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Contents

Stable positive Monte Carlo finite difference techniques for random parabolic partial differential equations

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1 Introduction

Integral Transform technique is a powerful method for solving random partial differential equations (RPDEs) in unbounded domains [1], but an alternative is needed in the case of bounded domains. In the deterministic case, the finite difference methods are the most used because they are easy to implement and efficient enough. But these methods extended to the random scenario have the drawback coming from the complexity of the computation of the statistical moments (the expectation and the standard deviation) arising from the operational random calculus throughout the iterative levels of the discretization steps and the necessity to store the information of all the previous levels of the iteration process [2, 3].

In this work we study the following RPDE of parabolic type often encountered in heat and mass transfer theory in heterogeneous media

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[p(x)\,\frac{\partial u(x,t)}{\partial x}\right] - q(x)\;u(x,t), \quad 0<x<1, \quad t>0\,, \tag{1}$$

$$u(0,t) = g_1(t), \quad t>0, \tag{2}$$

$$u(1,t) = g_2(t), \quad t>0, \tag{3}$$

$$u(x,0) = f(x), \quad 0\le x\le 1\,. \tag{4}$$

In this model (1)–(4) we will assume, without loss of generality, that involved s.p.'s: $p(x)$ and $q(x)$ in the coefficients, $f(x)$ in the initial condition and $g_i(t)$, $i=1,2$, in the boundary conditions, have one degree of randomness (finite degree of randomness [4]), i.e. they have the form

$$\left.\begin{array}{r} h(s)=F(s,A)\,, \\ A \text{ a r.v.}\,,\ F \text{ a differentiable real function of the variable } s. \end{array}\right\} \tag{5}$$

Then the s.p. $h(s)$ has sample differentiable trajectories, i.e, for a fixed event $\omega\in\Omega$, (Ω sample space) the real function $h(s,\omega)=F(s,A(\omega))$ is a differentiable function of the real

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variable s. In addition we assume that all the input data $p(x)$, $q(x)$, $f(x)$ and $g_i(t)$, $i = 1, 2$ are mean square continuous s.p.'s in variables x and t, respectively, $p(x)$ is also a mean square differentiable s.p. and the sample realizations of the random inputs $p(x)$, $q(x)$, $g_i(t)$, $i = 1, 2$ and $f(x)$ satisfy the following conditions:

$$0 < a_1 \leq p(x,\omega) \leq a_2 < +\infty\,, \quad x \in [0,1]\,, \text{ for almost every (a.e.) } \omega \in \Omega\,, \tag{6}$$

$$\frac{|p'(x,\omega)|}{p(x,\omega)} \leq b < +\infty\,, \qquad x \in [0,1]\,, \text{ for a.e. } \omega \in \Omega\,, \tag{7}$$

$$q_{\min} \leq q(x,\omega) \leq q_{\max}\,, \qquad x \in [0,1]\,, \text{ for a.e. } \omega \in \Omega\,, \tag{8}$$

$$g_i(t,\omega) \geq 0\,,\ i = 1,2, \qquad t > 0\,, \text{ for a.e. } \omega \in \Omega\,, \tag{9}$$

$$0 \leq f(x,\omega) \leq f_{\max}\,, \qquad x \in [0,1]\,, \text{ for a.e. } \omega \in \Omega\,, \tag{10}$$

where $p'(x)$ denotes the mean square derivative of $p(x)$.

2 Random finite difference scheme, numerical strategy and simulations

We develop a **stable** and **consistent** numerical random finite difference scheme preserving **positivity** of the solution stochastic process together with Monte Carlo technique that provides a useful tool to obtain accurate values of the expectation and the standard deviation of the approximating process even for large values of the time variable.

2.1 Random finite difference scheme

Let us consider the uniform partition of the spatial interval $[0, 1]$, of the form $x_i = ih$, $0 \leq i \leq M$, with $Mh = 1$. For a fixed time horizon, T, we consider $N + 1$ time levels $t^n = nk$, $0 \leq n \leq N$ with $Nk = T$. The numerical approximation of the solution s.p. of the random problem (1)–(4) is denoted by u_i^n, i.e. $u_i^n \approx u(x_i, t^n)$, $0 \leq i \leq M$, $0 \leq n \leq N$. Now, by using a forward first-order approximation of the time partial derivative and centred second-order approximations for the spatial partial derivatives in (1) one gets the following random numerical scheme for the spatial internal mesh points

$$\frac{u_i^{n+1} - u_i^n}{k} = p_i\,\frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{h^2} + p_i'\,\frac{u_{i+1}^n - u_{i-1}^n}{2h} - q_i\,u_i^n\,, 1 \leq i \leq M-1,\ 0 \leq n \leq N-1\,, \tag{11}$$

