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Contents

	Density-based uncertainty quantification in a generalized Logistic-type model $\ldots \ldots 1$
	Combined and updated <i>H</i> -matrices7
tr	Solving random fractional second-order linear equations via the mean square Laplace ansform
	Conformable fractional iterative methods for solving nonlinear problems 19
	$Construction \ of \ totally \ nonpositive \ matrices \ associated \ with \ a \ triple \ negatively \ realizable 24$
	Modeling excess weight in Spain by using deterministic and random differential equations31
ty	A new family for solving nonlinear systems based on weight functions Kalitkin-Ermankov pe
	Solving random free boundary problems of Stefan type
	Modeling one species population growth with delay
	On a Ermakov–Kalitkin scheme based family of fourth order
ci	A new mathematical structure with applications to computational linguistics and spe- alized text translation
m	Accurate approximation of the Hyperbolic matrix cosine using Bernoulli matrix polyno- ials
de	Full probabilistic analysis of random first-order linear differential equations with Dirac elta impulses appearing in control
	Some advances in Relativistic Positioning Systems
	A Graph–Based Algorithm for the Inference of Boolean Networks
m	Stability comparison of self-accelerating parameter approximation on one-step iterative sethods
m	Mathematical modelling of kidney disease stages in patients diagnosed with diabetes ellitus II
	The effect of the memory on the spread of a disease through the environtment 101
ti	Improved pairwise comparison transitivity using strategically selected reduced informa- on
	Contingency plan selection under interdependent risks
	Some techniques for solving the random Burgers' equation
de	Probabilistic analysis of a class of impulsive linear random differential equations via ensity functions

Probabilistic evolution of the bladder cancer growth considering transurethral resection 127
Study of a symmetric family of anomalies to approach the elliptical two body problem with special emphasis in the semifocal case
Advances in the physical approach to personality dynamics
A Laplacian approach to the Greedy Rank-One Algorithm for a class of linear systems 143
Using STRESS to compute the agreement between computed image quality measures and observer scores: advantanges and open issues
Probabilistic analysis of the random logistic differential equation with stochastic jumps156
Introducing a new parametric family for solving nonlinear systems of equations 162
Optimization of the cognitive processes involved in the learning of university students in a virtual classroom
Parametric family of root-finding iterative methods
Subdirect sums of matrices. Definitions, methodology and known results 180
On the dynamics of a predator-prey metapopulation on two patches
Prognostic Model of Cost / Effectiveness in the therapeutic Pharmacy Treatment of Lung Cancer in a University Hospital of Spain: Discriminant Analysis and Logit
Stability, bifurcations, and recovery from perturbations in a mean-field semiarid vegeta- tion model with delay
The random variable transformation method to solve some randomized first-order linear control difference equations
Acoustic modelling of large aftertreatment devices with multimodal incident sound fields 208
Solving non homogeneous linear second order difference equations with random initial values: Theory and simulations
A realistic proposal to considerably improve the energy footprint and energy efficiency of a standard house of social interest in Chile
Multiobjective Optimization of Impulsive Orbital Trajectories
Mathematical Modeling about Emigration/Immigration in Spain: Causes, magnitude, consequences
New scheme with memory for solving nonlinear problems
SP_N Neutron Noise Calculations
Analysis of a reinterpretation of grey models applied to measuring laboratory equipment uncertainties
An Optimal Eighth Order Derivative-Free Scheme for Multiple Roots of Non-linear Equa- tions
A population-based study of COVID-19 patient's survival prediction and the potential biases in machine learning
A procedure for detection of border communities using convolution techniques

Solving random free boundary problems of Stefan type

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1 Introduction

Free boundary problems describe several phenomena in nature, engineering and society, among others melting and freezing problems [1]. In these problems apart from determining the unknown function of the diffusion partial differential equation, we have an additional challenge concerning the calculus of evolution for the unknown moving boundary. In order to fit more realistically these type of problems, in this work we extend them into a random scenario using the mean square (m.s.) random calculus. We introduce *known* uncertainty, via considering random variables and stochastic processes following a certain probability distribution and depending on a finite degree of randomness [2, p.37]. In this work we study the following semi-infinite single-phase random melting problem for which the corresponding deterministic problem has an available exact solution [3, Chpts. 1 & 3]:

