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SOLUTION OF LINEAR AND NONLINEAR DIFFUSION PROBLEMS VIA STOCHASTIC DIFFERENTIAL EQUATIONS

Abstract

act The equation for nonlinear diffusion can be rearranged to a form that immediately leads to its stochastic analog. The latter contains a drift term that is absent when the diffusion coefficient is constant. The dependence of this coefficient on concentration (or temperature) is handled by generating many paths in parallel and approximating the derivative of concentration with respect to distance by the central difference. This method works for one-dimensional diffusion problems with finite or infinite boundaries and for diffusion in cylindrical or spherical shells. By mimicking the movements of molecules, the stochastic approach provides a deeper insight into the physical process. The parallel version of our algorithm is very efficient. The 99% confidence limits for the stochastic solution enclose the analytical solution so tightly that they cannot be shown graphically. This indicates that there is no systematic difference in the results for the two methods. Finally, we present a direct derivation of the stochastic method for cylindrical and spherical shells.

Keywordsnonlinear diffusion, stochastic differential equations, Wiener process,
Itô process, Kolmogorov backward equation

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1. Introduction

Heat and mass diffusion occur in many situations, both natural and industrial. The diffusion coefficient is often treated as a constant if its variation with temperature or concentration (respectively) is not very large. The transient case is then represented by a linear second-order partial differential equation (PDE), which has an analytical solution. Results for many such cases are summarized and organized in the definitive book by Crank [2]. If the variation is substantial, the transient case requires a numerical treatment, such as the Finite Element Method (FEM).

The relationship between the stochastic and differential equation approaches was established by Kolmogorov [6]. His forward equation was anticipated by the Fokker-Plank equation; his backward equation was new. Thus, it is well known [7, 10] that such a linear PDE can be recast (via the Fokker-Planck equation) as a first-order stochastic differential equation (SDE). Laso [7] emphasized the simplicity of the SDE and noted that it provides a more natural interpretation of transport phenomena. This is especially true in mass diffusion, where the random movement of the "particles" in the simulation mimic one component of the random movement of the molecules in the diffusion process. The principal contribution of his paper was to supply the stochastic equivalencies of all of the usual boundary conditions.

We showed how the one-dimensional nonlinear PDE could be converted to an SDE [1]. We extend this treatment by stating the general equation for nonlinear diffusion and converting it to an SDE. This leads to easy solutions of linear problems and new solutions of nonlinear. In particular, some common problems in two or three dimensions can be solved as one-dimensional SDEs by appropriately defining the physical regions corresponding to bins in the simulation. These examples were chosen to facilitate comparisons with transient solutions of the linear problem and steady-state solutions of the nonlinear.

2. Nonlinear diffusion

The general equation for diffusion is

$$\frac{\partial \theta}{\partial t} = \nabla \cdot \left[\alpha(\theta) \, \nabla \theta \right] \tag{1}$$

where θ is concentration or temperature, α is the diffusion coefficient, $\nabla \cdot$ is the divergence and ∇ is the gradient. To convert this to an SDE, we note that

$$\nabla^2 \left[\alpha(\theta) \,\theta \right] = \nabla \cdot \nabla \left[\alpha(\theta) \,\theta \right] = \nabla \cdot \left[\alpha \nabla \theta + \theta \, \frac{d\alpha}{d\theta} \,\nabla \theta \right] \tag{2}$$

where ∇^2 is the Laplacian. Thus

$$\nabla \cdot (\alpha \nabla \theta) = -\nabla \cdot \left[\theta \, \frac{d\alpha}{d\theta} \, \nabla \theta \right] + \nabla^2 \left[\alpha(\theta) \, \theta \right] \tag{3}$$

where the RHS of Equation (3) has the form of Laso's Equation (1).

We apply this equation in Cartesian, cylindrical, and spherical coordinates where the dependence is only on x, r, and r respectively.

When α is constant, Equation (1) reduces to

$$\frac{\partial\theta}{\partial t} = \alpha \nabla^2 \theta \tag{4}$$

which greatly simplifies the problem.

