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Semi-Integral Scheme for Simulation of Langevin Equation with Weak Inertia

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A stable and accurate algorithm for simulating massive damped Brownian motion is proposed and discussed. The algorithm, being fully integral for the friction and noise terms and predictor-corrector for the potential force in the Langevin equations, is stable upon changing time step and for various masses of the particle. In particular, the limit of zero inertia can be safely taken, and the algorithm yields naturally the corresponding overdamped case. The steady velocity of a particle moving in a titled periodic potential is calculated and three algorithms are compared.

KEY WORDS: Algorithm; massive damped; steady velocity; periodic potential.

In the past, several algorithms for numerical simulation of nonlinear stochastic differential equations (SDEs) have been provided,[(1)] for instance, one-step collocations,[(2, 3)] predictor-corrector schemes,[(4, 5)] Runge–Kutta (R-K) approaches.[(6, 7)] These methods of solving SEDs fire based on integration of the equations over one time step and Taylor expansion or predictor-corrector of the resulting equations. A subclass of SEDs that plays a major role in a lot fields is known as Langevin equations (LE) in mass weighted coordinate and velocity or momentum. Twenty years ago, Ermak and McCarmmon[(8)] proposed an idea of integral solution in the study of Brownian dynamics with hydrodynamic interactions. Very recently, the integral algorithms for solving the overdamped Langevin equations with additive white[(8)] and colored[(9)] noises were developed. For particular applications, such as molecular motors as a weak-inertia Brownian transport, the provided algorithms need to improve. Here, the final result of

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such speculation is presented and three different algorithms are compared: ALGO1, a basic Runge–Kutta method; ALGO2, an implicit algorithm; and proposed ALGO3, by using predictor-corrector approach for the potential force and analytical integration for the friction and noise terms.

The transport process of a massive Brownian particle moving in a nonlinear potential $V(x)$ subject to a white noise $\eta(t)$ and external fluctuations $F(t)$ is considered. The Langevin equation describing motion of the particles has the form

$$\dot{x}(t) = v(t) \tag{1}$$

$$m\dot{v}(t) = -\gamma v(t) + f(x) + \sqrt{2\gamma T}\,\eta(t) + F(t) \tag{2}$$

Where γ is the damping coefficient, $f(x) = -V'(x)$, T is the temperature of heat bath, as well as $\eta(t)$ satisfies $\langle \eta(t) \rangle = 0$ and $\langle \eta(t)\,\eta(t') \rangle = \delta(t - t')$.

We start from the fact that Eq. (2) can be regarded as a first-order ordinary differential equation if the latter three terms are treated and merged as a source term. Here it does not perform the Taylor expansion for deterministic terms like as the traditional methods. Integrating (2) and inserting into (1), we proceed as follows (ALGO3):

$$x(t + \Delta t) = x(t) + \int_t^{t+\Delta t} v(t')\,dt' \tag{3}$$

$$v(t') = \exp\left[-\frac{\gamma}{m}(t' - t) \right] v(t) + \frac{1}{m} \int_t^{t'} \exp\left[\frac{\gamma}{m}(s - t') \right] \times \{ f(x(s)) + \sqrt{2\gamma T}\,\eta(s) + F(s) \}\,ds \tag{4}$$

The integration for the potential force $f(x)$ in (3) and (4) is now computed by the second order R-K method within $[t, t + \Delta t]$ so that

$$\begin{aligned} x(t + \Delta t) = {} & x(t) + \frac{m}{\gamma}\left\{ 1 - \exp\left(-\frac{\gamma}{m}\Delta t \right) \right\} v(t) \\ & + \frac{1}{\gamma}[\alpha f(x(t)) + (1 - \alpha)\, f(x^*(t))] \\ & \times \left\{ \Delta t - \frac{m}{\gamma}\left[1 - \exp\left(-\frac{\gamma}{m}\Delta t \right) \right] \right\} \\ & + \frac{\sqrt{2\gamma T}}{m} Z_2(t) + \frac{1}{m} \int_t^{t+\Delta t} dt' \int_t^{t'} \exp\left[\frac{\gamma}{m}(s - t') \right] F(s)\,ds \end{aligned} \tag{5}$$

