NUMERICAL SOLUTION FOR THE NONLINEAR FOKKER-PLANCK EQUATION

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1. Introduction

Nonlinear Fokker-Planck (F.P.) equations are not amenable to closed form solutions in most of the cases. Some approximate methods have been developed, which are valid for certain cases [1,2]. It is possible to obtain exact numerical solution of the nonlinear Fokker-Planck equation and this will be the content of this talk.

The finite difference methods [3] employed to obtain the numerical solution, and a modified alogorithm, which reduces the computational time drastically, are discussed. The method is illustrated with a sample problem of diffusion in bistable potential [4].

Method of Solution

Let us consider the nonlinear F.P. equation of the form

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[f(x)P(x,t)\right] + \epsilon \frac{\partial^2 P(x,t)}{\partial x^2} \tag{1}$$

where f(x) is a nonlinear function of x. This is a second order partial differential equation, with boundary conditions specified by $P(x,t) \longrightarrow 0$ as $x \longrightarrow \pm \infty$. The initial conditions are given by specifying P(x,t) at t = 0. The finite difference method for solution of this equation proceeds as follows. A mesh structure is imposed on the variable x and t, the mesh widths being Δx and Δt respectively. Let j and k represent the x-mesh and t-mesh indices. Then the finite difference equations for P(x,t) at $t = t_{k+1}$ are given by

$$a_1 P_{j,k+1} + a_2 P_{j-1,k+1} + a_3 P_{j+1,k+1} - P_{j,k} = 0, \quad j = 2,\cdots(N-1) \tag{2}$$

Here N represents the number of meshes in the x-domain, k denotes the time step, previous to the time step under consideration. a_1, a_2 and a_3 are given by

$$a_1 = \left\{-f'(x_j) - \frac{2\epsilon}{\Delta x^2}\right\}\Delta t - 1.0 \tag{3}$$

$$a_2 = \left\{\frac{2\epsilon}{\Delta x^2} + \frac{f(x_j)}{2\Delta x}\right\}\Delta t \tag{4}$$

$$a_3 = \left\{\frac{2\epsilon}{\Delta x^2} + \frac{f(x_j)}{2\Delta x}\right\}\Delta t \tag{5}$$

$f'(x_j)$ denotes the first derivative of f(x) at $x = x_j$. Starting from the given initial distribution of P(x,t) at t = 0, the equations reduce to a tridiagonal set of equations involving $P_{j,k+1}, P_{j-1,k+1}$ and $P_{j+1,k+1}$. These equations are solved to obtain $P_{j,k+1}$ for j = 2,..N-1. Now the entire solution can be obtained in steps of Δt.

It can be easily seen that the other physical restrictions (1) $P(x,t)$ is non-negative for all x at all times and (2) $P(x,t)$ is normalized to unity at time t, are automatically satisfied, if one chooses an initial distribution, which is nonnegative and normalized to unity, (provided proper choice of Δx and Δt are made). Caution should be exercised in the choice of Δx and Δt, since finite difference approximations are valid only for small Δx and Δt. The choice of Δx is dictated by the accuracy with which $P(x,t)$ is computed at time t. It is essential that the function $P(x,t)$ does not vary much over the meshwidth Δx, since the finite difference approximation assumes $P(x,t)$ to be constant over the interval Δx. This in turn implies a small Δt, since the numerical procedure becomes unstable otherwise. It can be shown that, the numerical solution obtained with a large meshwidth Δx, depicts unphysical behaviour of being negative over some region of x. The normalization of $P(x,t)$ is also not preserved.

The computational time required for the numerical solution goes as N^2. As Δx is necessarily small, N is a large number in most cases and an appreciable amount of computational time is called for, to obtain accurate solutions. Hence it is advantageous to have algorithms which reduce the computer time requirements. The algorithm that has been developed by us, is based on continuous modification of Δx and the range in which $P(x,t)$ is computed. The method becomes transparent in the context of a particular example, which we will now discuss.