3. One-dimensional nonlinear diffusion into an infinite medium

In our earlier paper [1], we derived the stochastic equivalent of the nonlinear secondorder partial differential equation (PDE)

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial x} \left[\alpha(\theta) \frac{\partial\theta}{\partial x} \right] \tag{5}$$

The one-dimensional version of Equation (3) is

$$\frac{\partial}{\partial x} \left[\alpha(\theta) \frac{\partial \theta}{\partial x} \right] = -\frac{\partial}{\partial x} \left[\theta \frac{d\alpha}{d\theta} \frac{\partial \theta}{\partial x} \right] + \frac{\partial^2}{\partial x^2} \left[\alpha(\theta) \theta \right]$$
(6)

which yields

$$dX(t) = \frac{d\alpha}{d\theta} \frac{\partial\theta}{\partial x} dt + \sqrt{2\alpha(\theta)} \, dW(t) \tag{7}$$

from Laso's Equations (2) and (3). The origin of the terms in Equation (7) is obvious from Equation (6).

Equation (5) is a Cartesian version of Equation (1). In Equation (7), W is a onedimensional Wiener process [5], so X is a random variable. This equivalence depends on the generation of a great many paths in parallel [1] to yield $\theta(x, t)$.

Though computations were time consuming, we were able to demonstrate proof of concept. A remarkable increase in the speed of computation has made this simple method fast and accurate. We first demonstrate the speed and accuracy by studying nonlinear diffusion into an infinite medium.

4. Stochastic algorithm

Table 1 defines the variables and shows their values. For diffusion into an infinite medium, the algorithm corresponding to Equation (7) is

1. Set N_{bin} , N_b , Δx_b , Δx , Δt (see Table 1), and $\theta_j = 0$, $j = 1, \ldots, N_{\text{bin}}$ (according to initial condition, Equation (10)). This implies placing zero particles in the inner bins.

Parameter	Symbol	Value
Number of bins	$N_{\rm bin}$	100
Number of particles in boundary region	N_b	$100,000 \ (196,608)^{\dagger}$
Width of bin	Δx	0.01
Width of boundary region	Δx_b	0.05
Time step	Δt	$10^{-5} (10^{-6})$

 Table 1

 Simulation parameters.

[†] For parallel version

2. Calculate $N_0 = (\Delta x / \Delta x_b) N_b$.

- 3. Distribute N_b particles uniformly in $[-\Delta x_b, 0]$.
- 4. For each particle in the system, generate a random number ξ_i from the standard normal distribution and move each particle according to

$$X_i(t + \Delta t) = X_i(t) + \left(\frac{\theta_{j+1} - \theta_{j-1}}{2\Delta x}\right) \left.\frac{d\alpha}{d\theta}\right|_{\theta_j} \Delta t + \sqrt{2\alpha_j \Delta t} \,\xi_i \tag{8}$$

where α_j and θ_j are the values of α and θ for the bin in which the *i*th particle is located. From the boundary condition (Equation (9)), $\theta_0 = 1$.

- 5. For each bin, $(x_{j-1}, x_j]$, $x_j = j\Delta x$, calculate $\theta_j = N_j/N_0$, and hence $\alpha_j = f(\theta_j)$.
- 6. If any particle has reached the last bin, terminate the program; otherwise, return to 3.

The last step provides a termination in a finite time.

Our earlier work [1] showed that the central difference is, by far, the most accurate approximation of $\partial\theta/\partial x$. In all of our examples, α increases with θ . Consider the one-dimensional flow of heat from left to right. In (8), $d\alpha/d\theta > 0$ and $\theta_{j+1} < \theta_{j-1}$, so the additional term slows the rate of diffusion compared to the case where the conductivity is constant.

To demonstrate that our method can handle extreme variations in $\alpha(\theta)$, we examine the case where $\alpha(\theta) = e^{\theta}$ and compare the results with those of Crank [2]. The boundary and initial conditions are

$$\theta = 1, \, x = 0, \, t \ge 0 \tag{9}$$

$$\theta = 0, \, x > 0, \, t = 0 \tag{10}$$

Our Equation (5) corresponds to Equation (7.5) of Crank and our Equations (9) and (10) to his Eqs. (7.15) and (7.16). His iterative solution involving a change of variables is described starting on page 105 (7.2.1. Boltzmann's transformation). The next subsection (7.2.2. Numerical iterative methods) describes the solution of the resulting ODE via a double integration.

