A SECOND-ORDER STOCHASTIC LEAP-FROG ALGORITHM FOR LANGEVIN SIMULATION*

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Abstract

Langevin simulation provides an effective way to study collisional effects in beams by reducing the six-dimensional Fokker-Planck equation to a group of stochastic ordinary differential equations. These resulting equations usually have multiplicative noise since the diffusion coefficients in these equations are functions of position and time. Conventional algorithms, e.g. Euler and Heun, give only first order convergence of moments in a finite time interval. In this paper, a stochastic leap-frog algorithm for the numerical integration of Langevin stochastic differential equations with multiplicative noise is proposed and tested. The algorithm has a second-order convergence of moments in a finite time interval and requires the sampling of only one uniformly distributed random variable per time step. As an example, we apply the new algorithm to the study of a mechanical oscillator with multiplicative noise.

1 INTRODUCTION

Multiple Coulomb scattering of charged particles, also called intra-beam scattering, has important applications in accelerator operation. It causes a diffusion process of particles and leads to an increase of beam size and emittance. This results in a fast decay of the quality of beam and reduces the beam lifetime when the size of the beam is large enough to hit the aperture [1].

An appropriate way to study the multiple Coulomb scattering is to solve the Fokker-Planck equations for the distribution function in six-dimensional phase space. Nevertheless, the Fokker-Planck equations are very expensive to solve numerically even for dynamical systems possessing only a very modest number of degrees of freedom. Truncation schemes or closures have had some success in extracting the behavior of low-order moments, but the systematics of these approximations remains to be elucidated. On the other hand, the Fokker-Planck equations can be solved using an equivalent Langevin simulation, which reduces the six-dimensional partial differential equations into a group of stochastic ordinary differential equations. Compared to the Fokker-Planck equation, stochastic differential equations are not difficult to solve, and with the advent of modern supercomputers, it is possible to run very large numbers of realizations in order to compute low-order moments accurately. In general, the noise in these stochastic ordinary differential equations are multiplicative instead of additive since the dynamic friction coefficient and diffusion coefficient in the Fokker-Planck equations depend on the spatial position. An effective numerical algorithm to integrate the stochastic differential equation with multiplicative noise will significantly improve the efficiency of large scale Langevin simulation.

The stochastic leap-frog algorithms in the Langevin simulation are given in Section II. Numerical tests of this algorithms is presented in Section III. A physical application of the algorithm to the multiplicative-noise mechanic oscillator is given in Section IV. The conclusions are drawn in Section V.

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2 STOCHASTIC LEAP-FROG ALGORITHM

In the Langevin simulation, the stochastic particle equations of motion that follow from the Fokker-Planck equation are (Cf. Ref. [2])

$$\mathbf{r}' = \mathbf{v}, \tag{1}$$

$$\mathbf{v}' = \frac{\mathbf{F}}{m} - \nu\mathbf{v} + \sqrt{D}\mathbf{\Gamma}(t), \tag{2}$$

where $\mathbf{F}$ is the force including both the external force and the self-generated mean field space charge force, m is the mass of particle, ν is friction coefficient, D is the diffusion coefficient, and $\mathbf{\Gamma}(t)$ are Gaussian random variables with

$$\langle \Gamma_i(t) \rangle = 0, \tag{3}$$

$$\langle \Gamma_i(t)\Gamma_i(t') \rangle = \delta(t-t'). \tag{4}$$

In the case not too far from thermodynamic equilibrium, the friction coefficient is given as

$$\nu = \frac{4\sqrt{\pi}n(\mathbf{r})Z^4e^4\ln(\Lambda)}{3m^2(T(\mathbf{r})/m)^{3/2}} \tag{5}$$

and the diffusion coefficient D is $D = \nu kT/m$ [3]. Here, $n(\mathbf{r})$ is the density of particle, $T(\mathbf{r})$ is the temperature of of beam, Z is the charge number of particle, e is the charge of electron, Λ is the Coulomb logarithm, and k is the Boltzmann constant. For the above case, noise terms enter only in the dynamical equations for the particle momenta. In Eqn. (6) below, the indices are single-particle phase-space coordinate indices; the convention used here is that the odd indices correspond to momenta, and the even indices to the spatial coordinate. In the case of three dimensions, the dynamical equations then take the general form:

