STOCHASTIC TECHNIQUES FOR THE NUMERICAL SOLUTION OF ENGINEERING BOUNDARY VALUE PROBLEMS.

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Abstract. *This paper describes a family of stochastic methods based on Itô's theorem for the numerical solution of Dirichlet, Neumann and mixed boundary value problems. The major advantages of these techniques are:*

- *No mesh is needed. Only the geometry of the domain and the boundary conditions should be defined.*
- *The solution can be obtained at any point or at any part of the integration domain. It is not necessary to solve the whole domain, which can be of special interest in 3D applications.*
- *The error threshold can be controlled mainly with the step width of the random walk generation*
- *The algorithms can be easily parallelized.*
- *The same approach could be used to the numerical solution of stochastic partial differential equations.*

The theoretical approach is described, the corresponding algorithms are presented, and the general technique is applied to well-known engineering PDE equations of the elliptic and parabolic type.

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1 INTRODUCTION

From the origin of calculus in the 17th century by Isaac Newton and Gottfried Leibniz partial differential equations have been used to generate mathematical models of natural, economic and social phenomena. In general, these equations cannot be solved by analytical methods and, from the beginning of the 20th century, different approaches generating several discretization approximations have been developed (i.e. Ritz methods [1]). Since then a number of numerical methods, as Finite Differences, Finite Element Method, Boundary Element Method, Finite Calculus Techniques and many others have proved to give accurate results for quite difficult problems, both linear and nonlinear, in one, two and three dimensions.

In general, all these techniques imply some type of domain decomposition or discretization, and the solution of the problem must be obtained in the whole integration domain. As a consequence of the discretization, a set of algebraic equations (linear or nonlinear) must be solved.

A different approach to the solution of PDE's is presented in this paper. Probabilistic methods that have been developed from 1940 [2] may be used to solve both deterministic and stochastic differential equation by means of simulation techniques.

One of these possible techniques, based in Brownian motion particle simulation will be shown to be applied to elliptic and parabolic partial differential equations.

The advantages of this technique are:

- No mesh is needed. Only the geometry of the domain and the boundary conditions should be defined. This implies that the time-consuming discretization process in unnecessary.
- As it is not necessary to get the solution at every point of the domain, no system of equations must be solved.
- The solution can be obtained at any point or at any part of the integration domain. It is not necessary to determine the solution at the whole domain, and therefore there is not system of equations to solve, which can be of special interest in 3D and nonlinear problems.
- The error threshold can be controlled mainly with the step width of the random walk generation
- The algorithms can be easily parallelized.
- The same approach could be used to the numerical solution of stochastic partial differential equations [3].

In this paper the general technique for elliptic and parabolic differential equations will be presented, and will be applied to benchmark problems whose analytical solution is known.

2 PREVIOUS DEFINITIONS

2.1 Wiener processes.

A real stochastic process $\{W_t, t \geq 0\}$ is called a Wiener process if all the following requirements are accomplished:

- $W_0 = 0$
- $W_t - W_s$ is a random normal variable $N(0, t - s)$ for every t and s such that $t > s \geq 0$
- For every set of arguments $0 < t_1 < t_2 < \cdots < t_n$, the set of random variables $W_{t_1}, W_{t_{12}} - W_{t_1}, \ldots. W_{t_n} - W_{t_{-1}}$ are independent.
- W_t has continuous paths for every $t > 0$.

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2.2 Martigales

Consider a sequences of random variables $Z_1, Z_2 \ldots \ldots Z_n$ and the conditional expected value $E[Z_{n+1}|Z_1, Z_2 \ldots \ldots Z_n]$ for each n. The conditional expected value is the mean of Z_{n+1} if all values $Z_1, Z_2 \ldots \ldots Z_n$ are known. If $E[Z_{n+1}|Z_1, Z_2 \ldots \ldots Z_n] = Z_n$ the sequence, $Z_2 \ldots \ldots Z_n$ is a martingale.

The Wiener process is a Markov process as well as a martingale.

2.3 Itô's process

The stochastic process

$$dX = b(X(t), t)dt + \sigma(X(t), t)dB \tag{1}$$

in which dB is a standard Brownian motion (BM), is called an Itô's process and $b(X(t), t)$ and $\sigma(X(t), t)$ are functions both of time and the stochastic process $X(t)$. [4, 5]

2.4 Standard Brownian motion

A standard Brownian motion $B(t)$ is a Wiener process such that:
- $E[B(t)] = 0$
- $\Delta B = B(t + \Delta t) - B(t)$ has a probability distribution $N(0, s^2)$

Therefore $Var(\Delta B) = \Delta t = E(\Delta B^2) - \left(E(\Delta B)\right)^2 = E(\Delta B^2)$ and as the variance of ΔB is small it can be assumed that $\Delta t \approx \Delta B^2$. [6, 7]

2.5 Stochastic ordinary differential equations

An ordinary differential equation is only a rule which determines the change of a dependent variable which is a function of an independent variable expressed in terms of the function and its derivatives.

$$\boldsymbol{\frac{dX}{dt} = a(t, X)} \tag{2}$$

If non deterministic parameters appear in the differential system, the equation becomes a stochastic differential equation

$$\frac{dX}{dt} = a(t, X, Y) \tag{3}$$

where $Y(t)$ represents a stochastic process. It is obvious that in this case $X(t)$ is also a stochastic process and the solution will be the given by the probability distribution of $X(t)$.

2.6 Itô's integral

If one cannot integrate $a(t, X, Y)$ the stochastic ordinary differential equation can be rewritten as

$$\frac{dX}{dt} = b(X, t) + \sigma(X, t)\frac{dB(t)}{dt} \tag{4}$$

where $dB(t)$ is a standard brownian motion. The integral of the above equation is

$$X(t) = X_0 + \int_{t_0}^{t} b\big(s, X(s)\big)\, ds + \int_{t_0}^{t} \sigma\big(s, X(s)\big)dB(t) \tag{5}$$

This second integral $\int_{t_0}^{t} b\big(s, X(s)\big)dB(t)$ cannot be univocally defined, because W(s) variations are unbounded, given that $\sup \sum_{k=1}^{n-1}|B_{t_{k+1}} - B_{t_k}| = \infty$. The most correct definition

from a mathematical point of view was established by Itô in the forties and was the origin of the so called stochastic analysis [4, 5, 8, 9].

The most important property of Itô's integral is $E\left(\int_0^T G dB\right) = 0$ [10, 11].