5. Speed and accuracy

Figure 1a shows the essentially perfect agreement between the average values from the stochastic method with a step-size of 10^{-6} and Crank's solution. This was also true for

$$\alpha(\theta) = (1 - \lambda \theta)^{-1}, \ \lambda = 1/2$$

and

$$\alpha(\theta) = (1 - \lambda \theta)^{-2}, \ (1 - \lambda)^{-2} = 2$$

with that step-size and the same initial and boundary conditions. The results with a step-size of 10^{-5} were just as regular, but often showed a tendency to underestimate Crank's solution *very* slightly as shown in Figure 1b. In a few instances, this step-size produced results that were as good as (and sometimes better than) the smaller. Of course, the runs with the larger step-size took roughly 1/10 of the time.



Figure 1. θ vs. $x/(4t)^{1/2}$, $\alpha(\theta) = e^{\theta}$: a) $\Delta t = 10^{-6}$; b) $\Delta t = 10^{-5}$.

6. Parallel version of the algorithm

Trajectories of individual particles are independent, so the parallel version of the algorithm is straightforward. It is sufficient to distribute the trajectories (equally) among available processors (cores). Moreover, in the linear case (constant diffusion coefficient), the whole process can run asynchronously. For the nonlinear case (when the diffusion coefficient is a function of dimensionless concentration or temperature), consecutive time-steps have to be synchronized in the sense that the concentration vector α at time t must be known to calculate trajectories at time $t + \Delta t$ according to

Equation (8). Then the time-step run on node k, k = 1, ..., K, entails the following steps:

- 1. Distribute N_b/K particles uniformly in $[-\Delta x_b, 0]$.
- 2. For each particle in the system, move the particle according to Equation (8) and calculate new partial concentrations $\theta_i^k(t + \Delta t)$.

On completion, when all the values of $\theta_j^k(t + \Delta t)$ are known, the main core calculates and distributes the total concentration $\theta_j(t + \Delta t) = \sum_{k=1}^{K} \theta_j^k(t + \Delta t)$ and $\alpha_j(t + \Delta t) = f(\theta_j(t + \Delta t))$.

For optimal performance, the number of particles N_b should be a multiple of the number of cores, K. The program was written in C++ with OpenMPI Infiniband library. The tests were performed on a Hewlett-Packard Cluster Platform BL with a total of 17516 cores (12 cores per node); processors Intel Xeon (L5420, L5640, X5650, E5645, depending on the node), 2.26 - 2.66 GHz, 16 - 24 GB operating memory per node running under Scientific Linux 6.

	Table 2		
Execution times (average	value from 10 runs,	$N_b = 196,608)$ for	$\mathbf{r} \alpha(\theta) = e^{\theta}$

Number of cores	Time ([s] per iteration step)
1^{\dagger}	0.0554
1	0.1095
2	0.0508
4	0.0252
12	0.0078
24	0.0048

[†] Sequential version

Table 2 shows benchmarks for $\alpha(\theta) = e^{\theta}$. The times are in seconds per iteration step (average value from 10 runs). The number of particles, N_b , was 196,608. Thus, a time-step of 10^{-5} seconds implies a run time of approximately $10^5 \times 4.8 \times 10^{-3}$ seconds = 8 minutes to reach t = 1 (dimensionless units), which is very practical.

7. Nonlinear heat conduction in a one-dimensional homogeneous solid

After checking that our solutions to linear problems agreed with those of Laso [7], we used Equation (8) to calculate the transient solutions that approach the steady state. The initial and boundary conditions are

$$\theta = 0, \ 0 < x \le 1, \ t = 0$$

$$\theta = 1 \text{ at } x = 0, \ \theta = 0 \text{ at } x = 1 \text{ for } t \ge 0$$

A simple change of variable leads to the convenient boundary conditions shown above [7]. Our intervals are $(x_i, x_{i+1}]$, so our initial condition differs slightly from that of Laso. In particular, the initial condition $\theta = 0$, $0 < x \le 1$ does not violate the boundary condition $\theta = 1$ at x = 0. As noted by him, $\theta = 0$ at x = 1 is an absorbing boundary [4, 9]. All trajectories that reach the absorbing boundary are terminated. The algorithm for this case is:

- 6. Remove all particles that exit the last bin.
- 7. If the preset time has expired, terminate the program; otherwise, return to 3.