and

$$v(t+\Delta t)=\exp\left(-\frac{\gamma}{m}\Delta t\right)v(t)+\frac{1}{\gamma}\left[\alpha f(x(t))+(1-\alpha)f(x^*(t))\right]$$
$$\times\left[1-\exp\left(-\frac{\gamma}{m}\Delta t\right)\right]$$
$$+\frac{\sqrt{2\gamma T}}{m}Z_1(t)+\frac{1}{m}\int_t^{t+\Delta t}\exp\left[\frac{\gamma}{m}(s-t-\Delta t)\right]F(s)\,ds \tag{6}$$

Where $0\leqslant\alpha\leqslant 1$, $x^*(t)$ is also produced by Eq. (5) with $\alpha=1$ in the predictor steps[4, 5] and

$$Z_1(t)=\int_t^{t+\Delta t}\exp\left[\frac{\gamma}{m}(s-t-\Delta t)\right]\eta(s)\,ds \tag{7}$$

$$Z_2(t)=\int_t^{t+\Delta t}dt'\int_t^{t'}\exp\left[\frac{\gamma}{m}(s-t')\right]\eta(s)\,ds \tag{8}$$

Notice that Z_1 and Z_2 used in the corrector steps are the same as the predictor ones, they are two Gaussian random variables with zero mean as well as the standard deviations and cross correlation given by

$$\langle Z_1^2\rangle=\frac{m}{2\gamma}\left\{1-\exp\left(-\frac{2\gamma}{m}\Delta t\right)\right\} \tag{9}$$

$$\langle Z_2^2\rangle=\frac{m}{2\gamma}\left\{\frac{2m}{\gamma}\left[\Delta t-\frac{m}{\gamma}\left(1-\exp\left(-\frac{\gamma}{m}\Delta t\right)\right)\right]\right.$$
$$\left.-\left(\frac{m}{\gamma}\right)^2\left[1-\exp\left(-\frac{\gamma}{m}\Delta t\right)\right]^2\right\} \tag{10}$$

and

$$\langle Z_1Z_2\rangle=\frac{m^2}{2\gamma^2}\left\{1-2\exp\left(-\frac{\gamma}{m}\Delta t\right)+\exp\left(-2\frac{\gamma}{m}\Delta t\right)\right\} \tag{11}$$

To gain more insight, let us discuss the present algorithm with $\alpha=\frac{1}{2}$ (ALGO 3) in the cases of zero and finite inertia mass of the particle.

For weak inertia limit ($m\to 0$), Eq. (5) becomes

$$x(t+\Delta t)=x(t)+\frac{1}{2\gamma}\left[f(x(t))+f(x^*(t))\right]\Delta t+\sqrt{\frac{2T\,\Delta t}{\gamma}}\,\omega(t)+\frac{\Delta t}{\gamma}\bar{F}(t) \tag{12}$$

with

$$\bar{F}(t) = \frac{1}{\Delta t} \int_t^{t+\Delta t} F(s)\, ds \tag{13}$$

where $\omega(t)$ is a Gaussian random number with zero-mean and standard one.

On the other hand, the form of present LE (1) and (2) with the momentum degree of freedom is concerned with the following two-dimensional SEDs[1, 3, 4, 7]

$$\dot{q}_i = f_i(\mathbf{q}(t)) + g_{ij}(\mathbf{q}(t))\, \eta_i(t), \qquad i, j = 1, 2 \tag{14}$$

Here $q_1 = x$, $q_2 = p = mv$, $f_1 = m^{-1}p$, $f_2 = -\gamma m^{-1} p - V'(x) + F$, $g_{11} = g_{12} = g_{21} = 0$, and $g_{22} = \sqrt{2\gamma T}$. Performing predictor-corrector to first-order derivative of the potential in (14), one gets the R-K algorithm: ALGO1.[1, 6, 7] It can also obtained from Eqs. (5) and (6) under the conditions of intermediate-to-large m or small γ (i.e., the value of $(\gamma/m)\,\Delta t$ is small), namely,

$$\begin{aligned} x(t+\Delta t) &= x(t) + v(t)\,\Delta t \\ v(t+\Delta t) &= \left(1 - \frac{\gamma}{m}\,\Delta t\right) v(t) + \frac{1}{2m}\,[f(x(t)) + f(x^*(t))]\,\Delta t \\ &\quad + \frac{\sqrt{2\gamma T\,\Delta t}}{m}\,\omega(t) + \frac{\Delta t}{m}\,\bar{F}(t) \end{aligned} \tag{15}$$