where $p_i = p(x_i)$, $p'_i = p'(x_i)$ and $q_i = q(x_i)$. The resulting random discretized problem (1)–(4) can be rewritten in the following form

$$\left.\begin{array}{r} u_i^{n+1} = \dfrac{k}{h^2}\quad p_i - \dfrac{h}{2}p'_i\right)\, u_{i-1}^n + \left(1 - k\, q_i - \dfrac{2k}{h^2}p_i\right) u_i^n + \dfrac{k}{h^2}\quad p_i + \dfrac{h}{2}p'_i\right) u_{i+1}^n\,, \\ 1 \le i \le M-1\,,\ 1 \le n \le N-1\,, \\ u_0^n = g_1^n\,,\quad u_M^n = g_2^n\,,\quad 1 \le n \le N\,, \\ u_i^0 = f_i\,,\quad 0 \le i \le M\,, \end{array}\right\} \tag{12}$$

where $g_1^n = g_1(t^n)$, $g_2^n = g_2(t^n)$, and $f_i = f(x_i)$. We introduce the following definitions.

Definition 1 *A random numerical scheme is said to be $\|\cdot\|_p$-stable in the fixed station sense in the domain $[0,1]\times[0,T]$, if for every partition with $k = \Delta t$, $h = \Delta x$ such that $N\,k = T$ and $M\,h = 1$,*

$$\|u_i^n\|_p \le C\,,\quad 0 \le i \le M,\quad 0 \le n \le N\,, \tag{13}$$

where C is independent of the step-sizes h, k and the time level n.

Definition 2 *Let us consider a random finite difference scheme $F(u_i^n) = 0$ for a RPDE $\mathcal{L}(u) = 0$ and let the local truncation error $T_i^n(U(\omega))$ for a fixed event $\omega \in \Omega$ be defined by*

$$T_i^n(U(\omega)) = F(U_i^n(\omega)) - \mathcal{L}(U_i^n(\omega)),$$

where $U_i^n(\omega)$ denotes the theoretical solution of $\mathcal{L}(u)(\omega) = 0$ evaluated at (x_i, t^n). We call $T_i^n(U)$ by

$$\|T_i^n(U)\|_p = \left(\mathbb{E}\left[|T_i^n(U)|^p\right]\right)^{1/p} = \left(\int_\Omega |T_i^n(U(\omega))|^p f_{T_i^n(U)}(\omega)\ d\omega\right)^{1/p}.$$

With previous notation, the random finite difference scheme $F(u_i^n) = 0$ is said to be $\|\cdot\|_p$-consistent with the RPDE $\mathcal{L}(u) = 0$ if

$$\|T_i^n(U)\|_p \to 0 \ \ as\ \ h = \triangle x \to 0,\ k = \triangle t \to 0.$$

Theorem 1 *With the previous notation under conditions*

$$h \le \frac{2}{b}\,,\quad k \le \frac{h^2}{2a_2}\,,\ (If\ q_{max} < 0)\,,\quad k \le \frac{h^2}{2a_2 + h^2 q_{max}}\,,\ (If\ q_{max} \ge 0)\,, \tag{14}$$

on the discretized step-sizes $h = \Delta x$ and $k = \Delta t$, the random numerical solution s.p. $\{u_i^n\}$ of the random finite difference scheme (12) for the random partial differential model (1)–(10) is positive for $0 \le i \le M$ at each time-level $0 \le n \le N$ with $T = kN$. Furthermore the random finite difference scheme (12) is $\|\cdot\|_p$-stable in the fixed station sense taking the value

$$C = \alpha(T)\, G(T)\,,$$

where

$$\begin{array}{rcl} G(T) & = & \max_{0\le t\le T}\left\{g_{1,max}(T),\ g_{2,max}(T),\ f_{max}\right\} \\ g_{i,max}(T) & = & \max_{0\le t\le T}\{g_i(t,\omega)\,,\quad for\ a.e.\ \omega\in\Omega\}\,,\ i = 1,2\,. \end{array} \tag{15}$$

and

$$\alpha(T) = \left\{\begin{array}{ll} 1 & if\ \ q_{min} \ge 0\,, \\ e^{T|q_{min}|} & if\ \ q_{min} < 0\,. \end{array}\right. \tag{16}$$