Many other boundary conditions are possible [7], but we will use only the absorbing boundary for the rest of the examples. This facilitates comparison with other methods.

Figure 2 shows the close agreement with results calculated by the Finite Element Method (FEM).



Figure 2. Plane sheet, $\alpha(\theta) = e^{\theta}$.

8. Diffusion in a hollow cylinder

In our variables (assuming cylindrical symmetry of the diffusion, i.e. $\partial \theta / \partial \phi = \partial \theta / \partial z = 0$), Crank's equation (1.7) is

$$\frac{\partial \theta}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[r \,\alpha(\theta) \,\frac{\partial \theta}{\partial r} \right] \tag{11}$$

To facilitate comparisons with the plane-sheet (one-dimensional) case, we use the boundary and initial conditions

$$\theta = 1, r = 1, t \ge 0$$

$$\theta = 0, r = 2, t \ge 0$$

$$\theta = 0, 1 < r \le 2, t = 0$$

Completing the differentiation on the RHS of Equation (11), we get

$$\frac{\partial\theta}{\partial t} = \alpha(\theta) \frac{\partial^2\theta}{\partial r^2} + \left[\frac{d\alpha}{d\theta} \frac{\partial\theta}{\partial r} + \frac{\alpha}{r}\right] \frac{\partial\theta}{\partial r}$$
(12)

which has the form of Kolmogorov's backward equation [3]. Thus, the corresponding stochastic equation is

$$dR(t) = \left(\frac{d\alpha}{d\theta}\frac{\partial\theta}{\partial r} + \frac{\alpha}{r}\right)dt + \sqrt{2\alpha(\theta)}dW(t)$$
(13)

This equation may also be derived by applying Itô's formula [3] to change coordinates in Equation (7) from rectangular to polar (see Section 11).



Figure 3. Hollow cylinder: a) $\alpha(\theta) = e^{\theta}$; b) $\alpha(\theta) = 1 + 0.2\theta$.

We note that Equation (13) contains a drift term that is not present in Equation (7). This extra term pushes the process away from the origin. The influence of noise tends to move the process away from any concentrically confined area.

The algorithm corresponding to Equation (13) is as described in Sections 4 and 7, with the exception that we change Equation (8) to

$$R_i(t + \Delta t) = R_i(t) + \left[\left(\frac{\theta_{j+1} - \theta_{j-1}}{2\Delta r} \right) \left. \frac{d\alpha}{d\theta} \right|_{\theta_j} + \frac{\alpha_j}{R_i} \right] \Delta t + \sqrt{2\alpha_j \Delta t} \xi_i \qquad (14)$$

We applied our method to solve the SDE with $\alpha(\theta) = 1$, $\alpha(\theta) = e^{\theta}$ and $\alpha(\theta) = 1+0.2\theta$. For constant diffusion coefficient, α , the results were compared to the exact ones given by Crank [2, Equation (5.62)]. When α was a function of concentration, the steadystate solution was calculated from Crank's Equation (9.11), while the approximate solutions were obtained numerically using FEM. Figure 3 shows the close agreement with the curves calculated using FEM.