2.7 Itô's formula

Let $u = u(t, \bar{x})$ be a continuous function defined over $[t_0, T] \times \mathbb{R}^d$ taking values in $\mathbb{R}^d$ and with continuous partial derivatives. We will use the following notation:

$$\frac{\partial}{\partial t}u(t, \bar{x}) = u_t(t, \bar{x})$$

$$\frac{\partial}{\partial x}u(t, \bar{x}) = u_x(t, \bar{x}) \tag{6}$$

$$\frac{\partial^2}{\partial x^2}u(t, \bar{x}) = u_{x^2}(t, \bar{x})$$

For $i, j = 1 \ldots d$ let $\{X, t_0 \leq t \leq T\}$ be a stochastic process in $\mathbb{R}^d$. This process is defined by the following stochastic differential (Itô's process)

$$dX = b(X(t), t)dt + \sigma(X(t), t)dB \tag{7}$$

where dB is a standard Brownian motion. Then, the process defined by

$$Y(t) = u(t, X(t)), \forall t \in [t_0, T] \tag{8}$$

can be differentiated with respect the same Brownian motion

$$dY = u_t(t, X_t)dt + u_x(t, X_t)dX + \frac{1}{2}u_{x^2}(t, X_t)\sigma^2 dt =$$

$$= \left(u_t(t, X_t) + u_x(t, X_t)b(X(t), t) + \frac{1}{2}u_{x^2}(t, X_t)\sigma^2\right)dt + u_x(t, X_t)\,\sigma(X(t), t)dB \tag{9}$$

To prove this result we apply Taylor's expansion to u,

$$du = \frac{\partial u}{\partial X}\Delta X + \frac{\partial u}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 u}{\partial X^2}\Delta X^2 + \cdots \tag{10}$$

Itô's process can be rewritten as:

$$dX = b(X(t), t)dt + \sigma(X(t), t)\sqrt{dt}$$

$$(dX)^2 = (b(X(t), t))^2 dt^2 + (\sigma(X(t), t))^2 dt + 2b(X(t), t)dt\sigma(X(t), t)\sqrt{dt} \tag{11}$$

$$(dX)^2 = (\sigma(X(t), t))^2 dt$$

By replacing dX y $(dX)^2$ in the above Taylor expansion expression

$$du = \frac{\partial u}{\partial X}(b(X(t), t)dt + \sigma(X(t), t)dB) + \frac{\partial u}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 u}{\partial X^2}(\sigma(X(t), t))^2 dt$$

$$\tag{12}$$

$$du = \frac{\partial u}{\partial X}\sigma(X(t), t)dB + dt\left(b(X(t), t)\frac{\partial u}{\partial X} + \frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial^2 u}{\partial X^2}(\sigma(X(t), t))^2\right)$$

Which is known as Itô's formula.

3 ELLIPTIC PROBLEM GENERAL APPROACH

Let be the following elliptic partial differential equation in one spatial dimension

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$$Lu = -f(x) \tag{13}$$

with Dirichlet boundary condition

$$u(x) = g(x) \; si \; x \in \partial D \tag{14}$$

being ∂D the boundary of the integration domain D and L(.)

$$L(.) = \sum b_i \frac{\partial(.)}{\partial x_i} + \frac{1}{2}\sum\sum \sigma_{ij}\frac{\partial^2}{\partial x_i \partial x_j} \tag{15}$$

that will be applied to a function $u(t, X(t))$. The du differential can be written as

$$du = \frac{\partial u}{\partial X}\sigma(X(t), t)dB + dt\left(b(X(t), t)\frac{\partial u}{\partial X} + \frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial^2 u}{\partial X^2}\big(\sigma(X(t), t)\big)^2\right) \tag{16}$$

As the problem is steady state by definition

$$\frac{\partial u}{\partial t} = 0 \tag{17}$$

and therefore

$$du = \frac{\partial u}{\partial X}\sigma(X(t), t)dB + dt(L(u)) \tag{18}$$

or

$$du = \frac{\partial u}{\partial X}\sigma(X(t), t)dB - \big(f(x)\big)dt \tag{19}$$

This equation can be integrated as

$$\int_0^{\tau_x} du = \int_0^{\tau_x}\frac{\partial u}{\partial X}\sigma(X(t), t)dB - \int_0^{\tau_x}\big(f(x)\big)dt \tag{20}$$

being τ_x the so called stopping time, which is defined as the shortest time in which the stochastic process X reaches the boundary ∂D,

$$\tau_x = \inf\left(\frac{t}{X} \in \partial D\right) \tag{21}$$

and consequently

$$u(X^{\tau_x}) - u(X^0) = \int_0^{\tau_x}\frac{\partial u}{\partial X}\sigma(X(t), t)dB - \int_0^{\tau_x}\big(f(x)\big)dt \tag{22}$$

The expected value of these expressions is

$$E\big(u(X^{\tau_x})\big) - E\big(u(X^0)\big) = E\left(\int_0^{\tau_x}\frac{\partial u}{\partial X}\sigma(X(t), t)dB\right) - E\left(\int_0^{\tau_x}\big(f(x)\big)dt\right) \tag{23}$$

As we have defined the stopping time τ_x as the shortest time in which the stochastic process X reaches the boundary ∂D, if $u(X^0)$ is the value of $u(x)$ to obtain inside the integration domain,

$$E\big(g(X^{\tau_x})\big) - u(x) = E\left(\int_0^{\tau_x}\frac{\partial u}{\partial X}\sigma(X(t), t)dB\right) - E\left(\int_0^{\tau_x}\big(f(x)\big)dt\right) \tag{24}$$

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where $g(X^{\tau_x})$ is the boundary condition at the point in which the stochastic process X reaches the boundary ∂D. Remember that dB is a martingale and one of its properties is $E\left(\int_0^T G dB\right) = 0$.

Therefore

$$E\big(g(X^{\tau_x})\big) - u(x) = 0 - E\left(\int_0^{\tau_x}(f(x))dt\right) \tag{25}$$

and the Itô's formula becomes

$$u(x) = E\big(g(X^{\tau_x})\big) + E\left(\int_0^{\tau_x}(f(x))dt\right) \tag{26}$$

3.1 Problem solution in several variables

In the case of more than one variable the elliptic problem can be stated as

$$\text{L}u = -f(\bar{x})$$
$$u(\bar{x}) = g(\bar{x}) \; si \; \bar{x} \in \partial D \tag{27}$$
$$\text{L}(.) = \sum b_i \frac{\partial(.)}{\partial x_i} + \frac{1}{2}\sum\sum \sigma_{ij}\frac{\partial^2}{\partial x_i \partial x_j}$$

The corresponding stochastic process could be written as

$$d\bar{X} = \bar{b}(\bar{x}))dt + \bar{\bar{Z}}(\bar{x}))d\bar{B} \tag{28}$$

where b_i are the components of vector $\bar{b}(\bar{x})$.

The matrix $\bar{\bar{Z}}(x)$ is defined as follows [12]

$$\bar{\bar{C}} = \bar{\bar{Z}} * \bar{\bar{Z}}^T \tag{29}$$

where σ_{ij} are the components of the $\bar{\bar{C}}$ matrix. This matrix $\bar{\bar{Z}}$ can be easily determined if $\bar{\bar{C}}$ is symmetric, by using, for example, the Cholesky factorization technique.

The b_i and σ_{ij} components are the parameters of the differential operator $\text{L}(.)$.