$$\frac{\partial T(x,t,\omega)}{\partial t} = D(\omega) \frac{\partial^2 T(x,t,\omega)}{\partial x^2}, \quad D(\omega) = \frac{\kappa(\omega)}{c_p(\omega) \rho(\omega)}, \qquad 0 < x = x(t,\omega) < s(t,\omega), \quad \omega \in \Omega,$$
(1)

with the following random boundary and initial conditions

$$T(0,t,\omega) = T_{\rm w}(\omega), \quad t > 0, \ \omega \in \Omega \quad \text{(wall temperature)}, \tag{2}$$

$$T(s(t,\omega), t,\omega) = T_{\rm m}(\omega), \quad t > 0, \ \omega \in \Omega \quad \text{(melting front temperature)},$$
 (3)

$$T(x,0,\omega) = T_{\rm m}(\omega), \quad x > 0, \omega \in \Omega \quad \text{(initial temperature)},$$
(4)

$$s(0,\omega) = 0, \qquad \omega \in \Omega \qquad \text{(initial position of the interface)}, \tag{5}$$

and the velocity of the 2-stochastic process (2-s.p.) interface $s(t, \omega)$ is stated by a random Stefan's condition:

$$\frac{\mathrm{d}s(t,\omega)}{\mathrm{d}t} = -Q(\omega) \left. \frac{\partial T(s(t,\omega), t,\omega)}{\partial x} \right|_{x \to s(t,\omega)^{-}}, \quad Q(\omega) = \frac{\kappa(\omega)}{L(\omega) \rho(\omega)}, \ \omega \in \Omega.$$
(6)

Here the unknown 2-s.p. $T(x, t, \omega), \omega \in \Omega, 0 < x < s(t, \omega), t > 0$, represents the temperature of the material in the liquid phase, $D(\omega) > 0$ in (1) represents the diffusivity random variable (r.v.) involving the thermal conductivity r.v. $\kappa(\omega) > 0$, the specific heat r.v. $c_p(\omega) > 0$ and the density

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r.v. of the material $\rho(\omega) > 0$. The r.v. $Q(\omega) > 0$ appearing in the Stefan condition (6) involves the latent heat of fusion r.v. of the phase change material $L(\omega) > 0$ and the r.v.'s $\kappa(\omega) > 0$ and $\rho(\omega) > 0$. Since our purpose is numerical we assume a realistic random framework. In our models the involved 2-s.p.'s $T(x, t, \omega)$, $C(x, t, \omega)$ and $s(t, \omega)$ are defined in a complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and have p degrees of randomness [2, p.37], i.e., they only depend on a finite number p of random variables (r.v.'s)

$$g(x,t,\omega) = g(x,t,B_1(\omega),B_2(\omega),\ldots,B_p(\omega)) , \qquad (7)$$

where

$$\begin{array}{l}
B_i(\omega), \ 1 \le i \le p, \quad \text{are mutually independent r.v.'s,} \\
g \text{ is a differential real function of the variables } x, t.
\end{array}$$
(8)

For the treatment of the random moving boundary $s(t, \omega)$ we propose a boundary immobilization formulation or random front-fixing method based on a transformation of the original random problem

$$z = \frac{x(t,\omega)}{s(t,\omega)}, \quad \omega \in \Omega, \quad t > 0,$$
(9)

where z becomes the deterministic spatial variable of the immobilized random boundary problem. The new dependent variable

$$u(z,t,\omega) = T(x(t,\omega),t,\omega), \quad \omega \in \Omega,$$
(10)

is the solution s.p. of the random transformed problem

$$D(\omega) \frac{1}{s^2(t,\omega)} \frac{\partial^2 u(z,t,\omega)}{\partial z^2} + z \frac{s'(t,\omega)}{s(t,\omega)} \frac{\partial u(z,t,\omega)}{\partial z} = \frac{\partial u(z,t,\omega)}{\partial t}, \quad 0 < z < 1, \ t > 0, \ \omega \in \Omega, \ (11)$$

$$u(0,t,\omega) = T_{\mathbf{w}}(\omega), \quad t > 0, \quad \omega \in \Omega,$$
(12)

$$u(1,t,\omega) = T_{\rm m}(\omega), \quad t > 0, \quad \omega \in \Omega, \tag{13}$$