9. Diffusion in a hollow sphere

We applied our method to the problem of heat conduction in a hollow sphere with the inner surface r = 1 and outer surface r = 2. The concentration is a function of radius r and time t. The boundary and initial conditions are the same as those for the hollow cylinder. The diffusion equation in spherical coordinates, assuming symmetry, is [2, Equation (1.8)]

$$\frac{\partial\theta}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left[\alpha(\theta) r^2 \frac{\partial\theta}{\partial r} \right]$$
(15)

This is equivalent to

$$\frac{\partial\theta}{\partial t} = \alpha(\theta) \frac{\partial^2\theta}{\partial r^2} + \left[\frac{d\alpha}{d\theta} \frac{\partial\theta}{\partial r} + \frac{2\alpha}{r}\right] \frac{\partial\theta}{\partial r}$$
(16)

which is Kolmogorov's backward equation corresponding to the SDE

$$dR(t) = \left(\frac{d\alpha}{d\theta}\frac{\partial\theta}{\partial r} + \frac{2\alpha}{r}\right)dt + \sqrt{2\alpha(\theta)}\,dW(t) \tag{17}$$

The derivation of Equation (17) using Itô's formula is given in Section 11.

The extra drift term is similar to that for a cylinder but twice as strong. Thus, Equation (8) takes the form

$$R_i(t + \Delta t) = R_i(t) + \left[\left(\frac{\theta_{j+1} - \theta_{j-1}}{2\Delta r} \right) \left. \frac{d\alpha}{d\theta} \right|_{\theta_j} + \frac{2\alpha_j}{R_i} \right] \Delta t + \sqrt{2\alpha_j \Delta t} \,\xi_i \tag{18}$$

We used our method to solve the SDE with $\alpha(\theta) = 1$, $\alpha(\theta) = e^{\theta}$ and $\alpha(\theta) = 1 + 0.2\theta$. The results for the first case agreed closely with the exact values given by Crank's Equation (6.50). When α varied with θ , approximate solutions were obtained numerically using FEM. Figure 4 shows the very close agreement.



Figure 4. Hollow sphere: a) $\alpha(\theta) = e^{\theta}$; b) $\alpha(\theta) = 1 + 0.2\theta$.

10. Steady-state solutions

Crank [2] provides steady-state solutions for the case where the diffusion coefficient depends on concentration. His Equation (9.1) is

$$\frac{d}{dx}\left(\alpha \,\frac{d\theta}{dx}\right) = 0\tag{19}$$

and his solutions for the one-dimensional plane sheet, cylindrical shell, and spherical shell are given by his equations (9.7), (9.11), and (9.12) respectively. Our steady-state solutions were obtained by running the simulations until no further changes occurred. Figures 5a, b show the steady-state solutions for $\alpha(\theta) = e^{\theta}$ and $\alpha(\theta) = 1 + 0.2\theta$ respectively for the three cases.



Figure 5. Steady state: a) $\alpha(\theta) = e^{\theta}$; b) $\alpha(\theta) = 1 + 0.2\theta$.

11. Direct derivation of the SDEs for cylindrical and spherical coordinates

A vector-valued stochastic process $(\mathbf{X}_t)_{t\geq 0}$ is called a vector Itô process if $d\mathbf{X}_t = (dX_{1,t}, \ldots, dX_{n,t})$ is related to an underlying *n*-dimensional standard Brownian motion $(\mathbf{W}_t)_{t\geq 0} = (W_{1,t}, \ldots, W_{n,t})$ by

$$dX_{i,t} = a_{i,t}dt + \sum_{j=1}^{n} b_{ij,t}dW_{j,t}$$
(20)

Let $f = f(\boldsymbol{x}, t)$ be some sufficiently differentiable function on $\mathbb{R}^{n+1} = \mathbb{R}^n \times \mathbb{R}$, $\boldsymbol{x} = (x_1, \ldots, x_n)$. Then Itô's lemma for vector processes states that [8]

$$df(\boldsymbol{X}_t, t) = \frac{\partial f}{\partial t} dt + \sum_j \frac{\partial f}{\partial x_j} dX_{j,t} + \frac{1}{2} \sum_{j,k} \frac{\partial^2 f}{\partial x_j x_k} dX_{j,t} dX_{k,t}$$
(21)

where $dW_i dW_j = \delta_{ij} dt$, $dW_i dt = dt dW_i = 0$.

