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Constructing reliable approximations of the probability density function to the random heat PDE via a finite difference scheme

J. Calatayud[a], J.-C. Cortés[a,*], J.A. Díaz[b], M. Jornet[a]

[a] *Instituto Universitario de Matemática Multidisciplinar, Universitat Politècnica de València, Camí de Vera s/n, 46022, Valencia, Spain*
[b] *Departamento de Óptica, Facultad de Ciencias, Universidad de Granada, Granada, Spain*

Abstract

We study the random heat partial differential equation on a bounded domain assuming that the diffusion coefficient and the boundary conditions are random variables, and the initial condition is a stochastic process. Under general conditions, this stochastic system possesses a unique solution stochastic process in the almost sure and mean square senses. To quantify the uncertainty for this solution process, the computation of the probability density function is a major goal. By using a random finite difference scheme, we approximate the stochastic solution at each point by a sequence of random variables, whose probability density functions are computable, i.e., we construct a sequence of approximating density functions. We include numerical experiments to illustrate the applicability of our method.

Keywords: Uncertainty quantification, Random heat partial differential equation, Finite difference scheme, Probability density function, Numerical method.
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1. Introduction and motivation

Heat transfer modelling using partial differential equations has been extensively studied in the literature for many years, and it is currently an active field under research [1, 2, 3, 4, 5]. Information such as the diffusion coefficient, the initial distribution of temperature, etc., appears in the mathematical formulation of this class of problems. In practice, this key information needs to be established via measurements, which often involve uncertainties from measurement errors, material impurities, etc. These facts have motivated the mathematical modelling of heat transfer by using random partial differential equations. These differential equations are those in which the input data (initial and boundary conditions, forcing term and coefficients) are conveniently treated as random variables and stochastic processes. As a consequence, the solution to a random partial differential equation is not a classical function but a stochastic process. Apart from exact

*Corresponding author
Email addresses: jucagre@doctor.upv.es (J. Calatayud), jccortes@imm.upv.es (J.-C. Cortés), jadiaz@ugr.es (J.A. Díaz), marjorsa@doctor.upv.es (M. Jornet)

or approximate representations of the stochastic solution, say $u(x,t)$, an important goal in dealing with random partial differential equations is to compute its main statistical properties, such as the mean function, $\mu_u(x,t) = \mathbb{E}[u(x,t)]$, and the variance function, $\mathbb{V}[u(x,t)] = \mathbb{E}[u(x,t)^2] - \mu_u(x,t)^2$. However, a major objective is to compute the probability density function, $f_{u(x,t)}(u)$, of the stochastic solution for every (x,t) fixed, since from it one can calculate, not only the mean and the variance functions, but also higher one-dimensional statistical moments, $\mathbb{E}[u(x,t)^k]$, $k = 1, 2, \ldots$, provided they exist. Indeed, observe that

$$\mathbb{E}[u(x,t)^k] = \int_{\mathbb{R}} u^k f_{u(x,t)}(u)\,\mathrm{d}u, \quad k = 1, 2, \ldots$$

A powerful approach to deal with random partial differential equations is the so-called L^p-random calculus, and in particular, the mean square random calculus corresponding to $p = 2$, [6]. Convergence in L^2-random calculus is usually referred to as mean square (hereafter m.s.) convergence, [6, Ch. 4]. This approach has two key properties. The first one is the formal representation of the solution stochastic process, which coincides with the one of the deterministic case, i.e., when the random inputs are deterministic quantities. This fact allows retaining both the physical interpretation and the deterministic results via the random solution. The second one is a distinctive property of m.s. convergence compared to other types of stochastic convergences (almost surely, hereafter a.s., in probability, and in distribution), which is crucial to compute reliable approximations of the mean and the variance of the solution $u(x,t)$ (see [6, Th. 4.3.1]). If $u^M(x,t)$ is a sequence of random variables which is m.s. convergent to $u(x,t)$ as $M \to \infty$ for (x,t) fixed, i.e., $u^M(x,t) \xrightarrow[M\to\infty]{\text{m.s.}} u(x,t)$, then

$$\mathbb{E}[u^M(x,t)] \xrightarrow[M\to\infty]{} \mathbb{E}[u(x,t)] \quad \text{and} \quad \mathbb{V}[u^M(x,t)] \xrightarrow[M\to\infty]{} \mathbb{V}[u(x,t)].$$

In the context of heat transfer modelling via random partial differential equations, most of the contributions have focused on the construction of approximations of the solution stochastic process, and in the computation of its mean and variance as well, as we describe and reference in what follows. The calculation of the statistical moments is performed by taking advantage of the aforementioned key property of the m.s. convergence. Often, the methods and techniques that have been proposed to deal with random heat equations are analytic or numerical extensions of their deterministic counterparts. In the former case, we point out the following contributions [7, 8, 9, 10], where some important analytical techniques, such as Fourier series, homogeniza-tion method, polynomial chaos and Chebyshev wavelets together with Galerkin methods are, respectively, extended to the random setting to solve different formulations of the heat equation with uncertainties. In the latter case, i.e., using a numerical approach, the random heat equation has been extensively studied via random convergent numerical schemes [11, 12, 13, 14, 15], by applying stochastic finite elements [16, 17].

The computation of exact or approximate probability density function to random partial differential equations has been tackled only in few contributions [18, 19, 20], since the majority of the studies are addressed to construct approximations of the mean and the variance of the solution stochastic process.

A popular statistical technique to estimate the statistics of the stochastic solution is the Monte Carlo simulation [21]. It is easy to implement and robust. The mean square convergence rate of the sample mean towards the exact mean is proportional to $1/m$, where m is the number of realizations. This is a straightforward consequence of the central limit theorem. For nonparametric density estimations, a kernel density is constructed from a finite data sample. The method is

closely related to histograms. The properties of the density estimation depend on the kernel and the bandwidth chosen. Under certain smoothness of the target density function and optimality of the bandwidth selected, the mean square convergence rate of the kernel density estimate is $1/m^p$, $0 < p < 1$, [22, 23, 24]. This rate is slower than the typical $1/m$ convergence rate of parametric methods. For instance, according to [22], if the target density function is γ-H¨older continuous, $\gamma \in (0, 1]$, then the pointwise convergence rate is $O(1/m^p)$, where $p = \gamma/(2\gamma + 1) \leq 1/3$.