Consider the nonlinear F.P. equation given by

$$\frac{\partial P(x,t)}{\partial t} = -\left[(\gamma x - g x^3)\, P(x,t)\right] + \epsilon \frac{\partial^2 P(x,t)}{\partial x^2} \qquad (6)$$

(For relevance of this equation to diffusion in bistable potential, see [4]). We choose $\gamma = g = 1$ and $\epsilon = 0.5 \times 10^{-6}$. Consider the case where the initial condition is specified to be a Gaussian distribution of mean = .005 and variance = 1.0×10^{-6}. This is a sharply peaked function around the mean value. Hence, though the actual boundaries are at $\pm\infty$, one can set the boundaries at values close to the peak position (say x_{b1} and x_{b2}) to evaluate the initial evolution of $P(x,t)$. The number of meshes required to represent the function accurately is now determined as follows. Choose an arbitrary value of Δx and represent the initial distribution by the corresponding histogram. Compare the moments of the histogram, with the actual moments of the initial distribution. If the comparison is not good, decrease Δx until good comparison is achieved. Now with this value of Δx and with the boundary condition of $P(x,t+\Delta t)$ equal to zero at $x = x_{b1}$ and x_{b2}, solve for $P(x,t+\Delta t)$. This is continued for, say, ten steps of Δt (i.e. upto time $t = t_1$). Now the boundaries and Δx are modified based on the distribution of $P(x,t)$ at the time $t = t_1$. The evolution of $P(x,t)$ in the next few steps of Δt is obtained with the boundary conditions applied at the new boundaries and with the modified meshwidth. This is continued till $P(x,t)$ is obtained in the entire range of time.

2. Discussion

The numerical solution for the sample problem, using usual finite difference methods took one hour with Δx set equal to .0001. The modified algorithm required only ten minutes resulting in a reduction of computer time by a factor of ten. P(x,t) obtained using this algorithm has been shown in figure 1, at three typical times. It is seen that the expected nongaussian feature of P(x,t) is well represented. The first two moments of P(x,t) computed from this solution, were found to compare extremely well with the results of the Monte Carlo simulation of the corresponding nonlinear Langevin equation [4].

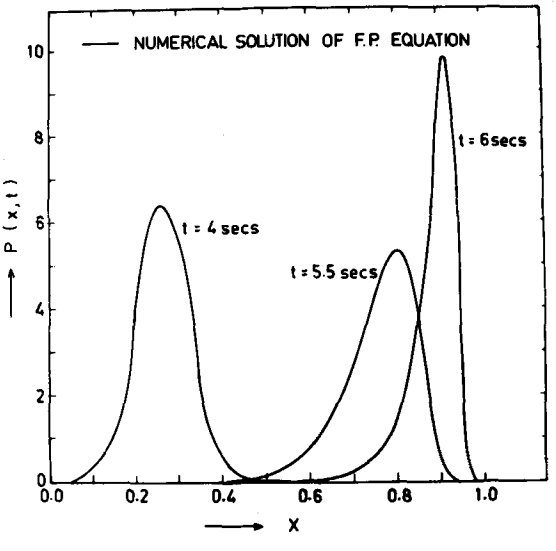

Fig.1 Numerical solution of (5) for $\gamma = g = 1$; $\epsilon = 0.5 \times 10^{-6}$ and an initial Gaussian distribution of mean = .005 and variance = 1.0×10^{-6}

The numerical solution to (5) was also obtained, in the case of a initial Gaussian distribution with zero mean and an initial variance of 1.0×10^{-6}. In this case, the steady state solution has two peaks at $x = \pm 1$. The numerical solution obtained for this case has been reported in (4). Since more than one peak is found, the modified algorithm discussed above could not be applied, asymptotically. This is because, in the above algorithm, uniform Δx is assumed in the entire x-domain, at any time t. A superior algorithm applicable in any general case, is possible, with variable mesh widths in the x-domain. The meshwidth in any region of x-domain, can be fixed based on the value of the first derivative of the function P(x,t) in that region. This algorithm is presently being developed by us.

References

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