11.1. Cylindrical coordinates

In cylindrical coordinates, $x = r \cos \phi$ and $y = r \sin \phi$. Then

$$f_1(x,y) = r = (x^2 + y^2)^{\frac{1}{2}}$$
(22)

and

$$f_2(x,y) = \phi = \arctan\frac{y}{x} \tag{23}$$

We have

$$\frac{\partial f_1}{\partial x} = \frac{x}{(x^2 + y^2)^{\frac{1}{2}}}, \quad \frac{\partial^2 f_1}{\partial x^2} = \frac{y^2}{(x^2 + y^2)^{\frac{3}{2}}}$$
(24)

$$\frac{\partial f_1}{\partial y} = \frac{y}{(x^2 + y^2)^{\frac{1}{2}}}, \quad \frac{\partial^2 f_1}{\partial y^2} = \frac{x^2}{(x^2 + y^2)^{\frac{3}{2}}}$$
(25)

Let (W_1, W_2) be a two-dimensional Wiener process, and let a two-dimensional Itô process be defined via

$$dX = a(t, x, y)dt + b(t, x, y)dW_1$$
(26)

and

$$dY = a(t, x, y)dt + b(t, x, y)dW_2$$
(27)

A coordinate transformation is specified by functions f_1 and f_2 defining two new coordinates r, ϕ . Inserting (22) into (21) we get the expression

$$dR = \frac{\partial f_1}{\partial x} dX + \frac{\partial f_1}{\partial y} dY + \frac{1}{2} \frac{\partial^2 f_1}{\partial x^2} dX dX + \frac{1}{2} \frac{\partial^2 f_1}{\partial y^2} dY dY$$
(28)

All of the other terms in the Itô formula are zero. Inserting (24)–(27) into (28) we get

$$dR = \frac{x}{(x^2 + y^2)^{\frac{1}{2}}} \left(a \, dt + b \, dW_1 \right) + \frac{y}{(x^2 + y^2)^{\frac{1}{2}}} \left(a \, dt + b \, dW_2 \right) + \frac{1}{2} \frac{b^2}{(x^2 + y^2)^{\frac{1}{2}}} \, dt$$
(29)

which is equivalent to

$$dR = \cos\phi \left(a \, dt + b \, dW_1\right) + \sin\phi \left(a \, dt + b \, dW_2\right) + \frac{b^2}{2r} \, dt \tag{30}$$

In our case, the concentration is a function of radius r and time t only and does not depend on the choice of ϕ . Hence, we can assume $\phi = 0$ simplifying (30) to

$$dR = (a + \frac{b^2}{2r}) dt + b \, dW_1 \tag{31}$$

11.2. Spherical coordinates

In spherical coordinates,

$$x = r \sin \psi \cos \phi, \ y = r \sin \psi \sin \phi, \ z = r \cos \psi$$

Then

$$f_1(x, y, z) = r = (x^2 + y^2 + z^2)^{\frac{1}{2}}$$
(32)

$$f_2(x, y, z) = \psi = \arccos \frac{z}{r}$$
(33)

$$f_3(x, y, z) = \phi = \arctan \frac{y}{x} \tag{34}$$

and

$$\frac{\partial f_1}{\partial x} = \frac{x}{(x^2 + y^2 + z^2)^{\frac{1}{2}}}, \quad \frac{\partial^2 f_1}{\partial x^2} = \frac{y^2 + z^2}{(x^2 + y^2 + z^2)^{\frac{3}{2}}}$$
(35)

$$\frac{\partial f_1}{\partial y} = \frac{y}{(x^2 + y^2 + z^2)^{\frac{1}{2}}}, \quad \frac{\partial^2 f_1}{\partial y^2} = \frac{x^2 + z^2}{(x^2 + y^2 + z^2)^{\frac{3}{2}}}$$
(36)

$$\frac{\partial f_1}{\partial z} = \frac{z}{(x^2 + y^2 + z^2)^{\frac{1}{2}}}, \quad \frac{\partial^2 f_1}{\partial z^2} = \frac{x^2 + y^2}{(x^2 + y^2 + z^2)^{\frac{3}{2}}}$$
(37)