In order to handle stiff problem caused by weak inertia, we now derive an implicit algorithm by using a farmer insertion for the friction term in (2) or (14): $\int_t^{t+\Delta t} \gamma v(s)\, ds = \gamma v(t+\Delta t)\,\Delta t$. The ALGO2 is obtained as

$$\begin{aligned} v(t+\Delta t) &= \frac{m}{m+\gamma\,\Delta t}\, v(t) + \frac{1}{2(m+\gamma\,\Delta t)}\,[f(x(t)) + f(x^*(t))]\,\Delta t \\ &\quad + \frac{\sqrt{2\gamma T\,\Delta t}}{m+\gamma\,\Delta t}\,\omega(t) + \frac{\Delta t}{m+\gamma\,\Delta t}\,\bar{F}(t) \end{aligned} \tag{16}$$

The present algorithm (ALGO3) has given the right prescription both for $m \to 0$ and large-m, it is believed that it should be very accurate even for finite m. To check this, we will test the above three algorithms computing the average steady velocity of a particle moving in a periodic potential $V(x) = -\sin(x)$ which is titled by a constant force $F(t) = F$. It has been solved analytically in the overdamped limit $m \to 0$.[11] After using a

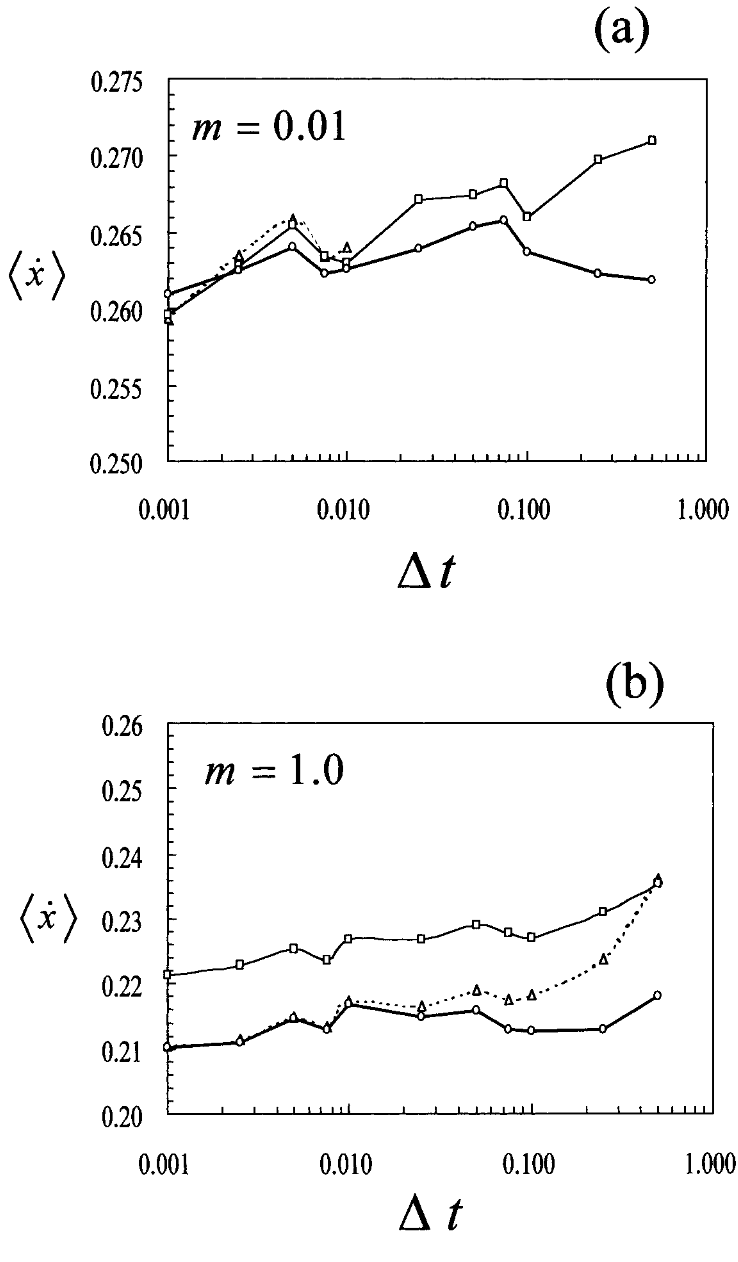

Fig. 1. Dependence of the steady velocity on time steps for $T = 1.0$, $F = 0.4$, as well as (a) $m = 0.01$, (b) $m = 1.0$. Dashed line with triangles, ALGO1; thin solid with squares, ALGO2; and thick solid line with circles, ALGO3.

