Stochastic Dynamic Solution of Nonlinear Differential Equations for Transport Phenomena

Monika Bargiel and Elmer M. Tory
Dept. of Mathematics and Computer Science, Mount Allison University, Sackville, NB, E0A 3C0, Canada

It is well known (van Kampen, 1981) that a *linear* second-order partial differential equation (PDE) such as

$$\frac{\partial\theta}{\partial t} = \alpha\frac{\partial^2\theta}{\partial x^2} \tag{1}$$

(where θ is the temperature T or the concentration C) can be recast, via the Fokker-Planck equation (FPE), as a first-order stochastic differential equation (SDE) such as

$$dX(t) = \sqrt{2\alpha}\,dW(t) \tag{2}$$

However, PDEs have been consistently preferred in chemical engineering applications. In Eq. 2, W is a one-dimensional Wiener process (Kloeden and Platen, 1992) which implies that X is a random variable. The common types of boundary conditions can also be transformed and the values of θ are obtained from the probability density function (pdf) $p(t, x)$ by a trivial rescaling (Laso, 1994). This pdf is estimated from a large number of individual solutions of the SDE.

Transformation of Nonlinear Problems to Stochastic Form

Suppose that we want to solve the *nonlinear* PDE

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial x}\left[\alpha(\theta)\frac{\partial\theta}{\partial x}\right] \tag{3}$$

To convert this to a SDE, we note that

$$\frac{\partial^2}{\partial x^2}[\alpha(\theta)\theta] = \frac{\partial}{\partial x}\left[\alpha(\theta)\frac{\partial\theta}{\partial x} + \frac{d\alpha}{d\theta}\frac{\partial\theta}{\partial x}\theta\right] \tag{4}$$

so

$$\frac{\partial}{\partial x}\left[\alpha(\theta)\frac{\partial\theta}{\partial x}\right] = -\frac{\partial}{\partial x}\left[\frac{d\alpha}{d\theta}\frac{\partial\theta}{\partial x}\theta\right] + \frac{\partial^2}{\partial x^2}[\alpha(\theta)\theta] \tag{5}$$

which has the form of Laso's Eq. 1 with

$$A(t, x) = \frac{d\alpha}{d\theta}\frac{\partial\theta}{\partial x} \tag{6}$$

Thus, the corresponding SDE is

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

Laso (1994) notes that sample paths for the diffusion process can be generated either sequentially or in parallel. If a great many paths are generated in parallel, nonlinear diffusion is a Pickard-Tory process (Pickard and Tory, 1987). The number of particles in $(x_k, x_{k+1}]$ at t_i provides an estimate of the value of θ and hence α. Given α, the trajectories are independent. Each particle moves, in each time step, according to the value of α corresponding to its position. However, α is also a random variable, being determined by the empirical estimate of θ which is itself evolving.

The algorithm corresponding to Eq. 7 is

(1) Set N_{bin}, N_b, Δx_b, Δx, Δt.
(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 bin, $(x_k, x_{k+1}]$, calculate $\theta_j = N_j/N_0$ and hence $\alpha_j = f(\theta_j)$.
(5) For each particle in the system, generate a random number ϕ_i from the standard normal distribution and move each particle according to

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

where α_j and θ_j are the values of α and θ for the bin in which the ith particle is located.

(6) If any particle has reached the last bin, terminate the program, otherwise return to 3.

The first three steps are those in Laso's algorithm. N_0 is the number of particles (in a bin) corresponding to the

Correspondence concerning this note should be addressed to E. M. Tory.

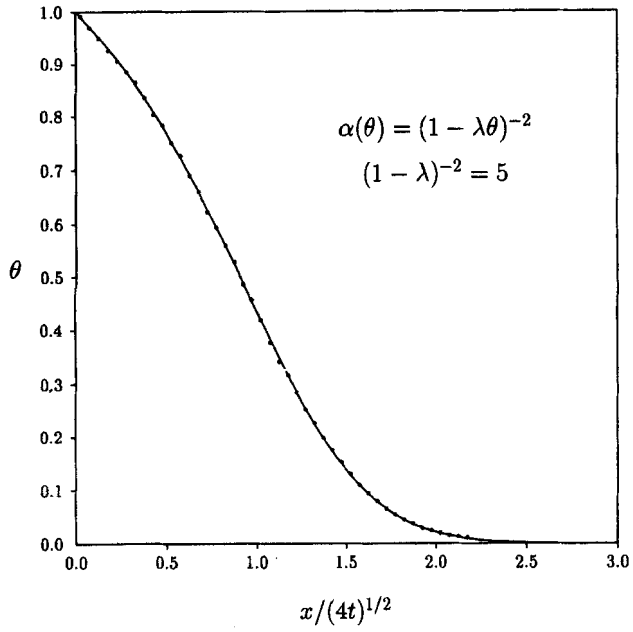

Figure 1. Nonlinear diffusion.

Points represent values averaged over 0.05 on the abscissa. The variation in α from $\alpha(0) = 1$ to $\alpha(1) = 5$ was the most extreme of the seven test cases.

boundary temperature or concentration. Thus, θ_j is the dimensionless temperature or concentration. This is a very simple way of rescaling the probability density. In the absence of a second boundary, some particles would eventually move beyond the last bin. The last step terminates the program before this happens.