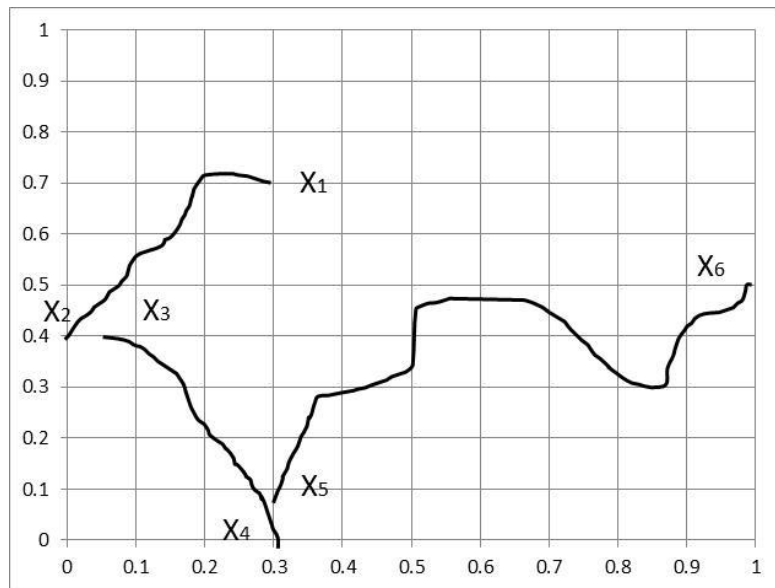## 3.2 Problems with Neumann boundary conditions

Figure 1 Particle random walk

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It must be noted that every particle follows a random walk determined by the Itô's stochastic process (Figure 1).

But in this case there are some Neumann boundary conditions. We describe now the procedure to take into account these boundaries. [13].

In a general case with Neumann boundary conditions and at least a Dirichlet boundary condition the procedure will be as follows:

$$Lu = -f(\bar{x})$$
$$u(\bar{x}) = g(\bar{x}) \ si \ \bar{x} \in \partial D_d \quad (30)$$
$$\frac{\partial\big(u(\bar{x})\big)}{\partial n} = c(\bar{x}) \ si \ \bar{x} \in \partial D_n$$

where ∂D_d are the boundaries in which Dirichlet conditions hold and ∂D_n the boundaries in which Neumann conditions are defined.

One should determine X_1 when the particle reaches a Neumann boundary before getting to a Dirichlet boundary.

$$u(X_5) = E\big(g(X^{\tau_x})\big) + E\left(\int_0^{\tau_x}(f(x))dt\right) = E\big(g(X_6)\big) + E\left(\int_{\tau_{X_5}}^{\tau_{X_6}}(f(x))dt\right) \quad (31)$$

The integration limits $\big[\tau_{X_5}, \tau_{X_6}\big]$ correspond to the time the particle takes to move from X_5 to X_6

If the coordinates X_4 correspond to a point located in a boundary with Neumann condition, the value $u(X_4)$ may be determined by Taylor expansion as

$$u(X_4) = u(X_5) - \frac{\partial u}{\partial y}(X_4)h_y = u(X_5) - c(X_4)h_y \quad (32)$$

In this way, the Neumann condition in X_4 is transformed to a Dirichlet condition and therefore:

$$u(X_3) = E\big(g(X^{\tau_x})\big) + E\left(\int_0^{\tau_x}(f(x))dt\right) = E\big(u(X_4)\big) + E\left(\int_{\tau_{X_4}}^{\tau_{X_5}}(f(x))dt\right) =$$
$$= E\big(u(X_5)\big) - E\big(c(X_4)h_y\big) + E\left(\int_{\tau_{X_4}}^{\tau_{X_5}}(f(x))dt\right) = \quad (33)$$
$$= E\big(g(X_6)\big) + E\left(\int_{\tau_{X_3}}^{\tau_{X_4}}(f(x))dt\right) + E\left(\int_{\tau_{X_5}}^{\tau_{X_6}}(f(x))dt\right) - E\big(c(X_4)h_y\big)$$

If this procedure is repeated with X_2 the solution at point X_1 can be written

$$u(X_1) = E\big(g(X^{\tau_x})\big) + E\left(\int_0^{\tau_x}(f(x))dt\right) = E\big(u(X_2)\big) + E\left(\int_{\tau_{X_1}}^{\tau_{X_2}}(f(x))dt\right) =$$
$$= E\big(u(X_3)\big) - E(c(X_3)h_x) + E\left(\int_{\tau_{X_1}}^{\tau_{X_2}}(f(x))dt\right) =$$

$$\quad (34)$$

$$= E\big(g(X_6)\big) + E\left(\int_{\tau_{X_1}}^{\tau_{X_2}}(f(x))dt\right) + E\left(\int_{\tau_{X_3}}^{\tau_{X_4}}(f(x))dt\right)$$
$$+E\left(\int_{\tau_{X_5}}^{\tau_{X_6}}(f(x))dt\right) - E\big(c(X_4)h_y\big) - E(c(X_3)h_x)$$

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In a general case Itô's formula can be written as

$$u(\bar{x}) = E\big(g(X^{\tau_x})\big) + E\left(\int_0^{\tau_x} (f(x))dt\right) + E\left(-\sum_i \frac{\partial u}{\partial n}(X_i)h_n\right) \tag{35}$$

where

$E\big(g(X^{\tau_x})\big)$ is the contribution of Dirichlet boundary conditions

$E\big(\int_0^{\tau_x}(f(x))dt\big)$ is the contribution of the input function

$E\left(-\sum_i \frac{\partial u}{\partial n}(X_i)h_n\right)$ is the contribution of Neumann boundary conditions

In these expressions X_i are the points where the particle reaches a Dirichlet boundary and h_n is a small value such that Taylor's expansions are accurate enough.

It is clear that for a unique simulation Neumann boundaries can be reached several times.

To explain more clearly the general technique we propose the following academic example.

$$\frac{\partial^2 u}{\partial x^2} + 3\frac{\partial^2 u}{\partial y^2} = -16 \tag{36}$$

with a rectangular boundary $D = (0,1)x(0,1)$ and mixed boundary conditions.

$$\frac{\partial u}{\partial x} = \beta(y) \quad x = 0$$
$$u = 0 \qquad x = 1$$

$$\tag{37}$$

$$\frac{\partial u}{\partial y} = \alpha(x) \quad y = 0$$
$$u = \gamma(x) \qquad y = 1$$

Itô's process is in this case:

$$d\bar{X} = \bar{b}(x)dt + \bar{\bar{Z}}(x)d\bar{B} \tag{38}$$

with $b_i = 0$, $\sigma_{11} = 2$, $\sigma_{12} = 0$, $\sigma_{21} = 0$, $\sigma_{22} = 6$.   :

To determine the $\bar{\bar{Z}}$ matrix we use $\bar{\bar{C}} = \bar{\bar{Z}} * \bar{\bar{Z}}^T$, this is to say

$$\begin{pmatrix} 2 & 0 \\ 0 & 6 \end{pmatrix} = \begin{pmatrix} z_{11} & z_{12} \\ z_{21} & z_{22} \end{pmatrix}\begin{pmatrix} z_{11} & z_{12} \\ z_{21} & z_{22} \end{pmatrix}^T \tag{39}$$

and therefore

$$\bar{\bar{Z}} = \begin{pmatrix} \sqrt{2} & 0 \\ 0 & \sqrt{6} \end{pmatrix} \tag{40}$$

If we apply now Itô's formula, the solution at point (x, y) is

$$u(\bar{x}) = E\big(g(X^{\tau_x})\big) + E\left(\int_0^{\tau_x}(f(x))dt\right) \tag{41}$$

In this example:

$$u(\bar{x}) = E\big(g(X^{\tau_x})\big) + E\left(\int_0^{\tau_x} 16\,dt\right) = E\big(g(X^{\tau_x})\big) + 16E\left(\int_0^{\tau_x} dt\right) =$$
$$= E\big(g(X^{\tau_x})\big) + 16E\,(T_x) \tag{42}$$

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where:

- $E\big(g(X^{\tau_x})\big)$ is the expected value of the particles positions when they reach for the first time a Dirichlet boundary condition.
- $E\,(T_x)$ is the expected value of the time the particles take to reach for the first time a Dirichlet boundary condition. In other words, the expected value of the particles stopping times.