In the present work, we will deal with the following heat partial differential equation on the spatial domain $[0, 1]$:

$$\begin{cases} u_t = \alpha u_{xx}, \quad x \in (0,1),\ t \in (0,T), \\ u(0,t) = A, \quad u(1,t) = B,\ t \in [0,T], \\ u(x,0) = \phi(x), \quad x \in [0,1]. \end{cases} \tag{1}$$

This is a first step of our research on approximating the density function of the heat equation. Other interesting cases remain pending for the future, for example the infinite domain case. At this point, we must point out that to the best of our knowledge the analysis of the random heat equation on infinite/semi-infinite domains have been carried out by some of the co-authors in previous contributions using an analytic approach via random integral transforms [25, 26]. However, it is very important to point out that in the above-mentioned contributions the goal has been to approximate the first statistical moments (mean and variance) of the solution rather than the first probability density function. In this new paper, we go further in two directions, first we provide reliable approximations for the first probability density function of the solution stochastic process, which is a more ambitious and desirable goal, and second, we construct random numerical schemes to compute the first probability density function rather than using an analytic approach. This latter point is completely new in dealing with the approximation of the first probability density function to the random heat equation.

For the sake of completeness, we recall that in a deterministic setting, the diffusion coefficient $\alpha > 0$, and the boundary conditions A and B are constants, and the initial condition $\phi(x)$ is a deterministic function. Then, its solution is a bivariate function $u(x, t)$. Sufficient conditions for the existence of a smooth classical solution $u(x, t)$ are given in the following result.

Proposition 1.1. *([27, Th. 3.1]) If ϕ is continuous on $[0, 1]$, piecewise C^1 on $[0, 1]$, $\phi(0) = A$ and $\phi(1) = B$, then $u(x,t)$ is continuous on $[0, 1] \times [0, \infty)$, is of class $C^{2,1}$ on $(0, 1) \times (0, \infty)$ and is a classical solution to (1).*

Moreover, under the conditions of Proposition 1.1, the solution to (1) is given by

$$u(x,t) = v(x,t) + xB + (1-x)A,$$

where

$$v(x,t) = \sum_{k=1}^{\infty} A_k e^{-k^2\pi^2\alpha t} \sin(k\pi x),$$

$$A_k = 2\int_0^1 \psi(y)\sin(k\pi y)\,dy, \quad \psi(y) = \phi(y) - yB - (1-y)A$$

(see [27, expressions (2.2) in p. 3, (2.3) in p.4 and (3.2)–(3.4) in p. 9]). This solution results from applying the classical method of separation of variables to (1) with homogeneous boundary conditions (case $A = B = 0$), and then doing a change of variables to adapt to the case $A \neq 0$ or $B \neq 0$.

Motivated by the arguments exhibited at the beginning of this section, hereinafter we will consider the randomization of the above heat diffusion problem (1). We then assume that the values of the input data depend on an experiment ω. The set of all experiments, called sample space and denoted by Ω, is equipped with a σ-algebra of events $\mathcal{F}$, and a probability measure $\mathbb{P}$ to form a complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$. The diffusion coefficient $\alpha = \alpha(\omega)$ and the boundary conditions $A = A(\omega)$ and $B = B(\omega)$ are random variables, and the initial condition $\phi(x) = \phi(x)(\omega)$ is assumed to be a stochastic process, being all of them defined in the probability space $(\Omega, \mathcal{F}, \mathbb{P})$. The term u is a stochastic process $u(x,t) = u(x,t)(\omega)$ that solves the random heat diffusion problem (1) in some probabilistic sense. Theorem 3.2 in ref. [27] proves that under square integrability of ϕ, A and B, there is a unique stochastic solution in the a.s. and m.s. senses [6]. Notice that, in this probabilistic scenario, we do not require $\phi(0) = A$ and $\phi(1) = B$.

Proposition 1.2. *([27, Th. 3.2]) The following statements hold:*

i) Almost sure (a.s.) solution: Suppose that $\phi \in \mathrm{L}^2([0,1] \times \Omega)$ and $A, B \in \mathrm{L}^2(\Omega)$. Then

$$u_t(x,t)(\omega) = \alpha(\omega)\, u_{xx}(x,t)(\omega)$$

a.s. for $x \in (0,1)$ and $t > 0$, where the derivatives are understood in the classical sense; $u(0,t)(\omega) = A(\omega)$ and $u(1,t)(\omega) = B(\omega)$ a.s. for $t \geq 0$; and $u(x,0)(\omega) = \phi(x)(\omega)$ a.s. for a.e. $x \in [0,1]$. Moreover, the process $u(x,t)(\omega)$ satisfying these conditions is unique.

ii) Mean square (m.s.) solution: Suppose that $\phi \in \mathrm{L}^2([0,1] \times \Omega)$, $A, B \in \mathrm{L}^2(\Omega)$ and $0 < a \leq \alpha(\omega) \leq b$, a.e. $\omega \in \Omega$, for certain $a, b \in \mathbb{R}$. Then

$$u_t(x,t)(\omega) = \alpha(\omega)\, u_{xx}(x,t)(\omega)$$

a.s. for $x \in (0,1)$ and $t > 0$, where the derivatives are understood in the m.s. sense; $u(0,t)(\omega) = A(\omega)$ and $u(1,t)(\omega) = B(\omega)$ a.s. for $t \geq 0$; and $u(x,0)(\omega) = \phi(x)(\omega)$ a.s. for a.e. $x \in [0,1]$. Moreover, the process $u(x,t)(\omega)$ satisfying these conditions is unique.

In addition, under the assumptions of Proposition 1.2, the solution to (1) is given by

$$u(x,t)(\omega) = v(x,t)(\omega) + xB(\omega) + (1-x)A(\omega), \tag{2}$$

where

$$v(x,t)(\omega) = \sum_{k=1}^{\infty} A_k(\omega) \mathrm{e}^{-k^2\pi^2\alpha(\omega)t} \sin(k\pi x), \tag{3}$$

$$A_k(\omega) = 2\int_0^1 \psi(y)(\omega) \sin(k\pi y)\, \mathrm{d}y, \quad \psi(y)(\omega) = \phi(y)(\omega) - yB(\omega) - (1-y)A(\omega). \tag{4}$$

The integral that defines $A_k(\omega)$ is understood in the sample path sense [6, Appendix A]. The convergence of the last series is considered a.s. or in $\mathrm{L}^2(\Omega)$, depending on whether we want $u(x,t)$ to be an a.s. or a m.s. solution, respectively.

As we are interested in computational uncertainty quantification, the existence of a solution in a probabilistic sense will not be a major concern. In contrast, our main goal is to construct reliable approximations of the probability density function of the solution, $u(x,t)$, to the random heat diffusion problem (1). To achieve this goal, we take advantage of a random numerical scheme together with a key probabilistic result that will be introduced later, to construct a sequence of approximating density functions. Afterwards, the proposed method will be presented in an algorithm. We will present numerical experiments aimed to show the capability of the proposed approach to quantify uncertainty in the random heat diffusion problem (1) via the computation of approximations to its probability density function.