In the spherical case, we consider the three-dimensional Wiener process (W_1, W_2, W_3) defined by

$$dX = a(t, x, y, z)dt + b(t, x, y, z)dW_1$$
(38)

$$dY = a(t, x, y, z)dt + b(t, x, y, z)dW_2$$
(39)

$$dZ = a(t, x, y, z)dt + b(t, x, y, z)dW_3$$
(40)

Then

$$dR = \frac{\partial f_1}{\partial x} dX + \frac{\partial f_1}{\partial y} dY + \frac{\partial f_1}{\partial z} dZ + + \frac{1}{2} \frac{\partial^2 f_1}{\partial x^2} dX dX + \frac{1}{2} \frac{\partial^2 f_1}{\partial y^2} dY dY + \frac{1}{2} \frac{\partial^2 f_1}{\partial z^2} dZ dZ$$
(41)

Inserting (35)-(40), we get

$$dR = \frac{x}{(x^2 + y^2 + z^2)^{\frac{1}{2}}} (a \, dt + b \, dW_1) + \frac{y}{(x^2 + y^2 + z^2)^{\frac{1}{2}}} (a \, dt + b \, dW_2) + \frac{z}{(x^2 + y^2 + z^2)^{\frac{1}{2}}} (a \, dt + b \, dW_3) + \frac{b^2}{(x^2 + y^2 + z^2)^{\frac{1}{2}}} dt$$
(42)

which is equivalent to

$$dR = \sin\psi\cos\phi(a\,dt + b\,dW_1) + \sin\psi\sin\phi(a\,dt + b\,dW_2) + + \cos\psi(a\,dt + b\,dW_3) + \frac{b^2}{r}dt$$
(43)

Assuming $\psi = \pi/2$ and $\phi = 0$,

$$dR = \left(a + \frac{b^2}{r}\right)dt + b\,dW_1\tag{44}$$

12. Conclusions

The stochastic method can solve any of the problems typically handled by separation of variables plus others that require numerical methods (such as FEM). The stochastic approach has the advantage of simplicity and clarity. It replaces a second-order partial differential equation with a first-order stochastic one. Linear and nonlinear diffusion are treated in the same way. The only difference is an added term in the latter. Stochastic solutions show clearly why nonlinear transfer is slower than linear. Unlike the classical approach (which is essentially a mathematical exercise), the simulation mimics the flow of heat or mass in the actual problem. Pedagogically, it reminds us that the actual process is random.

The stochastic approach is well-suited for parallel computation. Computing requirements are already modest, and further improvements in speed and capacity can be expected.

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References

- Bargieł M., Tory E.M.: Stochastic dynamic solution of nonlinear differential equations for transport phenomena. American Institute of Chemical Engineers Journal, vol. 42(3), pp. 889–891. doi:10.1002/aic.690420327, 1996.
- [2] Crank J.: The Mathematics of Diffusion. Oxford University Press, second ed., 1975.
- [3] Etheridge A.: A Course in Financial Calculus. Cambridge University Press, first ed., 2002.
- [4] Gardiner C.W.: Handbook of Stochastic Methods: for Physics, Chemistry and the Natural Sciences. Springer-Verlag New York, second ed., 1985.
- [5] Kloeden P.E., Platen E.: Numerical Solution of Stochastic Differential Equations. Springer-Verlag, Berlin-Heidelberg, first ed., 1992.
- Kolmogorov A.: Über die analytischen Methoden in der Wahrscheinlichkeitsrechnung. Mathematische Annalen, vol. 104(1), pp. 415–458, 1931.
- [7] Laso M.: Stochastic dynamic approach to transport phenomena. American Institute of Chemical Engineers Journal, vol. 40(8), pp. 1297–1311. doi: 10.1002/aic.690400804, 1994. ISSN 1547-5905.
- [8] Øksendal B.K.: Stochastic Differential Equations: An Introduction with Applications. Springer-Verlag, Berlin-Heidelberg, sixth ed., 2003.
- [9] Risken H.: The Fokker-Planck Equation: Methods of Solutions and Applications. Springer-Verlag, Berlin-Heidelberg, second ed., 1989.
- [10] Van Kampen N.: Stochastic Processes in Physics and Chemistry. Elsevier Amsterdam, third ed., 2007.

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