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AN IMPROVED WPE METHOD FOR SOLVING DISCONTINUOUS FOKKER-PLANCK EQUATIONS

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Abstract. In mathematical studies of molecular motors, the stochastic motor motion is modeled using the Langevin equation. If we consider an ensemble of motors, the probability density is governed by the corresponding Fokker-Planck equation. Average quantities, such as, average velocity, effective diffusion and randomness parameter, can be calculated from the probability density. The WPE method was previously developed to solve Fokker-Planck equations (H. Wang, C. Peskin and T. Elston, J. Theo. Biol., Vol. 221, 491-511, 2003). The WPE method has the advantage of preserving detailed balance, which ensures that the numerical method still works even when the potential is discontinuous. Unfortunately, the accuracy of the WPE method drops to first order when the potential is discontinuous. Here we propose an improved version of the WPE method. The improved WPE method a) maintains the second order accuracy even when the potential is discontinuous, b) has got rid of a numerical singularity in the WPE method, and c) is as simple and easy to implement as the WPE method. Numerical examples are shown to demonstrate the robust performance of the improved WPE method.

Key Words. Fokker-Planck equation, detailed balance, numerical solutions.

1. Introduction

Molecular motors are samll, and, as a result, the motor operation is dominated by high viscous friction and large thermal fluctuations from the surrounding fluid environment [1]. In general, a molecular motor has many internal and external degrees of freedom. One of these degrees of freedom is associated with the motor's unidirectional motion, the main biological function of the motor. For example, a kinesin dimer walks along a microtubule toward the positive end [5, 6]. There are many levels of models for molecular motors, from simple kinetic models with a few states to all atom molecular dynamics. In a modeling approach of intermediate level, the unidirectional motion is followed explicitly and the effects of other degrees of freedom are modeled in the mean field potential affecting the unidirectional motion [7, 8, 9].

To introduce this modeling approach of intermediate level, we consider the one dimensional motion of a small object in water. The motion of the object is governed by the Newton's second law:

$$m\frac{dv}{dt} = -\zeta v - \phi'(x) + \sqrt{2k_BT\zeta}\,\frac{dW(t)}{dt} \tag{1}$$

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where x is the coordinate along the dimension of motion, m is the mass and $v = \frac{dx}{dt}$ the velocity of the object, ζ is the drag coefficient, $\phi(x)$ a potential affecting the motion of object, and $W(t)$ is the Weiner process. The object is affected by a) the drag force $-\zeta v$, which is always opposing the motion, b) the force derived from the potential, and c) the Brownian force. Both the drag force and the Brownian force are caused by the bombardments of surrounding water molecules. The amplitude of Brownian force is related to the drag coefficient as $\sqrt{2k_BT\zeta}$, which is a result of the fluctuation-dissipation theorem [16, 17, 18]. Here k_B is the Boltzmann constant and T the absolute temperature [13].

In (1), there is a very short time scale associated with the object forgetting about its instantaneous velocity. It is called the time scale of inertia [11]. For both theoretical analysis and numerical solutions, it is more convenient to get rid of this short time scale and make the system non-stiff. We start by rewriting (1) as

$$\frac{dv}{dt} = -\frac{1}{t_0}\left[v - \left(-D\frac{\phi'(x)}{k_BT} + \sqrt{2D}\frac{dW(t)}{dt}\right)\right] \tag{2}$$

where $D = \frac{k_BT}{\zeta}$ is the diffusion coefficient, and $t_0 = \frac{m}{\zeta}$ has the dimension of time. In (2), in the absence of potential $\phi(x)$, the autocorrelation of the instantaneous velocity satisfies

$$\langle v(s)v(s+t)\rangle = \langle v^2(s)\rangle \exp\left(\frac{-t}{t_0}\right) \tag{3}$$

where $\langle\cdot\rangle$ denotes the average. It is clear that the object forgets about its current velocity after a small multiples of t_0. That is why t_0 is called the time scale of inertia. In the simple case where the object is a spherical bead of radius σ, the mass and the drag coefficient are respectively [1]

$$m = \frac{4}{3}\pi\rho\sigma^3 \quad , \qquad \zeta = 6\pi\eta\sigma \tag{4}$$

where ρ is the density and η the viscosity of water. The time scale $\frac{m}{\zeta}$ is proportional to the square of radius: $t_0 = \frac{m}{\zeta} = O\left(\sigma^2\right)$. Consequently, for small objects, the time scale $t_0 = \frac{m}{\zeta}$ is extremely small. For a bead of $1\mu m$ in diameter, the time scale of inertia is $t_0 = 56 \times 10^{-9}s = 56ns$ [10].

When t_0 is very small, (2) is well approximated by

$$v = \left[-D\frac{\phi'(x)}{k_BT} + \sqrt{2D}\frac{dW(t)}{dt}\right] \tag{5}$$

The reduction from (2) to (5) in the limit of small t_0 is called the Einstein-Smoluchowski limit [16, 14]. This reduction can be illustrated intuitively by considering a simple model equation: $y' = -\frac{1}{t_0}(y - f(t))$. The exact solution of the model equation is given by

$$\begin{aligned} y(t) &= f(t) + \exp\left(\frac{-t}{t_0}\right)(y(0) - f(t)) \\ &\quad + \frac{1}{t_0}\int_0^t \exp\left(\frac{-(t-s)}{t_0}\right)(f(s) - f(t))\,ds \end{aligned} \tag{6}$$

When t_0 is small and $t >> t_0$, the exact solution satisfies approximately $y(t) = f(t)$, which is comparable to (5). Writing (5) as a differential equation for x, we obtain

$$\frac{dx}{dt} = -D\frac{\phi'(x)}{k_BT} + \sqrt{2D}\frac{dW(t)}{dt} \tag{7}$$