2. Method

Consider the backward Euler method to formally approximate the solution process $u(x,t)$, [28]. We divide the spatial domain $[0,1]$ into equidistant points as $\{x_0,\dots,x_{M+1}\}$, where $x_i = ih$ and $h = 1/(M+1)$. We discretize the time domain $[0,T]$ as $\{t_0,\dots,t_N\}$, where $t_n = n\Delta t$ and $\Delta t = T/N$. The finite difference scheme corresponding to the backward Euler method is expressed via the following difference equation:

$$u^{N,M}_{n+1,i} = u^{N,M}_{n,i} + \eta(u^{N,M}_{n+1,i+1} - 2u^{N,M}_{n+1,i} + u^{N,M}_{n+1,i-1}),$$

where $\eta = \alpha(\Delta t)/h^2$ is a.s. positive. The term $u^{N,M}_{n,i}$ approximates $u(x_i,t_n)$. In matrix form,

$$\mathbf{u}^{N,M}_{n+1} = (\mathbf{I_M} - \eta\mathbf{L})^{-1}(\mathbf{u}^{N,M}_n + \eta\mathbf{c}), \tag{5}$$

where $\mathbf{u}^{N,M}_n = (u^{N,M}_{n,1},\dots,u^{N,M}_{n,M})^\top$, $\mathbf{c} = (A,0,\dots,0,B)^\top$ ($\top$ denotes the transpose operator for vectors and matrices), $\mathbf{I_M}$ is the $M\times M$ identity matrix and

$$\mathbf{L} = \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}$$

is also an $M\times M$ matrix.

This numerical method is stable for all η. The random difference equation (5) approximates the partial differential equation (1) with order $O(\Delta t) + O(h^2)$. We will take $N = N_M = (M+1)^2$, so that the local truncation error is given by $O(h^2)$. Therefore, we may drop the superscript N from the random difference equation (5):

$$\mathbf{u}^{M}_{n+1} = (\mathbf{I_M} - \eta\mathbf{L})^{-1}(\mathbf{u}^{M}_n + \eta\mathbf{c}). \tag{6}$$

This linear recurrence (6) has an explicit solution:

$$\mathbf{u}^{M}_n = \mathcal{A}^n\boldsymbol{\phi}^M + \left(\sum_{k=0}^{n-1}\mathcal{A}^k\right)\mathbf{b}, \tag{7}$$

where $\boldsymbol{\phi}^M = (\phi(x_1),\dots,\phi(x_M))^\top$, $\mathcal{A} = (\mathbf{I_M} - \eta\mathbf{L})^{-1}$ and $\mathbf{b} = \eta(\mathbf{I_M} - \eta\mathbf{L})^{-1}\mathbf{c}$, and from (7), we can compute explicitly each component $u^M_{n,i}$:

$$\begin{aligned} u^M_{n,i} &= (\mathcal{A}^n\boldsymbol{\phi}^M)_i + \left(\sum_{k=0}^{n-1}\mathcal{A}^k\right)(i,:)\mathbf{b} \\ &= (\mathcal{A}^n\boldsymbol{\phi}^M)_i + \eta\left(\sum_{k=0}^{n-1}\mathcal{A}^k\right)(i,:)\mathcal{A}(:,1)A + \eta\left(\sum_{k=0}^{n-1}\mathcal{A}^k\right)(i,:)\mathcal{A}(:,M)B, \end{aligned} \tag{8}$$

where $\mathcal{A}(i,:)$ denotes the i-th row of $\mathcal{A}$ and $\mathcal{A}(:,j)$ refers to the j-th column of $\mathcal{A}$.

From (8), we will derive the probability distribution of $u^M_{n,i}$ on account of the distributions of A, B, α and $\boldsymbol{\phi}^M$. We will distinguish two scenarios:

- Case 1: A is an absolutely continuous random variable (i.e. it has a density function) which is independent of the random vector $(\alpha, B, \boldsymbol{\phi}^M)$. In this case, α, B and $\boldsymbol{\phi}^M$ may take any type of probability distribution (continuous, discrete, etc.).

- Case 2: B is absolutely continuous and is independent of $(\alpha, A, \boldsymbol{\phi}^M)$. In this case, α, A and $\boldsymbol{\phi}^M$ may follow any kind of probability distribution (continuous, discrete, etc.).

Since the analysis of Case 2 is analogous to the one of Case 1, we will detail the study corresponding to Case 1, and for the Case 2 we summarize the main conclusions.

The following lemma allows computing the probability density function of $u_{n,i}^M$. The result is an extension of the Random Variable Transformation (RVT) technique (which has been extensively used [29, 30, 31]) when the transformation mapping consists of sums and products. Regarding notation, the probability density function of a random variable/vector X will be denoted as f_X hereafter, and its probability law will be written as $\mathbb{P}_X = \mathbb{P} \circ X^{-1}$.

Lemma 2.1. *Let U be an absolutely continuous random variable, independent of the random vector (Z_1, Z_2), where $Z_1 \neq 0$ a.s. Then $Z_1 U + Z_2$ is absolutely continuous, with density function $f_{Z_1 U+Z_2}(z) = \mathbb{E}[f_U((z - Z_2)/Z_1)/|Z_1|]$.*

Proof. Let C be a Borel set in $\mathbb{R}$. Then, using conditional probabilities,

$$\begin{aligned}
\mathbb{P}(Z_1 U + Z_2 \in C) &= \int_{\mathbb{R}^2} \mathbb{P}(Z_1 U + Z_2 \in C | Z_1 = z_1, Z_2 = z_2) \mathbb{P}_{(Z_1,Z_2)}(\mathrm{d}z_1, \mathrm{d}z_2) \\
&= \int_{\mathbb{R}^2} \mathbb{P}(z_1 U + z_2 \in C) \mathbb{P}_{(Z_1,Z_2)}(\mathrm{d}z_1, \mathrm{d}z_2) = \int_{\mathbb{R}^2} \int_{(C-z_2)/z_1} f_U(u)\, \mathrm{d}u\, \mathbb{P}_{(Z_1,Z_2)}(\mathrm{d}z_1, \mathrm{d}z_2) \\
&= \int_{\mathbb{R}^2} \int_C f_U\left(\frac{u - z_2}{z_1}\right) \frac{1}{|z_1|}\, \mathrm{d}u\, \mathbb{P}_{(Z_1,Z_2)}(\mathrm{d}z_1, \mathrm{d}z_2) \\
&= \int_C \int_{\mathbb{R}^2} f_U\left(\frac{u - z_2}{z_1}\right) \frac{1}{|z_1|} \mathbb{P}_{(Z_1,Z_2)}(\mathrm{d}z_1, \mathrm{d}z_2)\, \mathrm{d}u = \int_C \mathbb{E}\left[f_U\left(\frac{u - z_2}{z_1}\right) \frac{1}{|z_1|} \right] \mathrm{d}u.
\end{aligned}$$