Comparison of Solutions of Nonlinear Diffusion Equations

We solved Eq. 3 with $\theta = C/C_0$ and boundary and initial conditions (Crank, 1956)

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

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

for seven different diffusivity functions $\alpha(\theta)$ and plotted our results as θ vs. $x/(4t)^{1/2}$ as shown in Figure 1. The points are average values and the solid line is the curve calculated by Crank's method. Raw data and average values for all cases are given by Bargiel and Tory (1995). Table 1 shows the parameters used for these cases. When the central difference (Eq. 8) was used, agreement between the stochastic and traditional methods was almost perfect in five cases and excellent in the other two. The backward and forward differences gave results which were too large and too small, respectively, even for a time step of 10^{-6}. When the central difference was not used, a time step of 10^{-5} produced meaningless results. The temperature gradient has the physical meaning of a flux (Laso, 1994), but a SDE using this equivalence (Bargiel and Tory, 1995) worked less well than Eq. 8. Once the gradient is well established, the term in Δt in Eq. 8 is much less important than that in $\sqrt{\Delta t}$. Since the expected value of $|\phi_i|$ is 2.0, most particles move less than 0.01 in one time step. Thus, the central difference is less variable than the net flux between adjacent bins.

Table 1. Values of Parameters

Parameter	Symbol	Value
No. of particles in boundary region	N_b	10,000
Width of boundary region	Δx_b	0.05
No. of bins	N_{bin}	100
No. of particles corresponding to $\theta = 1$	N_0	2,000
Width of bin	Δx	0.01
Time step	Δt	10^{-5}

Discussion

The stochastic dynamic approach will work for virtually any $\alpha(\theta)$ encountered in practice. Our algorithm is only slightly slower than Laso's and is equally applicable to all of his eight fundamental boundary conditions. We used only one boundary condition (Eq. 9) because Crank's methods, which use the Boltzmann transformation, do not work (Crank, 1956, p. 149) when there is a second boundary condition at a finite distance.

In a real diffusion process, the astronomical number of particles ensures that random fluctuations have little or no significance in most cases. The simulation generates a much smaller number of trajectories and the histogram of bin-count frequencies forms a discrete approximation of what is essentially a continuous pdf. In all of our examples

$$\theta_2 > \theta_1 \Rightarrow \alpha(\theta_2) > \alpha(\theta_1) \tag{11}$$

This ensures that values of θ which are too high (low) in certain regions will cause diffusion rates there to be too high (low) also. Thus, the process is stable to perturbations and there is no need for smoothing provided that the number of trajectories is large enough to avoid extreme fluctuations. It follows that the advantages which Laso (1994) has cited also hold when the diffusion coefficient varies with temperature or concentration.

Each run took 2 to 3 h on a SUN SPARCstation 1+. Though these times would be much shorter with a modern workstation, the simplicity and versatility of the stochastic dynamic method will become more important as computational speed increases still further. Also, the method is well suited for parallel or vector computation. Thus, we will study other problems for which the SDE may have advantages.

Acknowledgments

We thank C. H. Hesse and several referees for helpful comments. This work was supported in part by the Natural Sciences and Engineering Research Council of Canada under grants OGP001268 and EQP0092826.

Notation

$A(t, x)$ = drift term
f = function relating α to θ
N_b = number of particles in boundary region corresponding to boundary temperature or concentration
N_{bin} = number of bins
N_j = number of particles in jth bin

N_0 = number of particles (in a bin) corresponding to the boundary temperature or concentration
t = time
t_i = particular value of t
Δt = time integration step
T = temperature
W = Wiener process
x = coordinate
x_k = particular value of x
Δx = width of bin
Δx_b = width of boundary region
X = random variable representing position
X_i = random variable representing position of ith particle

Greek letters

α_j = value of α for particles in jth bin
θ_j = value of θ for particles in jth bin
λ = constant
ϕ_i = random number from a standard Gaussian distribution

Literature Cited

Bargiel, M., and E. M. Tory, "Stochastic Dynamic Solution of Nonlinear Differential Equations for Transport Phenomena," Mount Allison Research Report M/CS 95-2 (May, 1995).

Crank, J., *The Mathematics of Diffusion*, 1st ed., Oxford University Press, Oxford (1956).

van Kampen, N. G., *Stochastic Processes in Physics and Chemistry*, North-Holland, Amsterdam (1981).

Kloeden, P. E., and E. Platen, *Numerical Solution of Stochastic Differential Equations*, Springer-Verlag, Berlin (1992).

Laso, M., "Stochastic Dynamic Approach to Transport Phenomena," *AIChE J.*, **40**(8), 1297 (1994).

Pickard, D. K., and E. M. Tory, "A Markov Model for Sedimentation: Fundamental Issues and Insights," *Advances in the Statistical Sciences*, Vol. IV, Stochastic Hydrology, I. B. MacNeill and G. J. Umphrey, eds., D. Reidel Publishing, Dordrecht (1987).

Manuscript received Jan. 19, 1995, and revision received May 12, 1995.