scale transformation,[12] the dimensionless damping coefficient is assumed to be unit one ($\gamma = 1.0$), the rescaled mass m, the temperature T, and the force F are three basic parameters of the model. The claim will be supported that the semi-integral algorithm proposed here (ALGO3) is convergence and stable on changing time step and various inertia mass of the particle.

In this paper, the numerical calculations for the steady velocity of the particle are done starting from $x(0) = \pi/2$ and $v(0) = 0$ with averaging over $N = 10^3$ stochastic realization. The average velocity of the particle at the stationary states is determined by

$$\langle \dot{x} \rangle = \frac{1}{t - t_a} \int_{t_a}^{t} \langle \dot{x}(s) \rangle \, ds = \frac{1}{N} \sum_{n=1}^{N} \frac{x_n(t) - x_n(t_a)}{t - t_a} \tag{17}$$

where $t > t_a$ and $(\gamma/m)\, t_a \gg 1$.

Dependence of the simulated results on time steps for weak and finite inertia mass of the particle is plotted in Figs. 1(a) ($m = 0.01$) and (b) ($m = 1.0$), respectively. Here the other parameters are $T = 1.0$ and $F = 0.4$. It is seen from Fig. 1(a) that the numerical data are same approximately for the three algorithms as $\Delta t < 0.01$, however, the data produced by

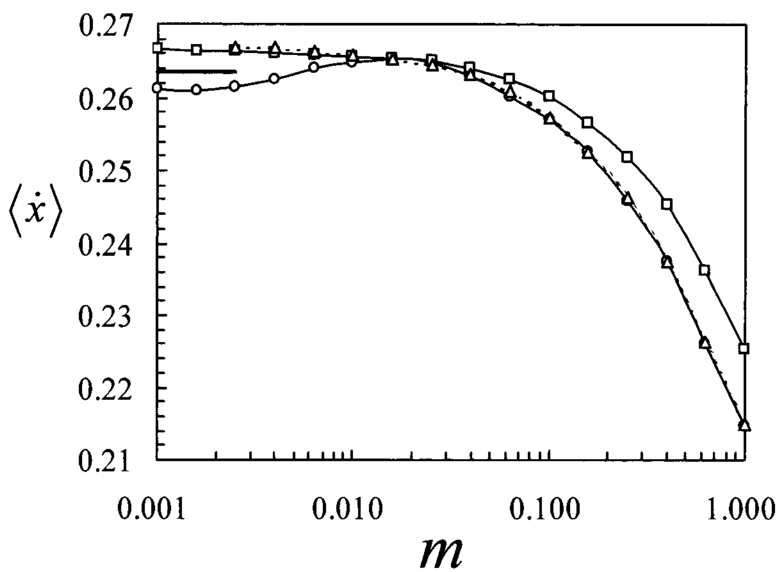

Fig. 2. The steady velocity as a function of m for $T = 1.0$ and $F = 0.4$. Dashed with triangles, ALGO1; thin solid line with squares, ALGO2; thin solid line with circles, ALGO3; and thick short line is theoretical data.