By using this key lemma, we are able to compute, for the Case 1, the probability density function of $u_{n,i}^M$ by taking into account the representation given in (8). Take

$$\begin{aligned}
U =& A, \\
Z_1 =& \eta \left(\sum_{k=0}^{n-1} \mathcal{A}^k \right)(i,:) \mathcal{A}(:,1), \\
Z_2 =& (\mathcal{A}^n \boldsymbol{\phi}^M)_i + \eta \left(\sum_{k=0}^{n-1} \mathcal{A}^k \right)(i,:) \mathcal{A}(:,M) B.
\end{aligned}$$

Let us justify that $Z_1 \neq 0$ a.s. The matrix $\mathbf{I_M} - \eta \mathbf{L}$ is an M-matrix, in the sense of ref. [32, p.10]: $\mathbf{I_M} - \eta \mathbf{L}$ has its offdiagonal entries nonpositive and, for the vector $\mathbf{r} = (\sin(\pi j/(M+1))_{j=1}^M$ with positive components, the image $(\mathbf{I_M} - \eta \mathbf{L})\mathbf{r}$ is written as $\lambda \mathbf{r}$, where $\lambda > 0$, so that $(\mathbf{I_M} - \eta \mathbf{L})\mathbf{r}$ has positive components. Moreover, $\mathbf{I_M} - \eta \mathbf{L}$ is an irreducible matrix, because its entries on the superdiagonal and on the subdiagonal are nonzero. By Theorem 2.7 in ref. [33], the entries of $\mathcal{A} = (\mathbf{I}_M - \eta \mathbf{L})^{-1}$ are positive. Thus, $Z_1 > 0$.

The assumption of independence between A and $(\alpha, B, \boldsymbol{\phi}^M)$ implies the independence between U and (Z_1, Z_2), by [34, p. 93]. By applying Lemma 2.1, we obtain

$$f_{u_{n,i}^M}(u) = \mathbb{E}\left[f_A\left(\frac{u - (\mathcal{A}^n \boldsymbol{\phi}^M)_i - \eta\left(\sum_{k=0}^{n-1} \mathcal{A}^k\right)(i,:)\mathcal{A}(:,M)B}{\eta\left(\sum_{k=0}^{n-1} \mathcal{A}^k\right)(i,:)\mathcal{A}(:,1)} \right) \frac{1}{\eta\left(\sum_{k=0}^{n-1} \mathcal{A}^k\right)(i,:)\mathcal{A}(:,1)} \right]. \tag{9}$$

For the Case 2, that is, if B is absolutely continuous and is independent of $(\alpha, A, \boldsymbol{\phi}^M)$, proceeding analogously we derive an alternative density function for $u_{n,i}^M$:

$$f_{u_{n,i}^M}(u) = \mathbb{E}\left[f_B\left(\frac{u - (\mathcal{A}^n \boldsymbol{\phi}^M)_i - \eta\left(\sum_{k=0}^{n-1} \mathcal{A}^k\right)(i,:)\mathcal{A}(:,1)A}{\eta\left(\sum_{k=0}^{n-1} \mathcal{A}^k\right)(i,:)\mathcal{A}(:,M)} \right) \frac{1}{\eta\left(\sum_{k=0}^{n-1} \mathcal{A}^k\right)(i,:)\mathcal{A}(:,M)} \right].$$

We approximate the density function of $u(x,t)$ as follows. Let $x^* \in (0,1)$ and $t^* \in (0,T)$. Consider a sequence of points in both partitions, $\{i_M/(M+1)\}_{M=1}^{\infty}$ and $\{n_M T/N_M\}_{M=1}^{\infty}$, where $i_M \in \{1,\dots,M\}$, $n_M \in \{0,\dots,N_M\}$ and $N_M = (M+1)^2$, such that $i_M/(M+1) \to x^*$ and $n_M T/N_M \to t^*$ as $M \to \infty$. For example, take $i_M = \lfloor x^*(M+1) \rfloor$ and $n_M = \lfloor t^* N_M/T \rfloor$, where $\lfloor \cdot \rfloor$ stands for the integer part. Then, the density function of $u(x^*,t^*)$ is

$$f_{u(x^*,t^*)}(u) = \lim_{M\to\infty} f_{u_{n_M,i_M}^M}(u). \tag{10}$$

At this point, we would like to remark that other finite difference schemes could be possible: forward Euler method, Crank-Nicholson method, etc. Our choice for the backward Euler method is due to its simplicity and being von Neumann stable for all η (stability means that all the eigenvalues of the matrix $(\mathbf{I_M} - \eta\mathbf{L})^{-1}$ have modulus less than or equal to 1; this is a necessary condition to assure the a.s. convergence of the discretizations to the true solution).

The case in which A and B are not absolutely continuous remains pending. One could think of performing the same analysis as before but isolating $\phi(x_j)$ in (8), instead of A or B. In such a case, one would assume that $\phi(x_j)$ is absolutely continuous and independent of $(\alpha, A, B, \phi(x_1), \dots, \phi(x_{j-1}), \phi(x_{j+1}), \dots, \phi(x_M))$. To achieve this independence, one may require $\phi(y_1), \dots \phi(y_m)$ to be independent, for every $y_1, \dots, y_m \in [0,1]$, $m \geq 1$. A process ϕ of this type exists by Kolmogorov's Extension Theorem [35, Th. 36.2, p. 486]. However, by [36, Example 1.2.5, p. 10], this process ϕ is not jointly measurable on $[0,1] \times \Omega$, so that ϕ cannot belong to $\mathrm{L}^2([0,1] \times \Omega)$. Hence, Proposition 1.2 on the existence of solution does not apply.

3. Computational aspects and algorithm

In this section we comment on computational aspects regarding the implementation of the probability density function (9).