Let a particle initially at position X_1 (see Figure 1). After a random walk as previously described the particle reaches the boundary at X_2 where a Neumann condition holds. Then the particle is reflected to X_3, and the process will be restarted at point $X_3 = X_2 + (h_x, 0)$. After the corresponding walk, the particle reaches the boundary at X_4 where again a Neumann condition holds. The particle is then reflected to $X_5 = X_4 + (0, h_y)$ and the process continues until the particle reaches a point in which a Dirichlet boundary condition holds (X_6). Then the process stops.

Let:

T_1 the time it takes the particle to go from X_1 to X_2
T_2 the time it takes the particle to go from X_3 to X_4
T_3 the time it takes the particle to go from X_5 to X_6

By using Itô's formula, the contribution of this particle to the solution is

$$u(X_1) = g(X_2) + 16(T_1) = u(X_2) + 16(T_1) \tag{43}$$

In this expression $u(X_2)$ can be expanded as $u(X_2)= u(X_3) - \frac{\partial u}{\partial x}(X_2)h_x$ and therefore

$$u = u(X_2) + 16(T_1) = u(X_3) - \frac{\partial u}{\partial x}(X_2)h_x + 16(T_1) \tag{44}$$

but

$$u(X_3) = g(X_4) + 16(T_2) = u(X_4) + 16(T_2) \tag{45}$$

and again

$$u(X_4) = u(X_5) - \frac{\partial u}{\partial y}(X_4)h_y \tag{46}$$

and the above expression (44) becomes

$$u = u(X_3) - \frac{\partial u}{\partial x}(X_2)h_x + 16(T_1) = u(X_5) - \frac{\partial u}{\partial y}(X_4)h_y - \frac{\partial u}{\partial x}(X_2)h_x + 16(T_1 + T_2) \tag{47}$$

Finally, as X_6 is a point in which a Dirichlet condition is stablished

$$u(X_5) = g(X_6) + 16(T_3) = 0 + 16(T_3) \tag{48}$$

and the contribution of this particles to the final solution is

$$u = 0 - \frac{\partial u}{\partial y}(X_4)h_y - \frac{\partial u}{\partial x}(X_2)h_x + 16(T_1 + T_2 + T_3) \tag{49}$$

3.3 Simulation procedures

The partial differential equation to solve is:

$$\mathrm{L}u = -f(x) \tag{50}$$

with the following boundary conditions:

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$$u(x) = g(x) \; si \; x \in \partial D_d$$

$$\frac{\partial u(x)}{\partial n} = t(x) \; si \; x \in \partial D_n$$

(51)

with $\partial D_d \cup \partial D_n = \partial D$ and $D_d \cap \partial D_n = \emptyset$, being ∂D the boundary of the integration domain D and

$$L(.) = \sum b_i \frac{\partial(.)}{\partial x_i} + \frac{1}{2} \sum \sum \sigma_{ij} \frac{\partial^2(.)}{\partial x_i \partial x_j}$$

(52)

As previously stated the solution is

$$u(\bar{x}) = E\big(g(X^{\tau_x})\big) + E\big(\int_0^{\tau_x}(f(x))dt\big) + E\left(-\sum_i \frac{\partial u}{\partial n}(X_i)h_n\right)$$

(53)

Then the simulation procedure is as follows:

3.3.1 Determine the Ito's process b_i y σ_{ij} coefficients:

$$d\bar{X} = \bar{b}(x)dt + \bar{\bar{Z}}(x)d\bar{B}$$

$$\begin{pmatrix} dx_1 \\ \vdots \\ dx_n \end{pmatrix} = \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix} dt + \begin{pmatrix} Z_{11} & \dots & Z_{1n} \\ \vdots & \ddots & \vdots \\ Z_{n1} & \dots & Z_{nn} \end{pmatrix} \begin{pmatrix} dB_1 \\ \vdots \\ dB_n \end{pmatrix}$$

(54)

$\bar{\bar{Z}}(x)$ is defined as the matrix calculated from the equation

$$\bar{\bar{C}} = \bar{\bar{Z}} * \bar{\bar{Z}}^T$$

(55)

where the parameters σ_{ij} are the elements of the $\bar{\bar{C}}$ matrix and the parameters b_i are the elements of the $\bar{b}(x)$ vector.

3.3.2 Set the s and h values, where s^2 is the variance of the Brownian motion process and h the increment to use in the Taylor series expansions.

The Brownian motion variance will determine the length of every leap of a particle for every time step.

The following figures show some examples of a Brownian motion process going on from the same point (x=0.6, y=2.7) with Dirichlet boundary condition at x=0 and Neumann condition at the reflecting border (Figures 2 and 3).
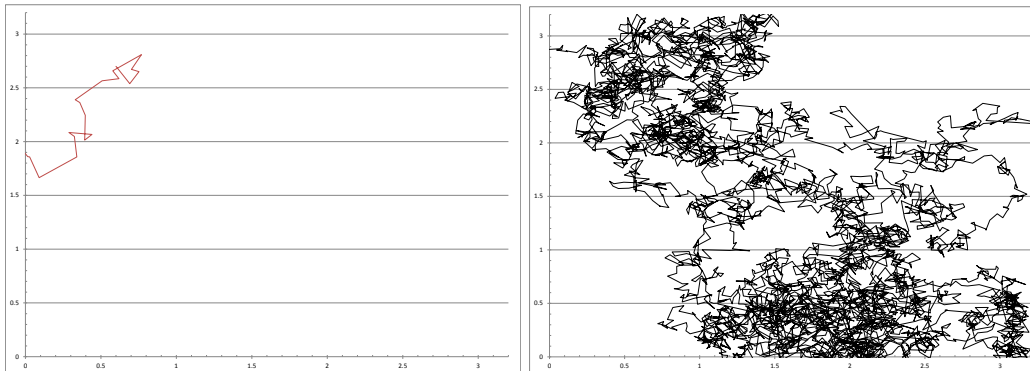
Standard deviation 0.1　　　　　　　　Standard deviation 0.05

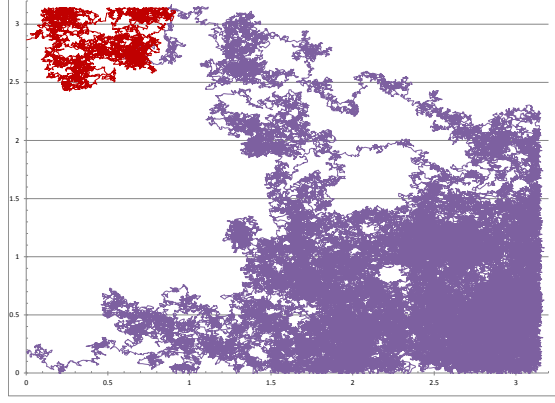**Figure 2. Examples of paths for different values of the BM standard deviation**

Figure 3. Two BM examples starting from the same point with the same standard deviation 0,01

A high value of the variance s^2 means a faster simulation process but it is generally less exact if the boundaries lie near the particle.