2.2 Numerical strategy and simulations

From a computational point of view, the handling of the random scheme (12) in a direct way makes unavailable the computation of approximations beyond a few first temporal levels. This is because, throughout the iterative temporal levels, $n = 1, \cdots, N$, it is necessary to store the symbolic expressions of all the previous levels of the iteration process collecting big and complex random expressions with which the expectation and the standard deviation must be computed. Furthermore, although the random expressions can be stored it does not guarantee that the two first statistical moments could be computed in a numerical way. For this reason we propose to use the random numerical scheme (12) together with the Monte Carlo technique avoiding the described computational drawbacks. The procedure is as follows: to take a number K of realizations of the random data involved in the random PDE (1)–(4) according to their probability distributions; to compute the numerical solution, $u_i^n(\omega_j)$, $j = 1, \cdots, K$, of the sampling deterministic difference schemes of (12); to obtain the mean and the standard deviation of these K numerical solutions evaluated in the mesh points $i = 1, \cdots, M-1$, at the last time-level N, denoted respectively by

$$\mathbb{E}_{\mathrm{MC}}^K[u_i^N] = \mu\left(u_i^N(\omega_1), u_i^N(\omega_2), \cdots, u_i^N(\omega_K)\right) . \tag{17}$$

$$\sqrt{\mathrm{Var}_{\mathrm{MC}}^K[u_i^N]} = \sigma\left(u_i^N(\omega_1), u_i^N(\omega_2), \cdots, u_i^N(\omega_K)\right) . \tag{18}$$

Example 1 *We consider the problem* (1)–(4) *with the random data*

$$p(x) = a\, e^{-x}\,,\ q(x) = -c\,,\ g_1(t) = e^{c\,t}\left(\frac{1}{2} + a\, t\right)\,,\ g_2(t) = e^{c\,t}\left(\frac{e^2}{2} + a\, e\, t\right)\,,\ f(x) = \frac{e^{2x}}{2}\,, \tag{19}$$

where the r.v. a follows a Gaussian distribution of mean $\mu = 0.5$ and standard deviation $\sigma = 0.1$ truncated on the interval $[0.4, 0.6]$, and the r.v. $c > 0$ has a beta distribution of parameters $(2; 4)$ truncated on the interval $[0.45; 0.55]$. We will assume that a and c are independent r.v.'s. Note all random input data $p(x)$, $q(x)$, $g_1(t)$, $g_2(t)$ and $f(x)$ are m.s. continuous and $p(x)$ is m.s. differentiable too. In addition, conditions (6)–(10) *are satisfied with*

$$a_1 = 0.4\, e^{-1}\,,\quad a_2 = 0.6\, e^{0}\,,\quad -0.55 \leq q(x,\omega) \leq -0.45\,,\ \omega \in \Omega\,,\quad 0 \leq f(x,\omega) \leq 3.69453\,.$$

From [5, Sec. 3.8.5.] the exact solution of problem (1)–(4), (19) *when both parameters a and c are deterministic, is given by*

$$u(x,t) = e^{c\,t}\left(a e^x t + \frac{e^{2x}}{2}\right)\,. \tag{20}$$

In our context, both a and c are r.v.'s, and expression (20) *must be interpreted as a s.p. Then, using the independence between r.v.'s a and c, the expectation and the standard deviation of s.p.* (20) *can be computed. Numerical convergence of the expectation and the standard deviation of the approximate solution s.p. using Monte Carlo (MC) technique is illustrated in the following way. With a fixed time $T = 1$, we have chosen both the spatial and temporal step-sizes $h = 0.0125$ and $k = 0.0001$, respectively, according to the stability conditions* (14) *and we have varied the number of realizations, K, of the r.v.'s a and c involved in the random problem* (1)–(4), (19). *Then, at the temporal level $N = 10000$ where the time $T = Nk = 1$ is achieved, we have*

computed the expectation (mean), $\mathbb{E}^K_{MC}[u_i^N]$ (17)*, and the standard deviation,* $\sqrt{\mathrm{Var}^K_{MC}[u_i^N]}$ (18)*, of the* K*-deterministic solutions,* u_i^N*, obtained to solve the* K*-deterministic difference schemes from* (12)*. Table 1 collects the RMSEs (Root Mean Square Errors) computed using the following expressions*

$$\mathrm{RMSE}\left[\mathbb{E}^K_{MC}[u_i^N]\right] = \sqrt{\frac{1}{M-1}\sum_{i=1}^{M-1}\left(\mathbb{E}[u(x_i,t^N)] - \mathbb{E}^K_{MC}[u_i^N]\,\right)^2}, \tag{21}$$

$$\mathrm{RMSE}\left[\sqrt{\mathrm{Var}^K_{MC}[u_i^N]}\right] = \sqrt{\frac{1}{M-1}\sum_{i=1}^{M-1}\left(\sqrt{\mathrm{Var}[u(x_i,t^N)]} - \sqrt{\mathrm{Var}^K_{MC}[u_i^N]}\right)^2}, \tag{22}$$

where $\mathbb{E}[u(x_i,t^N)]$ *and* $\sqrt{\mathrm{Var}[u(x_i,t^N)]}$ *denote the expectation and standard deviation of the exact solution s.p.* (20)*, respectively. It is observed the good behaviour of both approximations*