The computation of the powers $\mathcal{A}^k$ is especially demanding. Thus, it is better to consider the spectral decomposition of $\mathcal{A}$. The set of eigenvalues, μ_l, and eigenvectors, $\mathbf{s}^l$, of $\mathcal{A}$ is well-known [37]:

$$\mu_l = \frac{1}{2\eta(1 - \cos(l\pi h)) + 1}, \quad \mathbf{s}^l = (\sin(l\pi jh))_{j=1}^M, \tag{11}$$

for $l = 1, \ldots, M$. Let $\mathbf{D}$ be the diagonal matrix with $\mathbf{D}_{ll} = \mu_l$, and let $\mathbf{P} = [\mathbf{s}^1 \ldots \mathbf{s}^M]$ be the matrix whose column vectors are $\mathbf{s}^1, \ldots, \mathbf{s}^M$. Define $\mathbf{R} = \sqrt{2/(M+1)}\,\mathbf{P}$. Then $\mathbf{R}$ is an orthogonal $M \times M$ matrix, and the decomposition $\mathcal{A} = \mathbf{R}\mathbf{D}\mathbf{R}^\top$ holds. Hence, the powers of $\mathcal{A}$ can be computed as $\mathcal{A}^k = \mathbf{R}\mathbf{D}^k\mathbf{R}^\top$, which reduces notably the computational load.

On the other hand, the theoretical expression of the expectation from (9) is the following:

$$f_{u_{n,i}^M}(u) = \int_{\mathbb{R}^{M+2}} f_A\left(\frac{u - (\mathcal{A}^n\boldsymbol{\phi}^M)_i - \eta\left(\sum_{k=0}^{n-1}\mathcal{A}^k\right)(i,:)\mathcal{A}(:,M)B}{\eta\left(\sum_{k=0}^{n-1}\mathcal{A}^k\right)(i,:)\mathcal{A}(:,1)}\right) \times \frac{1}{\eta\left(\sum_{k=0}^{n-1}\mathcal{A}^k\right)(i,:)\mathcal{A}(:,1)}\,\mathbb{P}_{(\alpha,B,\boldsymbol{\phi}^M)}(\mathrm{d}\alpha, \mathrm{d}B, \mathrm{d}\boldsymbol{\phi}^M).$$

However, from a practical point of view, it is better to turn to Monte Carlo simulation to address the computation of (9), [21], as the integration is high-dimensional. Let $\alpha_{(j)}$, $B_{(j)}$ and $\boldsymbol{\phi}^M_{(j)}$, $j = 1, \ldots, m$, be m realizations of the random variables/vectors α, B and $\boldsymbol{\phi}^M$. Then we approximate (9) as

$$f_{u_{n,i}^M}(u) \approx \frac{1}{m}\sum_{j=1}^{m} f_A\left(\frac{u - (\mathcal{A}_{(j)}^n\boldsymbol{\phi}_{(j)}^M)_i - \eta_{(j)}\left(\sum_{k=0}^{n-1}\mathcal{A}_{(j)}^k\right)(i,:)\mathcal{A}_{(j)}(:,M)B_{(j)}}{\eta_{(j)}\left(\sum_{k=0}^{n-1}\mathcal{A}_{(j)}^k\right)(i,:)\mathcal{A}_{(j)}(:,1)}\right) \times \frac{1}{\eta_{(j)}\left(\sum_{k=0}^{n-1}\mathcal{A}_{(j)}^k\right)(i,:)\mathcal{A}_{(j)}(:,1)}. \tag{12}$$

When $m \to \infty$, this approximation becomes an a.s. limit by the law of large numbers.

Based on this proposed computational method, we provide Algorithm 1 for uncertainty quantification for the solution stochastic process $u(x,t)$ to the random heat partial differential equation (1).

Once we obtain $F(u)$ in Algorithm 1, we can perform uncertainty quantification with the density function $F(u)$, because $F(u) \approx f_{u(x^*,t^*)}(u)$. For example, the expectation and the variance of $u(x^*,t^*)$ may be approximated as

$$\mathbb{E}[u(x^*,t^*)] \approx \int_{\mathbb{R}} uF(u)\,\mathrm{d}u, \quad \mathbb{V}[u(x^*,t^*)] \approx \int_{\mathbb{R}} u^2F(u)\,\mathrm{d}u - \left(\int_{\mathbb{R}} uF(u)\,\mathrm{d}u\right)^2. \tag{13}$$

Any statistical moment of $u(x^*,t^*)$ may be approximated using the general formula

$$\mathbb{E}[g(u(x^*,t^*))] \approx \int_{\mathbb{R}} g(u)F(u)\,\mathrm{d}u,$$

where $g : \mathbb{R} \to \mathbb{R}$ is any deterministic function.

In the next section, we will illustrate the use of the proposed Algorithm 1 with three examples. We conclude this section by comparing our algorithm with kernel-based density estimations. Our algorithm applies plain Monte Carlo simulation to estimate the expectation (9). Therefore we

Algorithm 1 Approximation for the density function of the solution $u(x^*, t^*)$.

procedure F($u(x^*, t^*)$)

x^*

t^*

T

A ▷ probability distribution

B ▷ probability distribution

α ▷ probability distribution

$\phi(x)$ ▷ stochastic process

M

$N_M = (M+1)^2$

$i = \lfloor x^*(M+1) \rfloor$

$n = \lfloor t^* N_M / T \rfloor$

$\mathbf{D} = \mathrm{diag}(\mu_1, \ldots, \mu_M)$, ▷ where the entry μ_l is defined by (11)

$\mathbf{R} = \sqrt{2/(M+1)}\,[\mathbf{s}^1 \ldots \mathbf{s}^M]$ ▷ where the vector $\mathbf{s}^l$ is defined by (11)

$\mathcal{A} = \mathbf{R}\mathbf{D}\mathbf{R}^\top$

$\mathcal{A}^n = \mathbf{R}\mathbf{D}^n\mathbf{R}^\top$

$\sum_{k=0}^{n-1} \mathcal{A}^k = \mathbf{R}(\sum_{k=0}^{n-1} \mathbf{D}^k)\mathbf{R}^\top$

$$F(\alpha, B, \boldsymbol{\phi}^M) = f_A\left(\frac{u - (\mathcal{A}^n\boldsymbol{\phi}^M)_i - \eta\left(\sum_{k=0}^{n-1}\mathcal{A}^k\right)(i,:)\mathcal{A}(:,M)B}{\eta\left(\sum_{k=0}^{n-1}\mathcal{A}^k\right)(i,:)\mathcal{A}(:,1)}\right)\frac{1}{\eta\left(\sum_{k=0}^{n-1}\mathcal{A}^k\right)(i,:)\mathcal{A}(:,1)}$$

for $j = 1$ to m **do** ▷ obtain m realizations for α, B, ϕ^M

$\alpha_{(j)}$

$B_{(j)}$

$\boldsymbol{\phi}^M_{(j)}$

end for

$F(u) = \frac{1}{m}\sum_{j=1}^{m} F(\alpha_{(j)}, B_{(j)}, \boldsymbol{\phi}^M_{(j)})$ ▷ compute the sample mean

end procedure

obtain pointwise estimates of the density function at mean square error rate $O(m^{-1})$, where m is the number of realizations. The algorithm has a parametric nature (i.e. from known distributions and samples, compute the parameter mean). By contrast, a kernel density construction estimates the unknown density function at mean square error rate $O(m^{-p})$, for certain $0 < p < 1$ (see Section 1 and the references therein). It is of nonparametric nature (i.e. from samples only, infer an unknown probability distribution), thus slower than parametric methods. In addition, each realization of the kernel density estimate requires the computation of the heat equation solution. Hence, overall, our method is proved to be faster.