The h value has to be small enough to fulfill the Taylor expansion conditions but large enough to guarantee that the particle is always inside the domain of integration. In this paper a value of h five times the standard deviation of the Brownian motion process has been used, this is to say

$$h = 5\sqrt{\Delta t} = 5s$$

3.3.3 Obtain the solution in $\bar{x}$.

To obtain the problem solution we must calculate

$$u(\bar{x}) = E\big(g(X^{\tau_x})\big) + E\left(\int_0^{\tau_x}(f(x))dt\right) + E\left(-\sum_i \frac{\partial u}{\partial n}(X_i)h_n\right) \tag{56}$$

A possibility is to use Montecarlo method: we select a large number of particles for each point in which the solution must be evaluated.

From $\bar{x}$, every one of these particles performs, for each Δt, a random step defined by Itô's process, namely

$$d\bar{X} = \bar{b}(x)dt + \bar{\bar{Z}}(x)d\bar{B} \tag{57}$$

where dB is a standard Brownian motion with Gaussian distribution $N(0, s^2)$

Remember that the time spent for each particle to reach a boundary in which a Dirichlet condition holds, τ_x, is called stopping time.

The contribution of a particle to the solution is

$$u_j = \frac{\big(g(X^{\tau_x})\big) + \left(\int_0^{\tau_x}(f(x))dt\right) + \left(-\sum_i \frac{\partial u}{\partial n}(X_i)h_n\right)}{N} \tag{58}$$

where i is the number of times the particle reaches a boundary with Neumann condition, N the number of particles used in the simulation and τ_x the time spent for each particle to reach a boundary in which a Dirichlet condition holds (the so called stopping time). In equation (58):

- $g(X^{\tau_x})$ is the contribution of Dirichlet type boundary conditions. It is evaluated as the value of the boundary condition at the point first reached by the particle.
- $\int_0^{\tau_x}(f(x))dt$ is the contribution of the input function at the solution and must be evaluated until the stopping time.

- $-\sum_i \frac{\partial u}{\partial n}(X_i)h_n$ is the contribution of Neumann type boundary conditions. A particle may reach a Neumann type condition never, once or more times before reaching a point in which a Dirichlet boundary condition holds.

The final solution estimation is:

$$u = \sum_{j=1}^{N} u_j \tag{59}$$

3.4 Two dimensional examples

3.4.1 Let Ω be the unit circle defined as $x^2 + y^2 \leq 1$ in Cartesian coordinates. We state the following differential operator.

$$\Delta U = 0 \tag{60}$$

with boundary conditions

$$U(r,0) = U(r,2\pi) = 0$$

$$U(1,\theta) = \sin\left(\frac{\theta}{2}\right), \quad 0 < \theta < 2\pi \tag{61}$$

The analytical solution of this problem is $U = sin\left(\frac{\theta}{2}\right)\sqrt{r}$ (See Figure 4)

The Itô's process governing the particles motion is

$$d\bar{X} = \bar{b}(x)dt + \bar{\bar{Z}}(x)d\bar{B} \tag{62}$$

In this case $b_i = 0$, $\sigma_{i,j} = 1 \ \forall \ i = j$ and $\sigma_{i,j} = 0 \ \forall \ i \neq j$. Therefore, as $\bar{\bar{C}} = \bar{\bar{Z}} * \bar{\bar{Z}}^T$ and $\bar{\bar{C}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, it results that $\bar{\bar{Z}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.
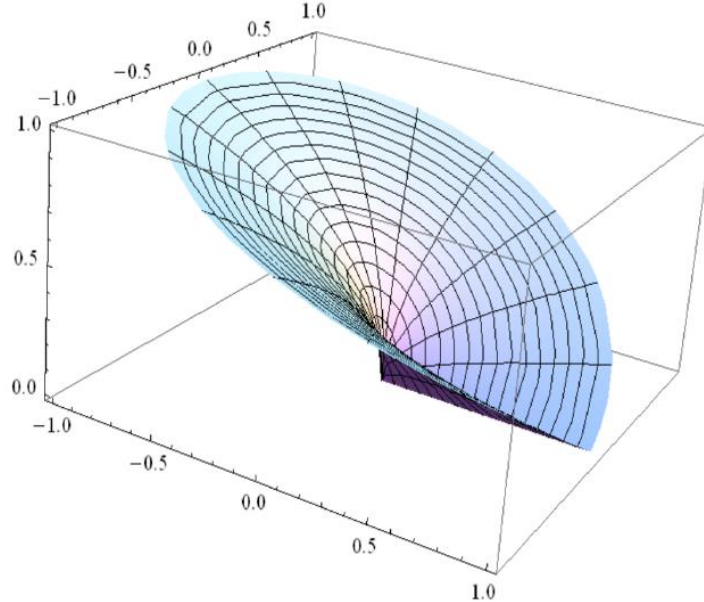

Figure 4. Analytical solution of the problem stated in section 3.4.1

It follows that $dx_1 = dB_1$ and $dx_2 = dB_2$

The numerical solution is:

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$$u(\bar{x}) = E\big(g(X^{\tau_x})\big) + E\Big(\int_0^{\tau_x}(f(x))dt\Big) \tag{63}$$

because in this example there are not Neumann boundary conditions. In this case $f(x) = 0$, and therefore

$$u(\bar{x}) = E\big(g(X^{\tau_x})\big) \tag{64}$$

where τ_x is the stopping time of each particle.

Figure 5 shows the comparison between the exact (analytical) solution and the simulation for different points of the integration domain.

For radii in the [0.3 al 0.9] interval 5.000 particles have been generated with a process standard deviation of 0.01.