$$s(0,\omega) = 0, \qquad \omega \in \Omega, \tag{14}$$

$$s'(t,\omega) = -\frac{Q(\omega)}{s(t,\omega)} \left. \frac{\partial u(z,t,\omega)}{\partial z} \right|_{z \to 1^{-}}, \quad t > 0, \quad \omega \in \Omega,$$
(15)

where $s'(t, \omega)$ denotes the first mean square derivative $\frac{ds(t,\omega)}{dt}$, $\omega \in \Omega$. The mean square operational calculus developed in (11) and (15) is legitimated when

$$\frac{\partial^2 u(z,t,\cdot)}{\partial z^2}, \quad \frac{\partial u(z,t,\cdot)}{\partial z}, \quad \frac{s'(t,\cdot)}{s(t,\cdot)}, \quad \frac{1}{s(t,\cdot)}, \text{ and } \frac{1}{s^2(t,\cdot)}$$
(16)

lie in $L_4(\Omega)$, see [4, Sec. 3].

With the immobilised boundary we can use a random finite difference method [5] constructing random difference schemes for both unknowns the temperature s.p. and the melting interface. Both difference schemes will be executed simultaneously because the melting interface is used to compute the temperature. Let us consider the uniform partition of the spatial domain [0, 1] taking a step size h in order to obtain equally spaced points $z_i = ih$, $0 \le i \le M$, such that Mh = 1. For a fixed time τ and a small initial time $t^0 > 0$, we take a step size k and N + 1 intermediate time levels are generated $t^n = nk + t^0$, $0 \le n \le N$, with $\tau = Nk + t^0$. The random difference scheme for determining the approximation $u_i^n(\omega) = u^n(z_i, t^n, \omega)$ to the unknown s.p. temperature $u(z, t, \omega), \omega \in \Omega$, is given by

$$u_{i}^{n+1}(\omega) = a_{i}^{n}(\omega) u_{i-1}^{n}(\omega) + b^{n}(\omega) u_{i}^{n}(\omega) + c_{i}^{n}(\omega) u_{i+1}^{n}, \quad \omega \in \Omega,$$

$$1 \leq i \leq M - 1, \quad 0 \leq n \leq N - 1,$$

$$u_{0}^{n}(\omega) = T_{w}(\omega), \quad u_{M}^{n}(\omega) = T_{m}(\omega), \quad 0 \leq n \leq N,$$

$$u_{i}^{0}(\omega) = \frac{T_{m}(\omega) - T_{w}(\omega)}{\operatorname{erf}(\beta)} \operatorname{erf}(\beta z_{i}) + T_{w}(\omega), \quad 0 \leq i \leq M.$$

$$(17)$$

with the random coefficients

$$a_{i}^{n}(\omega) = \frac{k}{h^{2}(s^{n}(\omega))^{2}} \left(D(\omega) + \frac{Q(\omega)\Delta^{n}(\omega)}{4} z_{i} \right)$$

$$b^{n}(\omega) = 1 - \frac{2kD(\omega)}{h^{2}(s^{n}(\omega))^{2}}$$

$$c_{i}^{n}(\omega) = \frac{k}{h^{2}(s^{n}(\omega))^{2}} \left(D(\omega) - \frac{Q(\omega)\Delta^{n}(\omega)}{4} z_{i} \right)$$

$$i \leq i \leq M-1, \quad 0 \leq n \leq N-1, \quad (18)$$

being $\Delta^n(\omega) = 3u_M^n(\omega) - 4u_{M-1}^n(\omega) + u_{M-2}^n(\omega)$. The random difference scheme for determining the approximation $s^n(\omega) = s(t^n, \omega)$ to the melting interface s.p. $s(t, \omega), \omega \in \Omega$ takes the form

$$s^{n+1}(\omega) = s^{n}(\omega) - \frac{k \ Q(\omega) \ \Delta^{n}(\omega)}{s^{n}(\omega) \ 2h}, \quad 0 \le n \le N-1,$$

$$s^{0}(\omega) = 2 \ \beta(\omega) \ \sqrt{D(\omega) \ t^{0}}, \quad t^{0} > 0, \omega \in \Omega,$$

$$\beta(\omega) \ e^{\beta(\omega)^{2}} \operatorname{erf}(\beta(\omega)) = \frac{Q(\omega) \ (T_{w}(\omega) - T_{m}(\omega))}{D(\omega) \ \sqrt{\pi}}.$$

$$(19)$$

For small enough values of the step-size h together with the hypothesis

$$\frac{k}{h^2} < 2 t^0 \beta_{\min}^2 \,, \tag{20}$$

where $\beta_{\min} = \min\{\beta(\omega) : \omega \in \Omega\}$, one guarantees the positivity and stability of the solution s.p.'s of the random difference schemes (17)–(18) and the time increasing behaviour of the melting interface s.p. obtained from (19).