On the other hand, our algorithm is more robust than a kernel-based density estimate. Indeed, as we only require the estimation of a mean, see (9), we do not need to impose any regularity condition on the densities (the Law of Large Numbers assures convergence in any situation); any discontinuity point or peak will be correctly captured by our method. On the contrary, kernel density estimates are highly influenced by smoothness; without prior knowledge on the features of the target density function, the optimal kernel may not be known. The kernel distribution estimate may consider wrong tails, for instance.

Methods based on finite-dimensional representations of the stochastic solution (discretizations, finite-term expansions, etc.) and on considering the density functions of such representations, correctly capture the density features (discontinuities, differentiability points, support, etc.), see [38, 39] for example.

4. Numerical examples

Here, we show three numerical examples for (1) by considering a variety of probability distributions for each random input. Take $T = 3$, so that the domain of the partial differential equation becomes $(0, 1) \times (0, 3)$, and let $u(x, t)$ be the solution stochastic process to (1), whose existence is guaranteed by [27, Th. 3.2]. We will approximate its probability density function at a point (x^*, t^*) by utilizing (10). Consider $i_M = \lfloor x^*(M + 1) \rfloor$, $n_M = \lfloor t^* N_M / T \rfloor$. These points satisfy $i_M/(M + 1) \to x^*$ in the partitions, and $n_M T/N_M \to t^*$ as $M \to \infty$.

We will set particular distributions for α, A, B and ϕ. It will be assumed that A is absolutely continuous and independent of (α, B, ϕ), so that Lemma 2.1 is applicable. The expectation (9) will be approximated via Monte Carlo simulation, with $m = 20,000$ realizations of each random variable. This m value has been checked to be enough in order to ensure good approximations of (9). The algorithm has been implemented in the software Mathematica$^{\circ R}$, version 11.2 (Wolfram Research, Inc.: Champaign, IL, USA, 2017).

We will choose different stochastic processes ϕ. In Example 4.1, its sample paths will be exactly computable. In Example 4.2, by contrast, the process will be decomposed via an infinite Karhunen-Lo`eve-type expansion. In this case, a dimensionality reduction of the random space must be carried out to simulate ϕ, by truncating the series. These two situations cover the range of possibilities for a given initial condition $\phi(x)$: finite or infinite-dimensional randomness. The latter case always requires parametrizing the random space by a set of a finite number of random variables. This methodology was used in our recent contribution [38]. Finally, the purpose of the last example, Example 4.3, will only be to illustrate how our method is able to capture non-differentiability points, in contrast to kernel density estimates.

In the examples, we will observe fast convergence of (9) as M increases, although the error may not be monotonically decreasing.

For the sole purpose of validating our density approximations, we will compare our compu-tations for the expectation and the variance (13) with the method proposed in the reference [7].

In [7], the authors proposed a novel methodology to estimate the expectation and the variance of the solution to the heat equation, by considering explicit series expressions. Their use of the mean square calculus restricted their analysis to these two statistics. Suppose that α, A, B and ϕ are independent. The idea in ref. [7] is as follows: from (2)–(4), the expectation of $u(x, t)$ may be approximated as

$$\mathbb{E}[u(x,t)] = \mathbb{E}[v(x,t)] + x\mathbb{E}[B] + (1-x)\mathbb{E}[A], \tag{14}$$

being

$$\mathbb{E}[v(x,t)] \approx \sum_{k=1}^{K} \mathbb{E}[A_k]\mathbb{E}[\mathrm{e}^{-k^2\pi^2\alpha t}]\sin(k\pi x) \tag{15}$$

and

$$\mathbb{E}[A_k] = 2\int_0^1 \mathbb{E}[\psi(y)]\sin(k\pi y)\,\mathrm{d}y, \quad \mathbb{E}[\psi(y)] = \mathbb{E}[\phi(y)] - y\mathbb{E}[B] - (1-y)\mathbb{E}[A], \tag{16}$$

where the order of truncation K must be sufficiently large to achieve the desired accuracy. Notice that the independence hypothesis between α and ϕ has been used in (15). Concerning the variance of $u(x, t)$, we compute

$$\mathbb{V}[u(x,t)] = \mathbb{V}[v(x,t)] + x^2\mathbb{V}[B] + (1-x)^2\mathbb{V}[A], \tag{17}$$

$$\begin{aligned}\mathbb{V}[v(x,t)] \approx & \sum_{k_1,k_2=1}^{K} \mathbb{C}\mathrm{ov}[A_{k_1}, A_{k_2}]\mathbb{E}[\mathrm{e}^{-(k_1^2+k_2^2)\pi^2\alpha t}]\sin(k_1\pi x)\sin(k_2\pi x) \\ & + \sum_{k_1,k_2=1}^{K} \mathbb{E}[A_{k_1}]\mathbb{E}[A_{k_2}]\mathbb{C}\mathrm{ov}[\mathrm{e}^{-k_1^2\pi^2\alpha t}, \mathrm{e}^{-k_2^2\pi^2\alpha t}]\sin(k_1\pi x)\sin(k_2\pi x),\end{aligned} \tag{18}$$

$$\mathbb{C}\mathrm{ov}[A_{k_1}, A_{k_2}] = 4\int_0^1\int_0^1 \mathbb{C}\mathrm{ov}[\psi(y_1), \psi(y_2)]\sin(k_1\pi y_1)\sin(k_2\pi y_2)\,\mathrm{d}y_1\,\mathrm{d}y_2, \tag{19}$$

$$\mathbb{C}\mathrm{ov}[\psi(y_1), \psi(y_2)] = \mathbb{C}\mathrm{ov}[\phi(y_1), \phi(y_2)] + y_1y_2\mathbb{V}[B] + (1-y_1)(1-y_2)\mathbb{V}[A], \tag{20}$$

for a large level of truncation K. The independence assumptions have been used in (17), (18) and (20). The approximations derived with these expressions from [7] must be similar to those calculated with our density functions.