For 0.2 and 0.1 radii 15.000 particles have been generated with a process standard deviation of 0.001.
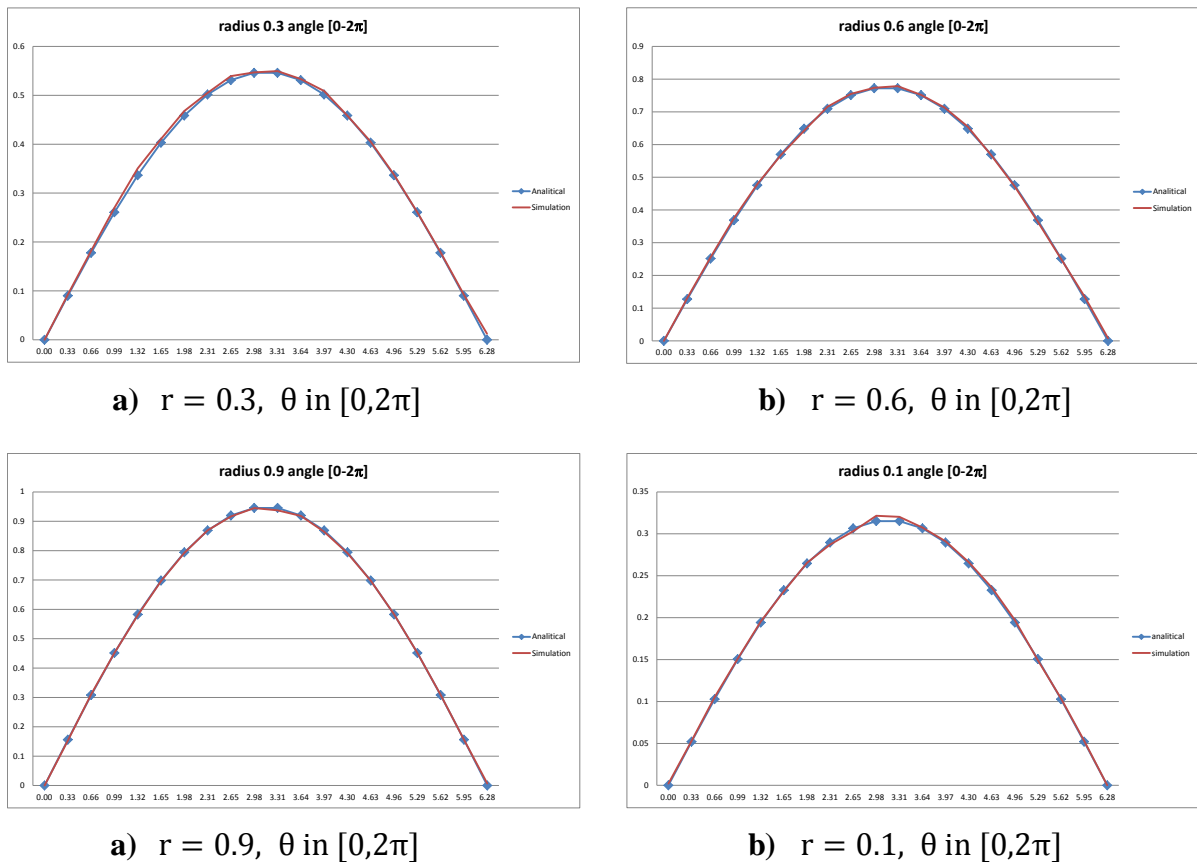

a) r = 0.3, θ in [0,2π]   **b)** r = 0.6, θ in [0,2π]

a) r = 0.9, θ in [0,2π]   **b)** r = 0.1, θ in [0,2π]

Figure 5. Simulation vs. analytical solutions of problem 3.4.1 for different domain points

3.4.2 Consider the following problem, in which both Dirichlet and Neumann boundary conditions are defined:

$$\Delta U = 0, \quad 0 \leq X \leq \pi \quad 0 \leq Y \leq \pi \tag{65}$$

with boundary conditions

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$$u(x = 0, y) = -\frac{1}{\tanh(\pi)}[\cosh(y) - \tanh(\pi)\,senh(y)]$$

$$\left.\frac{\partial u}{\partial x}\right|_{(\pi,y)} = 0; \quad 0 \le y \le \pi$$

(66)

$$\left.\frac{\partial u}{\partial y}\right|_{(x,0)} = cos(x)$$

$$\left.\frac{\partial u}{\partial y}\right|_{(x,\pi)} = 0 \quad 0 \le x \le \pi$$

The analytical solution, shown in Figure 6, is:

$$u(x, y) = -\frac{1}{\tanh(\pi)}[\cosh(y) - \tanh(\pi)\,senh(y)]\cos(x) \tag{67}$$

The Itô's process governing the particles motion is

$$d\bar{X} = \bar{b}(x)dt + \bar{\bar{Z}}(x)d\bar{B} \tag{68}$$
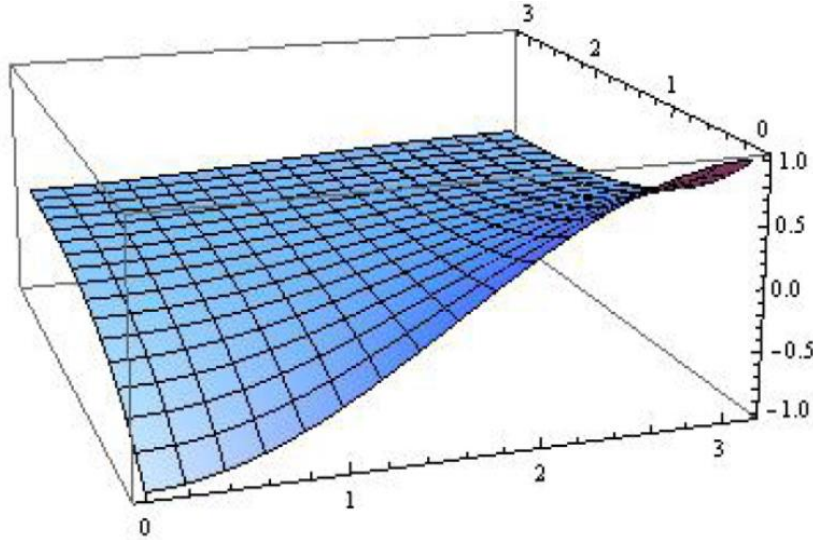
Therefore $dx_1 = dB_1$ and $dx_2 = dB_2$

Figure 6. Analytical solution of problem stated in section 3.4.2

The simulation solution is

$$u(\bar{x}) = E\big(g(X^{\tau_x})\big) + E\left(\int_0^{\tau_x}(f(x))dt\right) + E\left(-\sum_i \frac{\partial u}{\partial n}(X_i)h_n\right) \tag{69}$$

because in this case $f(x) = 0$

15.000 particles have been generated for each point, the h value is 0.05 and the standard deviation of the Brownian motion is 0.01.