K	RMSE $\left[\mathbb{E}^K_{\mathrm{MC}}[u_i^N]\right]$	RMSE $\left[\sqrt{\mathrm{Var}^K_{\mathrm{MC}}[u_i^N]}\right]$	CPU,s $\left[\mathbb{E}^K_{\mathrm{MC}}/\sqrt{\mathrm{Var}^K_{\mathrm{MC}}}\right]$
50	$1.45604e-02$	$1.32856e-02$	630.516
200	$1.11710e-02$	$1.84435e-03$	982.375
800	$1.08512e-02$	$1.06139e-03$	2052.330
3200	$4.20138e-03$	$6.01374e-03$	6209.480
12800	$2.07183e-04$	$1.69504e-03$	22600.100

Table 1: RMSEs and CPU time (in seconds) spent to compute the approximations to the expectation (mean), $\mathbb{E}^K_{\mathrm{MC}}$, and the standard deviation, $\sqrt{\mathrm{Var}^K_{\mathrm{MC}}}$ in the level time $N = 10000$, for $K \in \{50, 200, 800, 3200, 12800\}$ MC realizations, on the spatial domain $[0+h, 1-h]$, $x_i = ih$, $1 \leq i \leq 79$, $h = 0.0125$.

the expectation and the standard deviation as the number K *of simulations increases. That is, the accuracy of the approximations to both statistical moments increases when the number of MC simulations is growing. In this sense, Figure 1 and Figure 2 reflects the improvement of the approximations considering the study of the relative errors. Computations have been carried out by Mathematica© software version 12.0.0.0, for Windows 10Pro (64-bit) AMD Ryzen Threadripper 2990WX, 3.00 GHz 32 kernels.*

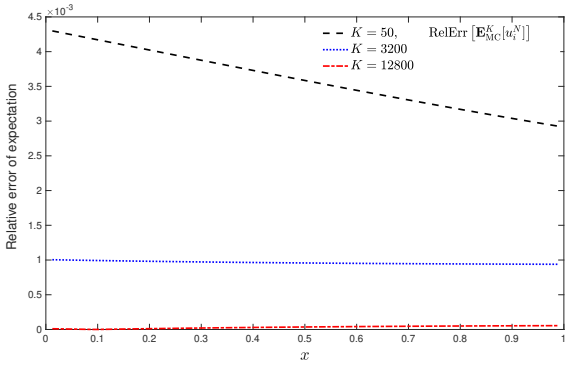

Figure 1: Relative errors of the approximations to the expectation (mean), $\mathbb{E}^K_{\mathrm{MC}}[u_i^N]$.

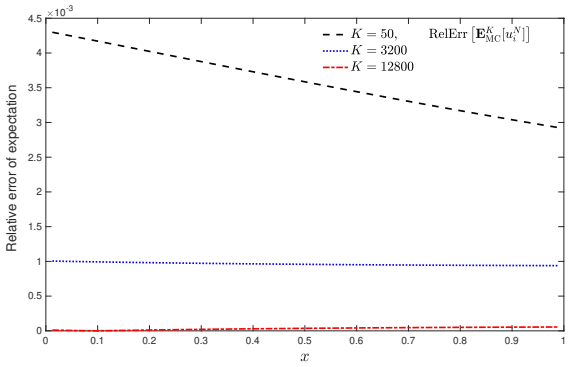

Figure 2: Relative errors of the approximations to the standard deviation, $\sqrt{\mathrm{Var}^K_{\mathrm{MC}}[u_i^N]}$.

3 Conclusions and future work

The random scheme (12) developed is consistent, conditionally stable and positive. This random scheme combined with the MC method solves the computational problem of methods random iterations as it avoids collapsing in the calculation of symbolic expressions to few temporary steps. In this way, it is possible the computation of the mean and the standard deviation. The convergence strategy used is to choose the discretization step-size h and k, verifying the stability conditions, and increase the number of MC realizations until that the errors no longer change substantially. This method can even be applied to non-linear or two-dimensional problems.

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