In order to compute the mean and the standard deviation of the approximated solutions from (17)–(19) firstly we need to overcome the trouble of solving the random non-linear equation appearing on (19). Then we use a Monte Carlo technique taking a number K of realizations and solve the corresponding sampling deterministic non-linear equations associated. Each sampled solution $\beta(\omega_K)$ will be taken in the difference scheme (19) as well as a number K of realizations of the random data involved in (17)–(19) according to their probability distributions. Finally, the K sampling deterministic difference schemes associated to (17)–(19) will be solved and the mean and the standard deviation of the K results can be computed. Now in order to undo the variable change for computing the mean and the standard deviation of the solution s.p. $T(x, t, \omega)$ of (1) we use the transformation (9) which allows us to compute the mean of the r.v. $x(t, \cdot)$ at a fixed time t,

$$\mu[x(t,\omega)] = z \ \mu[s(t,\omega)] \,, \quad 0 \le z \le 1 \,.$$
(21)

Then the mean of the temperature s.p. above computed $\mu[u(z,t,\omega)]$ is assigned to the mean of the space variable $\mu[x(t,\omega)]$ given by (21).

In order to illustrate and validate the random solid-liquid phase change simulation results obtained in our study, we are going to consider a block of ice of negligible thickness. The data taken have been considered mutually independent and truncated r.v.'s., see Table 1.

$T_{ m w}$	$10^{\circ}C$
$T_{ m m}$	$0^{\circ}\mathrm{C}$
Thermal Conductivity $(\kappa(\omega))$	$\kappa(\omega) \sim N_{[0.5,0.7]}(0.60, 0.10) \text{ W/m}^{o}\text{C}$
Density of the liquid (ρ)	1 kg/l
Specific heat (c_p)	$4.1868 \text{ J/g}^{\circ}\text{C}$
$D(\omega) = \frac{\kappa(\omega)}{c_p \rho}$	$D(\omega) = 14.3308 \kappa(\omega) \mathrm{mm}^2/\mathrm{min}$
Latent heat of fusion $(L(\omega))$	$L(\omega) \sim N_{[0.31, 0.35]}(0.33, 0.02) \text{ KJ/g}$
$Q(\omega) = \frac{\kappa(\omega)}{L(\omega)\rho}$	$Q(\omega) = 6 \frac{\kappa(\omega)}{L(\omega)} \text{ mm}^2/^\circ \text{C min}$

Table 1: Thermophysical properties of water and other data of the example.

The study of the numerical convergence of these approximations has been treated by means of the analysis of their absolute errors in two stages at a fixed time τ . Firstly, we have fixed the step-sizes (h, k) verifying the sufficient stability condition (20) and we have varied the number Kof Monte Carlo realizations comparing their absolute differences, AbsDiff, between two successive realizations { $K_{\ell}, K_{\ell+1}$ } using the following expressions

$$AbsDiff \left[\mu \left(u_{K_{\ell}K_{\ell+1}}(z_{i},\tau,\omega) \right) \right] = \left| AbsErr \left[\mu \left(u_{K_{\ell+1}}(z_{i},\tau,\omega) \right) \right] - AbsErr \left[\mu \left(u_{K_{\ell}}(z_{i},\tau,\omega) \right) \right] \right|,$$

$$AbsDiff \left[\sigma \left(u_{K_{\ell}K_{\ell+1}}(z_{i},\tau,\omega) \right) \right] = \left| AbsErr \left[\sigma \left(u_{K_{\ell+1}}(z_{i},\tau,\omega) \right) \right] - AbsErr \left[\sigma \left(u_{K_{\ell}}(z_{i},\tau,\omega) \right) \right] \right|,$$

$$AbsDiff \left[\mu \left(s_{K_{\ell}K_{\ell+1}}(t^{n},\omega) \right) \right] = \left| AbsErr \left[\mu \left(s_{K_{\ell+1}}(t^{n},\omega) \right) \right] - AbsErr \left[\mu \left(s_{K_{\ell}}(t^{n},\omega) \right) \right] \right|,$$