Figure 5 shows the comparison between the exact (analytical) solution and the simulation for different points of the integration domain.
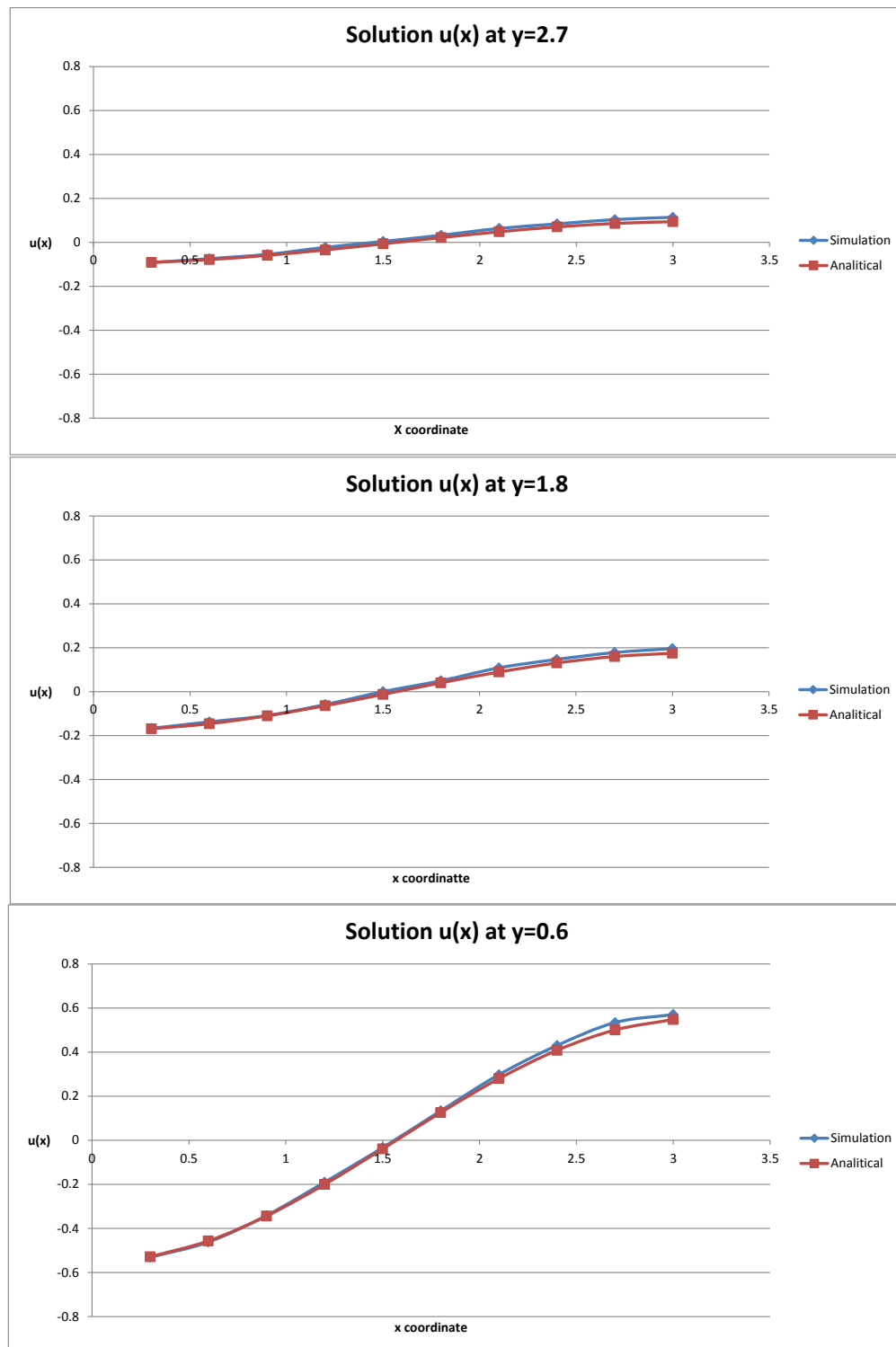
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Figure 7. Simulation vs. analytical solutions of problem 3.4.2 for different domain points

4 PARABOLIC PROBLEM GENERAL APPROACH

Consider the following partial differential equation:

$$\mathrm{L}(u) = -f(\bar{x}, t) \tag{70}$$

with boundary and initial conditions:

$$u(\bar{x}, t) = g(\bar{x}, t) \; si \; \bar{x} \in \partial D_d$$

$$\frac{\partial u(\bar{x}, t)}{\partial n} = c(\bar{x}, t) \; if \; \bar{x} \in \partial D_n \qquad (71)$$

$$u(\bar{x}) = l(\bar{x}) \; if \; t = 0$$

with $t > 0$, $\bar{x} \in D$, $\partial D_d \cup \partial D_n = \partial D$ and $D_d \cap \partial D_n = \emptyset$, being ∂D the boundary of the integration domain D. The $L(.)$ operator can be written as

$$L(.) = -\frac{\partial(.)}{\partial t} + \sum b_i \frac{\partial(.)}{\partial x_i} + \frac{1}{2} \sum \sum \sigma_{ij} \frac{\partial^2}{\partial x_i \partial x_j} \qquad (72)$$

where the time *t* may be considered as a new coordinate in the process.

In the n-dimensional case

$$d\bar{X} = \bar{b}(x)dt + \bar{\bar{Z}}(x)d\bar{B} \qquad (73)$$

that can also be written as

$$\begin{pmatrix} dx_0 \\ dx_1 \\ \vdots \\ dx_n \end{pmatrix} = \begin{pmatrix} -1 \\ b_1 \\ \vdots \\ b_n \end{pmatrix} dt + \begin{pmatrix} 0 & \cdots & 0 \\ Z_{11} & \cdots & Z_{1n} \\ \vdots & \ddots & \vdots \\ Z_{n1} & \cdots & Z_{nn} \end{pmatrix} \begin{pmatrix} dB_0 \\ dB_1 \\ \vdots \\ dB_n \end{pmatrix} \qquad (74)$$

where x_0 is the time coordinate and x_i, $i \in (0, n)$ the spatial coordinates.

At every time interval dt, the particle moves randomly in the space (x_i) and goes back a fixed time increment dt.

If the particle reaches a Neumann boundary condition, the particle bounces back and continues the random motion inside the integration domain.

The initial condition $u(\bar{x}) = l(\bar{x})$ if $t = 0$ is, in this process, considered as a Dirichlet boundary condition.

The particle random motion may stop because:

- Particle reaches a Dirichlet boundary in the space (x_i)
- Particle reaches time t=0, because, as it was stated before, this initial condition works as a Dirichlet Condition for this simulation process.

4.1 Two dimensional parabolic example

To explain more clearly the general technique we propose the following academic example:

The PDE to solve is:

$$\frac{\partial u}{\partial t} = \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \qquad (75)$$

with integration domain $0 \le x \le 2$, $0 \le y \le 4$, $t \ge 0$ (see Figure 8) and boundary conditions

$$\frac{\partial u(x = 0, y, t)}{\partial x} = 0, \qquad u(x, y = 0, t) = 0$$

$$\frac{\partial u(x = 2, y, t)}{\partial x} = 0, \quad u(x, y = 4, t) = 0 \qquad (76)$$

_____

and the inital condition

$$u(x, y, t = 0) = 7 \tag{77}$$

$$u(x, y = 4, t) = 0$$

$$\frac{\partial u(x = 0, y, t)}{\partial x} = 0 \qquad\qquad \frac{\partial u(x = 2, y, t)}{\partial x} = 0$$

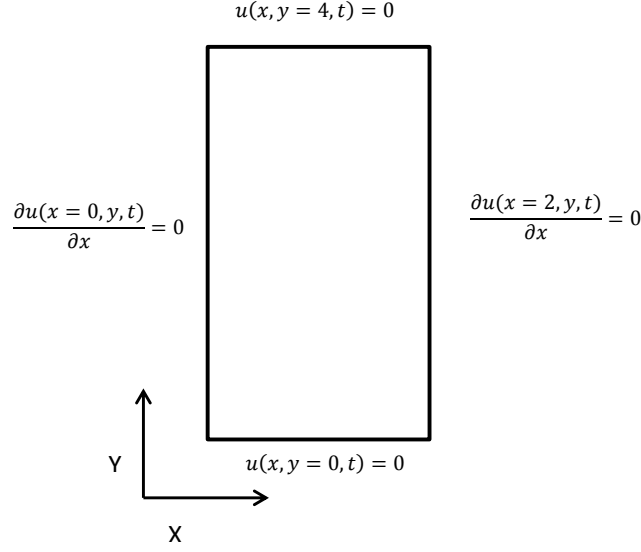Y $u(x, y = 0, t) = 0$

X

Figure 8. Integration domain for the problem presented in section 4.1

The analytical solution for this problem is:

$$u(x, y, t) = \frac{14}{\pi} \sum_{n=1}^{\infty} (1 - \cos(n\pi)) \left(\frac{1}{n}\right) e^{\left(\frac{-t\pi^2 n^2}{16}\right)} \sin\left(\frac{n\pi y}{4}\right) \tag{78}$$