Example 4.1. Let $A \sim$ Gamma(3, 1), $B = -1$ (constant), $\alpha \sim$ Triangular(1, 2) and $\phi(x) = D\cos x + \mathrm{e}^{\sin(Ex^2)}$, where $D \sim$ Binomial(20, 0.2) and $E \sim$ Uniform(-1, 0). By Proposition 1.2, there exists a unique solution stochastic process $u(x, t)$, both in the a.s. and m.s. senses, which is given by (2)–(4). It is assumed that A, α, D and E are independent random variables. We are under the conditions of Case 1. Let $(x^*, t^*) = (0.25, 2.4)$. In Figure 1, we plot the approx-imations (9) for M = 9, 11, 13, 15, 17, 19, 21. We observe non-monotone convergence. More-over, the density function obtained for $M = 19$ coincides visually with the density function of $\lim_{t\to\infty} u(x, t) = xB + (1-x)A = -0.25 + 0.75A$, which is given by

$$f_A\left(\frac{x+0.25}{0.75}\right)\frac{1}{0.75} \tag{21}$$

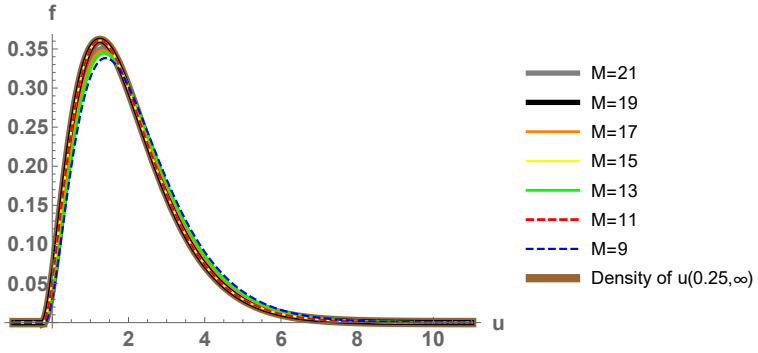

Figure 1: Example 4.1: plot of $f_{u^M_{n_M,i_M}}(u)$ given by (9) for $M = 9, 11, 13, 15, 17, 19, 21$, and the asymptotic density (21).

(apply the RVT method to the transformation $-0.25 + 0.75A$, [6, p. 24–25]). This is because $\lim_{t\to\infty} u(x, t) = xB + (1 - x)A$ holds exponentially in t, so for $t = 2.4$ we have $u(0.25, 2.4) \approx u(0.25, \infty) = -0.25 + 0.75A$.

Table 1 shows the approximations for $\mathbb{E}[u(x^*, t^*)]$ and $\mathbb{V}[u(x^*, t^*)]$. Table 2 presents these computations by means of the procedure in ref. [7] (see (14)–(20)). We clarify the fact that the results reported in Table 2 are not cited; they are calculated here based on the methodology from the reference. The agreement of the results demonstrates the validity of the probability density functions plotted in Figure 1. Moreover, notice that the results coincide with the asymptotic limit $\mathbb{E}[u(0.25, \infty)] = \mathbb{E}[-0.25 + 0.75A] = 2$ and $\mathbb{V}[u(0.25, \infty)] = \mathbb{V}[-0.25 + 0.75A] = 1.6875$.

M	9	11	13	15	17	19	21
$\mathbb{E}[u^M_{n_M,i_M}]$	2.199	2	2.142	2	2.110	2	2.090
$\mathbb{V}[u^M_{n_M,i_M}]$	1.912	1.688	1.845	1.688	1.809	1.688	1.786

Table 1: Example 4.1: approximations for $\mathbb{E}[u(x^*, t^*)]$ and $\mathbb{V}[u(x^*, t^*)]$ obtained with (13).

K	1	2	3	4	5
$\mathbb{E}[u(x^*, t^*)]$	2	2	2	2	2
$\mathbb{V}[u(x^*, t^*)]$	1.688	1.688	1.688	1.688	1.688

Table 2: Example 4.1: approximations for $\mathbb{E}[u(x^*, t^*)]$ and $\mathbb{V}[u(x^*, t^*)]$ as in ref. [7] (see (14)–(20)).

Thus, the best choice for uncertainty quantification for $u(0.25, 2.4)$ is $M = 19$, or even the density function of $u(0.25, \infty)$ given by (21).

Example 4.2. Let us consider $A \sim \text{Normal}(-1, 1)$, $B = -1$ (constant), $\alpha \sim \text{Triangular}(1, 2)$ and

$$\phi(x) = \sum_{j=1}^{\infty} \frac{\sqrt{2}}{j^{3/2}\sqrt{1 + \log j}} \sin(j\pi x)\xi_j, \tag{22}$$

where $\xi_1, \xi_2, \ldots$ are independent and identically distributed random variables, with density function

$$f_{\xi_1}(\xi) = \frac{\sqrt{2}}{\pi(1+\xi^4)}, \quad \xi \in \mathbb{R}.$$

Since $\xi_1, \xi_2, \ldots$ have zero expectation and unit variance, and $\{\sqrt{2}\sin(j\pi x)\}_{j=1}^{\infty}$ is an orthonormal basis of $L^2([0,1])$, the series in (22) corresponds to a Karhunen-Loève expansion [40, Th. 5.28]. Karhunen-Lo`eve expansions are Fourier-type series that decompose square integrable processes in terms of the eigenvalues and eigenfunctions of the covariance integral operator. Here we give a test series explicitly, where the set of eigenvalues is $\{1/(j^3(1+\log j))\}_{j=1}^{\infty}$ and the set of eigenfunctions is $\{\sqrt{2}\sin(j\pi x)\}_{j=1}^{\infty}$. The covariance of the process ϕ is given by [40, p. 203]

$$\mathbb{C}\mathrm{ov}[\phi(x), \phi(y)] = \sum_{j=1}^{\infty} \frac{2}{j^3(1+\log j)} \sin(j\pi x)\sin(j\pi y),$$

and its covariance integral operator is $C\varphi(x) = \int_0^1 \mathbb{C}\mathrm{ov}[\phi(x), \phi(y)]\varphi(y)\mathrm{d}y$, $x \in [0,1]$, $\varphi \in L^2([0,1])$. The convergence of the series is understood in $L^2([0,1] \times \Omega)$. Proposition 1.2 tells us that there is a unique solution stochastic process $u(x,t)$, both in the a.s. and m.s. senses, which is given by (2)–(4).

