N_{PE} \sim \varepsilon^{-(N_a)/\alpha},$$

Note that it is desirable to match $\alpha$ with the accuracy of solutions of problem (10) and piecewise polynomial functions, so for the cubic splines $\alpha = 4$, for the quintic splines $\alpha = 6$.

Comparing the orders of magnitude of $N_{MC}$ and $N_{PE}$, one can see that the CPA is more effective than Monte Carlo method at

$$N_a \leq 2\alpha.$$

7. A numerical example

Consider the numerical solution of the boundary value problem with random coefficients

$$L(u) u = - \sum_{i=1}^{2} \frac{\partial}{\partial x_i} (a_i \frac{\partial}{\partial x_i} u) = f, \quad (x, y) \in D,$$

$$u = 0, x \in \partial D,$$

where $D = [0, 1] \times [0, 1]$, $f = 2\pi^2 \sin(\pi x) \sin(\pi y)$, $a_i$ are independent random constants, with supports $[0.85, 1.15]$, $a_i(t) = 10p((t-1.5)/10)$, where $p(t)$ is the Irwin-Hall distribution

$$p(x) = \begin{cases} x^2/2; & t \in [0, 1]; \\ -x^2 + 3x - 3/2; & t \in [1, 2]; \\ (x^2 - 6x + 9)/2; & t \in [2, 3]. \end{cases}$$

To construct a probabilistic extension of the solution $u^h(x, y, a_1, a_2)$, in the domain of the supports $a_i$, we construct uniform grids $\omega_i = \{0.85, 0.925, 1.0, 1.075, 1.15\}$ and numerically solve 25 problems $a_1 \in \omega_1$, $a_2 \in \omega_2$. We will use the FEM with linear elements on uniform grids $D^h = \{x_i = i/10| i = 0, ..., 10\} \times \{y_i = i/10| i = 0, ..., 10\}$. Figure 1 shows the calculation of $u^h(x, y, a_1, a_2)$. From the values $(a_1, a_2, u^h(x, y, a_1, a_2))$ on the grid $\omega_1 \times \omega_2$ we construct a piecewise linear surface $s(t_1, t_2)$, shown in blue lines. Then, the value $u^h(x, y, a_1, a_2)(z)$ is calculated using the integral

$$u^h(x, y, a_1, a_2)(z) = \int_{\Gamma_z} \frac{a_1(t)a_2(z)}{|s'_z(t, z)|} dt, \quad (12)$$
where $\Gamma_z$ is the curve of intersection of the surface $s(t_1, t_2)$ and the plane $z = 1.0083$. Thus, $\xi(t_1)$ are the roots of the equation $z = s(t_1, \xi(t_1))$. The curve $\Gamma_z$ is shown in red.

By calculating the integrals (12) for different $z \in [0.8768, 1.1862]$ it is possible to construct an approximation of the probability density function. In figure 2 shows a piecewise polynomial approximation of the probability density function $u^h(x_5, y_5, a_1, a_2)$.

8. Conclusion
In this paper, we use the computational probabilistic analysis to solve elliptic partial differential equations with random coefficients. This method has the following advantages: it leads to unrelated deterministic problems, the method is universal and sufficiently accurate, it allows one to construct the probability density functions of numerical solutions. The use of probabilistic extensions generally suffers from the curse of dimensionality. Therefore, this method is effective only for a small number of random variables.
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