$$\dot{x}_1 = F_1(x_1, x_2, x_3, x_4, x_5, x_6) + \sigma_{11}(x_2, x_4, x_6)\xi_1(t)$$

$$\dot{x}_2 = F_2(x_1)$$

$$
\begin{aligned}
\dot{x}_3 &= F_3(x_1,x_2,x_3,x_4,x_5,x_6) + \sigma_{33}(x_2,x_4,x_6)\xi_3(t) \\
\dot{x}_4 &= F_4(x_3) \\
\dot{x}_5 &= F_5(x_1,x_2,x_3,x_4,x_5,x_6) + \sigma_{55}(x_2,x_4,x_6)\xi_5(t) \\
\dot{x}_6 &= F_6(x_5) \qquad (6)
\end{aligned}
$$

In the dynamical equations for the momenta, the first term on the right hand side is a systematic drift term which includes the effects due to external forces and damping. The second term is stochastic in nature and describes a noise force which, in general, is a function of position. The noise $\xi(t)$ is first assumed to be Gaussian and white as defined by Eqns. (3)-(4). The stochastic leap-frog algorithm for Eqns. (6) is written as

$$
\bar{x}_i(h) = \bar{D}_i(h) + \bar{S}_i(h) \qquad (7)
$$

The deterministic contribution $\bar{D}_i(h)$ can be obtained using the deterministic leap-frog algorithm. Here, the deterministic contribution $\bar{D}_i(h)$ and the stochastic contribution $\bar{S}_i(h)$ of the above recursion formula for one-step integration are found to be

$$
\begin{aligned}
\bar{D}_i(h) &= \bar{x}_i(0) + hF_i(\bar{x}_1^*,\bar{x}_2^*,\bar{x}_3^*,\bar{x}_4^*,\bar{x}_5^*,\bar{x}_6^*); \\
&\quad \{i=1,3,5\} \\
\bar{D}_i(h) &= \bar{x}_i^* \\
&\quad + \frac{1}{2}hF_i\left[x_{i-1} + hF_{i-1}(\bar{x}_1^*,\bar{x}_2^*,\bar{x}_3^*,\bar{x}_4^*,\bar{x}_5^*,\bar{x}_6^*)\right]; \\
&\quad \{i=2,4,6\} \\
\bar{S}_i(h) &= \sigma_{ii}\sqrt{h}W_i(h) + \frac{1}{2}F_{i,k}\sigma_{kk}h^{3/2}\tilde{W}_i(h) \\
&\quad + \frac{1}{2}\sigma_{ii,j}F_j h^{3/2}\tilde{W}_i(h) \\
&\quad + \frac{1}{4}F_{i,kl}\sigma_{kk}\sigma_{ll}h^2\tilde{W}_i(h)\tilde{W}_i(h); \\
&\quad \{i=1,3,5;\ j=2,4,6;\ k,l=1,3,5\} \\
\bar{S}_i(h) &= \frac{1}{\sqrt{3}}F_{i,j}\sigma_{jj}h^{3/2}\tilde{W}_j(h) \\
&\quad + \frac{1}{4}F_{i,jj}\sigma_{jj}^2h^2\tilde{W}_j(h)\tilde{W}_j(h) \\
&\quad \{i=2,4,6;\ j=1,3,5\} \\
\bar{x}_i^* &= \bar{x}_i(0) + \frac{1}{2}hF_i(\bar{x}_1,\bar{x}_2,\bar{x}_3,\bar{x}_4,\bar{x}_5,\bar{x}_6) \\
&\quad \{i=1,2,3,4,5,6\} \qquad (8)
\end{aligned}
$$

where $\tilde{W}_i(h)$ is a series of random numbers with the moments

$$
\langle \tilde{W}_i(h) \rangle = \langle (\tilde{W}_i(h))^3 \rangle = \langle (\tilde{W}_i(h))^5 \rangle = 0 \qquad (9)
$$

$$
\langle (\tilde{W}_i(h))^2 \rangle = 1, \quad \langle (\tilde{W}_i(h))^4 \rangle = 3 \qquad (10)
$$