In order to sample from $\phi(x)$, we need to truncate the series in (22). Truncating up to order $N = 5$, we are accounting for more than 99.5% of the total variance of $\phi(x)$, $\int_0^1 \mathbb{V}[\phi(x)]\,\mathrm{d}x = \sum_{j=1}^{\infty} 1/(j^3(1+\log j))$, [40, p. 204]. Thus, we will use

$$\phi(x) = \sum_{j=1}^{5} \frac{\sqrt{2}}{j^{3/2}\sqrt{1+\log j}} \sin(j\pi x)\xi_j.$$

It is assumed that A, α, $\xi_1, \ldots, \xi_5$ are independent random variables. We are under the conditions required by Case 1. Let $(x^*, t^*) = (0.25, 0.3)$. Figure 2 shows the approximations (9) for values of $M = 9, 11, 13, 15, 17, 19, 21, 23$. Convergence is achieved, so that the density function of $u(x^*, t^*)$ has been accurately approximated.

Table 3 shows the approximations for $\mathbb{E}[u(x^*, t^*)]$ and $\mathbb{V}[u(x^*, t^*)]$ obtained with (13). No-tice that the convergence is non-monotone. We compare these estimates to the procedure in ref. [7] (see (14)–(20)), whose values are tabulated in Table 4. The results reported in Table 4 are not cited; they are calculated here based on the methodology from the reference. Again, the agreement of the results demonstrates the validity of the probability density functions plotted in Figure 2.

M	9	11	13	15	17	19	21	23
$\mathbb{E}[u^M_{n_M,i_M}]$	−0.979	−0.977	−0.981	−0.981	−0.984	−0.984	−0.986	−0.985
$\mathbb{V}[u^M_{n_M,i_M}]$	0.624	0.546	0.603	0.549	0.599	0.551	0.586	0.552

Table 3: Example 4.2: approximations for $\mathbb{E}[u(x^*, t^*)]$ and $\mathbb{V}[u(x^*, t^*)]$ obtained with (13).

Thereby, the best truncation order for uncertainty quantification for $u(0.25, 0.3)$ is $M = 23$.

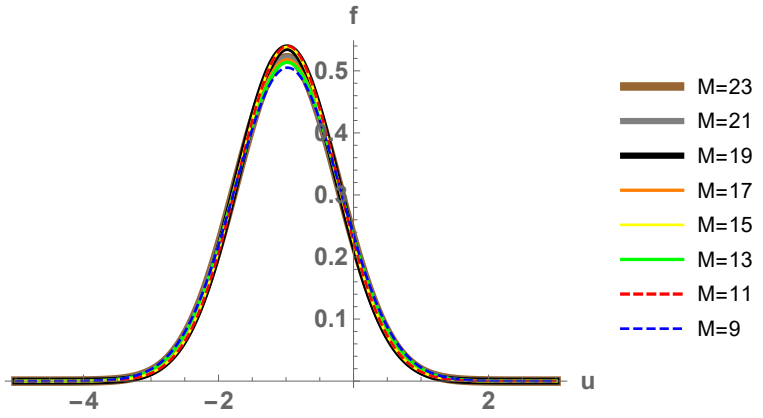

Figure 2: Example 4.2: plot of $f_{u^M_{n_M,i_M}}(u)$ given by (9) for $M = 9, 11, 13, 15, 17, 19, 21, 23$

K	1	2	3	4	5
$\mathbb{E}[u(x^*, t^*)]$	−0.987	−0.987	−0.987	−0.987	−0.987
$\mathbb{V}[u(x^*, t^*)]$	0.563	0.563	0.563	0.563	0.563

Table 4: Example 4.2: approximations for $\mathbb{E}[u(x^*, t^*)]$ and $\mathbb{V}[u(x^*, t^*)]$ as in ref. [7] (see (14)–(20)).

Example 4.3. Consider $A \sim$ Triangular$(-1, 1)$, $B \sim$ Uniform$(1, 1.1)$, $\alpha = 1$ (constant) and $\phi(x) = e^{\sin(Ex^2)}$, where $E \sim$ Uniform$(-1, 0)$. By Proposition 1.2, there is a unique solution $u(x, t)$, given by (2)–(4). The random quantities are assumed to be independent. Let $(x^*, t^*) = (0.25, 0.05)$. In Figure 3, we depict the approximations (9) for $M = 17, 21, 25, 29$. We also plot a kernel density estimate, using Silverman's rule to determine the bandwidth and Gaussian kernel. We observe that the shape of the density f_A influences the densities of the discretizations a lot. There are three peaked points which are captured by our algorithm. In contrast, the kernel density estimate smooths out the approximation by drawing tails and is not capable of capturing the density features. Obviously, other choices of kernel and bandwidth would give different and maybe more suitable approximations, but a priori we do not have information about the pointwise properties of the target density.

5. Conclusions

In this paper, we have proposed a computational method to quantify the uncertainty of the random heat partial differential equation on a bounded domain via the approximation of its probability density function. The method is based on constructing a sequence of approximating density functions via a finite difference scheme. The numerical examples show that the convergence is achieved quickly, albeit with non-monotone decreasing error. Our approach improves the published contributions on heat transfer stochastic modelling, in which the approximation of the expectation and the variance was the main goal. Moreover, our method could be applied to other relevant random differential equations, in which the computation of the probability density

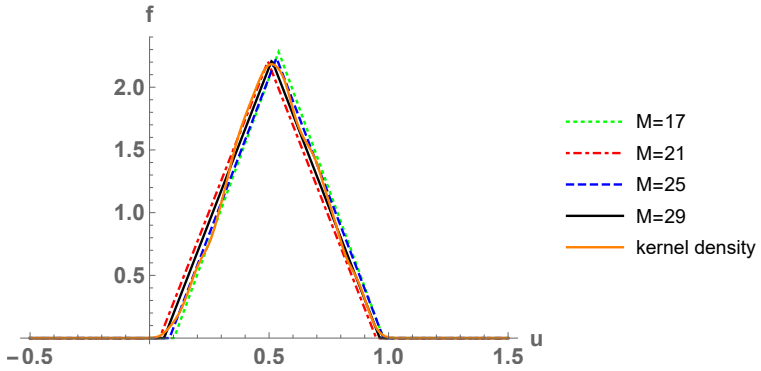

Figure 3: Example 4.3: plot of $f_{u^M_{n_M,i_M}}(u)$ given by (9) for $M = 17, 21, 25, 29$

function is a major goal. In general, the idea is always similar: use a discretization numerical scheme (Euler, Runge-Kutta, etc.) and determine the density function of the discretized solution, which is employed as an approximation to the true density function. In order to derive the density of the discretized solution, it seems that the governing differential equation must be linear, to express the recursive equations of the finite difference scheme in closed-form.

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Conflict of Interest Statement

The authors declare that there is no conflict of interests regarding the publication of this article.

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