ALGO1 takes numerical overflow when $\Delta t > 0.01$ (i.e., $(\gamma/m)\,\Delta t > 1$). Clearly, ALGO3 is the most stable algorithm on changing time steps. From Fig. 1(b) one observes that both ALGO1 and ALGO3 versus time steps are convergence for the massive damped cases, and up to $\Delta t = 0.25$ ALGO3 reproduced the $\Delta t = 0.001$ value quite well. But the results calculated by ALGO2 are symmetrically larger than that of other two algorithms. So it is concluded that ALGO3 has a range of convergence larger than either ALGO1 or ALGO2. We stress again that also for ALGO3 the limit $m \to 0$ and finite Δt can be safely taken.

The steady velocity of the particle as a function of inertia mass is shown in Fig. 2 for $T = 1.0$ and $F = 0.4$. The theoretical value is $\langle \dot{x} \rangle_{th} = 0.2635$ in the overdamped limit. It is observed that ALGO2 and ALGO3 can approach to this exact value from two different directions, however, ALGO1 occurs numerical overflow when $m < 3 \times 10^{-3}$. Moreover, ALGO3 is also in keeping with the calculated results of ALGO1 when massive inertia is taken, but ALGO2 does not. Therefore, the present algorithm can be applied to the underdamped cases.

Finally, the average velocity of the particle for various inertia as a function of the temperature is shown in Fig. 3. Here the parameters of

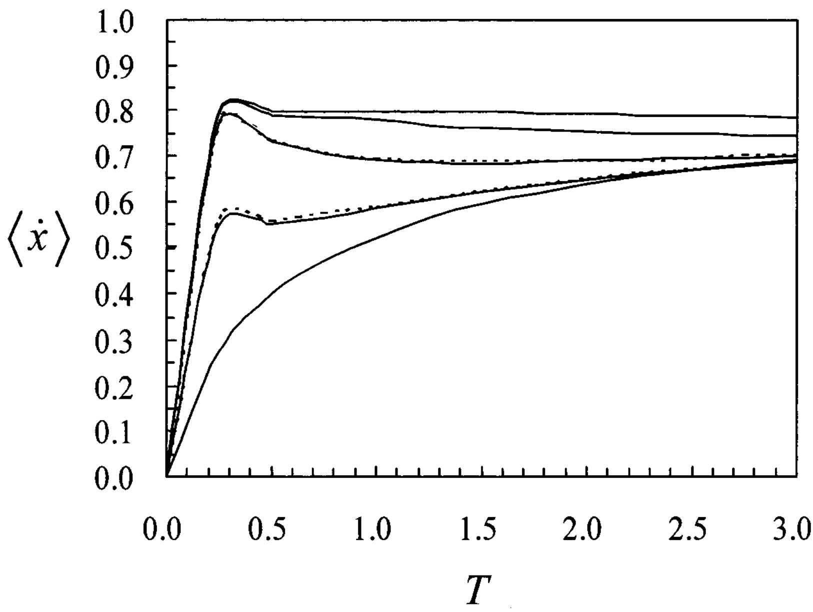

Fig. 3. The steady velocity calculated by ALGO3 (solid lines) and ALGO1 (dashed lines) as a function of the temperature for $F = 0.8$ and for five values $m = 40$, 20, 10, 5 and 2 for top to bottom.

simulating algorithm are $\Delta t = 0.1$, $t = 10^3$ and $t_a = 5 \times 10^2$. The results show that the steady velocity can achieve a local maximum at a finite temperature when $m > 5.0$ and $F > 0.5$. Thus a peak phenomenon is observed, here the inertia of the particle acts as a surrogate to a time-oscillating filed appeared in the stochastic resonance.

In summary, a stable and accurate semi-integral approach for simulating Langevin equations covering with a widely varying parameter values is proposed. Which has the nice properties that it can be reduced to the predictor-corrector algorithms for the overdamped and underdamped SEDs. Through the studies on the steady velocity of a particle with various inertia in a titled periodic potential, it is found that the present scheme gives a larger range of convergence for time steps comparing with the differential schemes. Any value of inertia mass of the particle can be considered and the stiff difficult has been avoided. Moreover, the average steady velocity of the particle is shown as a local peak function of the temperature.

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