The stochastic process approach is

$$\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) - \frac{\partial u}{\partial t} = 0$$

$$L(.)u(x)) - f(x)$$

$$f(x) = 0 \tag{79}$$

$$L(.) = \sum_i b_i \frac{\partial.}{\partial x_i} + \frac{1}{2} \sum_{ij} \sigma_{ij} \frac{\partial^2}{\partial x_i \partial x_j}$$

In this case $i = 0, 1, 2$ y $j = 0, 1, 2$.
The Itô process can be written as

$$d\bar{X} = \bar{b}(x)dt + \bar{\bar{Z}}(x)d\bar{B} \tag{80}$$

or

$$\begin{pmatrix} dx_0 \\ dx_1 \\ dx_2 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix} dt + \begin{pmatrix} 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} \begin{pmatrix} dB_0 \\ dB_1 \\ dB_2 \end{pmatrix} \tag{81}$$

with $dB = N(0, dt)$.

_____

The estimate of the solution is

$$u(\bar{x}) = E\big(g(X^{\tau_x})\big) + E\left(\int_0^{\tau_x}(f(x))dt\right) + E\left(-\sum_i \frac{\partial u}{\partial n}(X_i)h_n\right) \qquad (82)$$

The second and third addends are null because $f(x) = 0$ and all Neumann boundary conditions are also null.

Then

$$u(\bar{x}) = E\big(g(X^{\tau_x})\big) \qquad (83)$$

where τ_x is the already defined stopping time.

Suppose we want to calculate the problem solution at a point with coordinates (x, y, t). As always, the simulation solution is to generate a number of particles at this point and apply the above described technique..
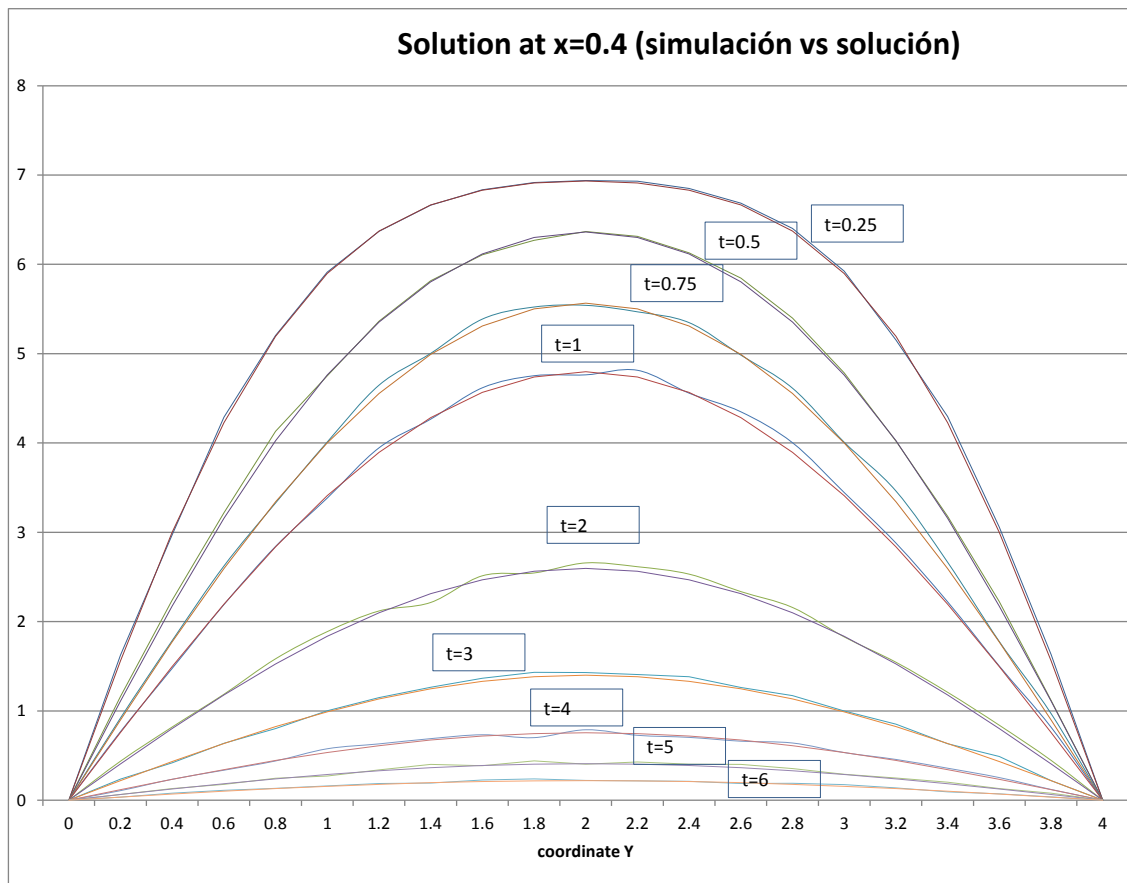

Figure 9. Solution of the problem proposed in section 4.1

5 CONCLUSIONS

A simulation stochastic method to solve partial differential equations (of elliptic and parabolic type) has been presented. The analysis of the specific boundary and (in the parabolic type) initial conditions has been carried out. A number of academic examples, with known analytical solutions, have been used as benchmarks, and the simulation solution has agreed very well with the exact solutions in all cases.

The main advantages of this technique are:

- No domain discretization is necessary.

- No need for a solver, because there are not systems of equations in the solution process
- It is not necessary to solve the PDE in the whole integration domain. The solution can be obtained only where it is needed (a point, several points, a particular area of the domain).
- In parabolic problems, to obtain the solution at time T_f it is not necessary to obtain it at intermediate times $(T_0; T_f)$.
- The approximation error is a function of the number of particles generated in the simulation, and decreases as the number of particles increases. This is so because the solution is an expected value, and because of the central limit theorem the variance will decrease as the number of elements (particles) increases.
- The speed of the process increases as the variance of the stochastic process (Itô's process) increases. However, near the boundaries, the variance should be kept small enough as the walk does not go outside the domain
- As the solution estimate is an expected value, parallel methods may be applied in a very easy way. For instance, the same accuracy will be obtained with a CPU generating a 10.000 particles simulation as with 100 CPU's generating a 100 particles simulation each. As the only process that can be considered time consuming is the particles generation and the corresponding random walk, the process time can be directly divided by the number of CPU's in the cluster.

6 AKNOWLEGMENTS

7 REFERENCES

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