This can not only be achieved by choosing true Gaussian random numbers, but also by using the sequence of random numbers following:

$$
\tilde{W}_i(h) = \begin{cases} -\sqrt{3}, & R < 1/6 \\ 0, & 1/6 \le R < 5/6 \\ \sqrt{3}, & 5/6 \le R \end{cases} \qquad (11)
$$

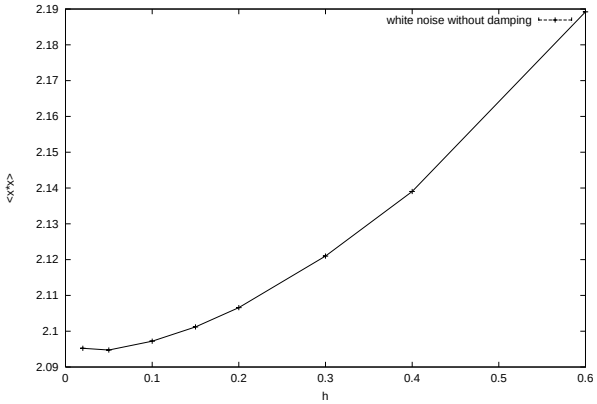

Figure 1: Zero damping convergence test. $\langle x^2(t) \rangle$ at $t = 6$ as a function of step size with white Gaussian noise. Solid lines represent quadratic fits to the data points (diamonds).

where R is a uniformly distributed random number on the interval (0,1). This trick significantly reduces the computational cost in generating random numbers.

3 NUMERICAL TESTS

The above algorithm was tested on a one-dimensional stochastic harmonic oscillator with a simple form of the multiplicative noise. The equations of motion were

$$
\begin{aligned}
\dot{p} &= F_1(p,x) + \sigma(x)\xi(t) \\
\dot{x} &= p \qquad (12)
\end{aligned}
$$

where $F_1(p,x) = -\gamma p - \eta^2 x$ and $\sigma(x) = -\alpha x$. The stochastic leapfrog integrator for this case is given by Eqns. (8) (white noise) with the substitutions $x_1 = p$, $x_2 = x$.

As a first test, we computed $\langle x^2 \rangle$ as a function of time-step size. To begin, we took the case of zero damping constant ($\gamma = 0$), where $\langle x^2 \rangle$ can be determined analytically. The curve in Fig. 1 shows $\langle x^2 \rangle$ at $t = 6.0$ as a function of time-step size with white Gaussian noise. Here, the parameters η and α are set to 1.0 and 0.1. The analytically determined value of $\langle x^2 \rangle$ at $t = 6.0$ is 2.095222. The quadratic convergence of the stochastic leap-frog algorithm is clearly seen in the numerical results. We also verified that the quadratic convergence is present for nonzero damping ($\gamma = 0.1$). At $t = 12.0$, and with all other parameters as above, the convergence of $\langle x^2 \rangle$ as a function of time step is shown by the curve in Fig. 2. As a comparison against the conventional Heun's algorithm [5], we computed $\langle x^2 \rangle$ as a function of t using $100,000$ numerical realizations for a particle starting from $(0.0, 1.5)$ in the (x,p) phase space. The results along with the analytical solution and a numerical solution using Heun's algorithm are given in Fig. 3. Parameters used were $h = 0.1$, $\eta = 1.0$, and $\alpha = 0.1$. The advantage in accuracy of the stochastic leap-frog algorithm over Heun's algorithm is clearly displayed, both in terms of error amplitude and lack of a systematic drift.

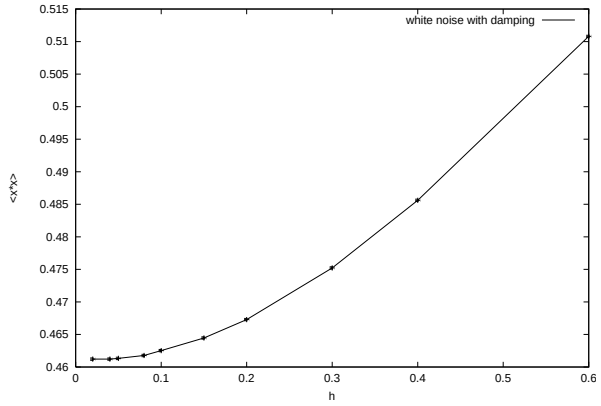

Figure 2: Finite damping ($\gamma = 0.1$) convergence test. $\langle x^2(t)\rangle$ at $t = 12$ as a function of step size with white Gaussian noise. Solid lines represent quadratic fits to the data points (diamonds).