$$AbsDiff \left[\sigma \left(s_{K_{\ell}K_{\ell+1}}(t^{n},\omega) \right) \right] = \left| AbsErr \left[\sigma \left(s_{K_{\ell+1}}(t^{n},\omega) \right) \right] - AbsErr \left[\sigma \left(s_{K_{\ell}}(t^{n},\omega) \right) \right] \right|,$$

$$(22)$$

where AbsErr represents the absolute error of the mean and the standard deviation between the exact values, $u(z_i, \tau, \omega)$ and $s(t^n, \omega)$, and the approximated ones denoted by $u_K(z_i, \tau, \omega)$ and $s_K(t^n, \omega)$. Figure 1 shows how the successive absolute differences (22) decrease as the number of Monte Carlo realizations $K_{\ell} \in \{10, 20, 40, 80, 160\}$ increases for the fixed step-sizes (h, k) =(0.05, 8e - 04). In the second stage about the study of the convergence of the approximations to the both statistical moments, we have taken a fixed number of Monte Carlo realizations K, K = 1280, and we have refined the step-sizes (h, k) according to the stability condition (20). The approximations getting better due to the decreasing of the absolute errors as step-sizes decreasing up to the values (h, k) = (0.025, 2e - 04). Table 2 collects the maximum value for these absolute errors.

2 Conclusions and Future work

In this work a random free boundary problem has been addressed from the m.s. calculus point of view for the first time to our knowledge. The methodology used combines a random front-fixing method, random finite difference schemes and Monte Carlo technique. The random scheme combined with the Monte Carlo method solves the computational problem associated with random iterative methods 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 of



(c) AbsDiff(Mean of melting interface s.p.)

(d) AbsDiff(S.Deviation of melting interface s.p.)

Figure 1: Absolute differences over the $\tau = 5.1$ minutes for both statistical moments of the approximations s.p. between two successive realizations $\{K_{\ell}, K_{\ell+1}\}, K_{\ell} \in \{10, 20, 40, 80, 160\}$. The step-sizes (h, k) = (0.05, 8e - 04) are fixed and $t^n = t^0 + nk, 0 \le n \le N = 6250$ in $[t^0 = 0.1, \tau = 5.1]$.

(h,k)	(M,N)	$\ \operatorname{AbsErr}\left[\mu\left(u_{K}(z_{i},\tau,\omega)\right)\right]\ _{\infty}$ °C	$\ \operatorname{AbsErr}\left[\sigma\left(u_{K}(z_{i},\tau,\omega)\right)\right]\ _{\infty}$ °C
(0, 1, 2, 105, 0, 02)	(10, 1600)	1.0464a 02	1 1250
(0.1, 5.125e - 05)	(10, 1000)	1.9404e - 02	1.1550e – 05
(0.05, 8.0e - 04)	(20, 6250)	5.7560e - 03	5.4689e - 04
(0.025, 2.0e - 04)	(40, 25000)	2.2727e - 03	4.0980e - 04
(h,k)	(M,N)	$\ \operatorname{AbsErr}\left[\mu\left(s_{K}(t^{n},\omega)\right)\right]\ _{\infty}$ mm	$\ \operatorname{AbsErr}\left[\sigma\left(s_{K}(t^{n},\omega)\right)\right]\ _{\infty}$ mm
(0.1, 3.125e - 03)	(10, 1600)	1.3208e - 01	1.9869e - 02
(0.05, 8e - 04)	(20, 6250)	2.0884 e - 02	1.4453e - 02
(0.025, 2e - 04)	(40, 25000)	7.4025e - 03	1.3079e - 02

Table 2: Maximum values of the absolute errors for both statistical moments of the approximate temperature s.p. and the approximate melting interfaces s.p. from $t^0 = 0.1$ up to $\tau = 5.1$ minutes. The step-sizes (h, k) are refined while the number of the Monte Carlo realizations is the fixed value K = 1280. The values M and N are the spatial and temporal levels, respectively.

the approximate temperature s.p. and the approximate melting interface s.p. The numerical comparisons with the statistical moments of the exact solutions for the temperature and the melting interface allow to check the reability of the approximations computed. This method is suitable to be used to solve other types of Stefan problems.

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