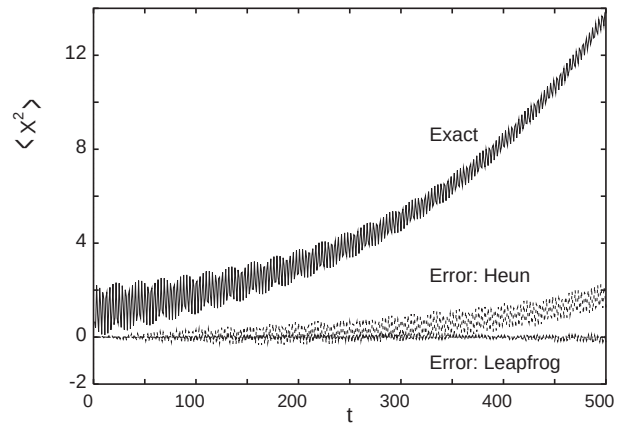

Figure 3: Comparing stochastic leap-frog and the Heun algorithm: $\langle x^2(t)\rangle$ as a function of t. Errors are given relative to the exact solution.

4 APPLICATION

In this section, we apply our algorithm to studying the approach to thermal equilibrium of an oscillator with multiplicative noise. The governing equations are:

$$\begin{aligned} \dot{p} &= -\omega_0^2 x - \lambda x^2 p - \sqrt{2D}x\xi_2(t) \\ \dot{x} &= p \end{aligned} \tag{13}$$

where the diffusion coefficients $D = \lambda kT$, λ is the coupling constant, and ω_0 is the oscillator angular frequency without damping. In Fig. 4, we display the time evolution of the average energy with multiplicative noise from the simulations and the approximate analytical calculations [6]. The analytic approximation resulting from the application of the energy-envelope method is seen to be in reasonable agreement with the numerical simulations for $kT = 4.5$. The slightly higher equilibrium rate from the analytical calculation is due to the truncation in the energy envelope equation using the $\langle E^2(t)\rangle \approx 2\langle E(t)\rangle^2$ relation which yields an upper bound on the rate of equilibration of the average energy [6].

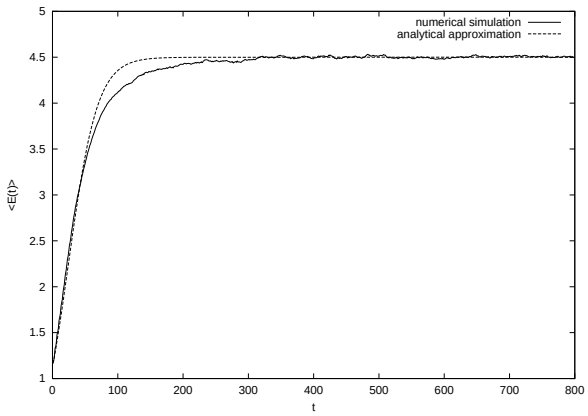

Figure 4: Temporal evolution of the scaled average energy $\langle E(t)\rangle$ with multiplicative noise from numerical simulation and analytical approximation.

5 CONCLUSIONS

We have presented a stochastic leap-frog algorithm for Langevin simulation with multiplicative noise. This method has the advantages of retaining the symplectic property in the deterministic limit, ease of implementation, and second-order convergence of moments for multiplicative noise. Sampling a uniform distribution instead of a Gaussian distribution helps to significantly reduce the computational cost. A comparison with the conventional Heun's algorithm highlights the gain in accuracy due to the new method. Finally, we have applied the stochastic leap-frog algorithm to a nonlinear mechanic-oscillator system to investigate the the nature of the relaxation process.

6 ACKNOWLEDGMENTS

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