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Numerical simulations of generalized Langevin equations with deeply asymptotic parameters

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Abstract

A unified algorithm for solving Langevin equations with deeply asymptotic parameters is proposed and tested. The method consists of identifying solvable linear friction and implementing the force evaluations by use of the Runge–Kutta method. We apply the present scheme to the periodic motion of an overdamped particle subjected to a multiplicative white noise. The accurate calculations for the temporal velocity of the particle and its correlation function can be realized by introducing an inertial term. It is shown that the fluctuation around the steady quantity increases with decreasing time step in the overdamped white-noise algorithm, however, a massive white-noise technique greatly reduces this spurious drift, and the result can converge to the correct value if the added inertia approaches zero. The other application is the simulation of generalized Langevin equation with an exponential memory friction, this allows us to treat a weak non-Markovian process.

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Keywords: Langevin equations; Damping integration; Stability; Deeply asymptotic parameters

1. Introduction

Numerical methods to solve stochastic differential equations (SDEs) have been discussed extensively in the literature [1–3]. Very recently, Hershkovitz [4] has derived a fourth-order algorithm by means of the Taylor expansion, which allows for very low friction. Drozdov and Brey [5], Forbert and Chin [6] have also used the operator factorization method [7] to yield a fourth-order Langevin algorithm. Superiority of

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these higher-order algorithms is the stability of the calculated results and large time steps being followed. The different time scale in SDEs is referred to as a stiff problem, here, the stiffness may come from two aspects: the white noise limit of the colored noise and the overdamped limit (weak inertia) of the system. Indeed, in many situations, stochastic processes with deeply asymptotic parameters are physically relevant. Unfortunately, from an algorithm viewpoint, those limits cannot be taken, namely, different algorithms have to apply to different parameter regions. A family of implicit schemes which are well suited to stiff stochastic systems and avoid some of the pitfalls inherent in fully implicit schemes that have been suggested by some authors [8,9]. The necessity of choosing the step small not only implies that the amount of computations increases, but also, more importantly, that the computational error increases. Moreover, the implicit algorithm cannot be applied to the opposite limits such as a strong damping or a long correlation time.

In particular, additive noise disappears from the noise-averaged form of the dynamical equation, but in the case of multiplicative noise with an intensity function $g(x)$, which should lead to dramatic changes of system behavior. Two classical illustrations are the Kubo oscillator [10] and the state-dependent diffusion [11–14]. For spatial periodic systems there the velocity of particle and its correlation function are two important output signs [15,16]. It stems from the fact that during a change of the noise $\xi(t)$ also the random variable $x(t)$ changes and therefore $\langle g(x(t))\xi(t)\rangle$ is no longer zero, and this average leads to the "spurious" drift. So that the velocity of particle at any time has to evaluate from the differential quotient of the coordinate. The problem is made more severe by the fact that the temporal velocity $\dot{x}(t) \propto (\Delta t)^{-1/2}$ becomes relatively large as $\Delta t \to 0$. This implies that calculated results should not convergent and thus the direct integration algorithm is not valid. In this paper, we will present an expanding for the original problem, which includes deeply asymptotic parameters such as inertia of the particle and correlation time of the noise.

The structure of this paper is as follows. In Section 2, the algorithm is described, the fundamental mismatch between the exponential nature of the iteration collocation and the Gaussian character of the integration of noise is shown in the resulting algorithm. In Section 3, the damping-integration approach is expanded to solve a generalized Langevin equation (GLE). Two examples in Section 4 are, respectively, the overdamped state-dependent transport and the energy relaxation of a system with a weak memory friction. Further, we demonstrate the necessity and superiority of the proposed algorithm. Finally, Section 5 offers a summary.

2. Damped-integration algorithm

An operating model of multiplicative white noise induced transport is simply written as

$$\dot{x}(t) = f(x) + g(x)\xi(t), \tag{1}$$

with $\langle\xi(t)\rangle = 0$ and $\langle\xi(t)\xi(t')\rangle = 2\delta(t-t')$. In order to remove the difficulty mentioned in Section 1, we introduce an inertial term into Eq. (1) and use a weak Ornstein–Uhlenbeck noise $\varepsilon(t)$ (with a small correlation time) [18–20] to mimic the white noise $\xi(t)$, i.e.

$$\dot{x}(t) = v(t), \tag{2}$$

$$m\dot{v}(t) + \gamma v(t) = f(x) + g(x)\varepsilon(t), \tag{3}$$

$$\dot{\varepsilon}(t) = -\frac{1}{\tau_c}\varepsilon + \frac{1}{\tau_c}\eta(t), \tag{4}$$

where m is the mass of the particle, γ denotes the viscous damping coefficient, $f(x) = -U'(x)$ ($U(x)$ is the potential), $g(x)$ is the noise strength, τ_c is the correlation time of the colored noise, and $\eta(t)$ satisfies $\langle\eta(t)\rangle = 0$ and $\langle\eta(t)\eta(t')\rangle = 2\delta(t-t')$. This describes practically a general motion of a particle with inertia subjected to a multiplicative colored noise.

If the r.h.s. of Eq. (3) is regarded as a source term, we can perform the integration of the velocity variable during a step interval $[t, t+\Delta t]$, then the present algorithm is processed as follows:

$$v(t+\Delta t) = \exp\Big(-\frac{\gamma}{m}\Delta t\Big)v(t) + \frac{1}{m}\int_t^{t+\Delta t}\exp\Big[-\frac{\gamma}{m}(t+\Delta t-s)\Big]\cdot\{f(x(s)) + g(x(s))\varepsilon(s)\}\,\mathrm{d}s, \tag{5}$$

$$x(t+\Delta t) = x(t) + \frac{m}{\gamma}\Big[1-\exp\Big(-\frac{\gamma}{m}\Delta t\Big)\Big]v(t) + \frac{1}{\gamma}\int_t^{t+\Delta t}\Big\{1-\exp\Big[-\frac{\gamma}{m}(t+\Delta t-s)\Big]\Big\} \cdot [f(x(s)) + g(x(s))\varepsilon(s)]\,\mathrm{d}s, \tag{6}$$

$$\varepsilon(t+\Delta t) = \exp(-\Delta t/\tau_c)\varepsilon(t) + \frac{1}{\tau_c}\int_t^{t+\Delta t}\exp[-(t+\Delta t-s)/\tau_c]\eta(s)\,\mathrm{d}s. \tag{7}$$

There are many ways to evaluate numerically the integrations in the r.h.s. of Eqs. (5) and (6), such as the one-step collocation via the Taylor expansion [3,18,19] and the fourth-order stochastic Runge–Kutta (S-R-K) algorithm [17]. Here, the deterministic integrations of Eqs. (5) and (6) are evaluated directly by means of the second method, and for the multiplicative factor of the colored noise, we use the S-R-K averaging $\bar{g}(x(t))$ to instead of $g(x(t))$ and depart it from the stochastic integration, because the noise is always a rapidly varying quantity. Thus the present damping-integration algorithm is obtained as

$$x(t+\Delta t) = x(t) + \frac{m}{\gamma}\Big[1-\exp\Big(-\frac{\gamma}{m}\Delta t\Big)\Big]v(t) + F_x + \frac{1}{\gamma}\bar{g}(x(t))\Big\{\tau_c[1-\exp(-\Delta t/\tau_c)] - \frac{m\tau_c}{\gamma\tau_c - m}\Big[\exp(-\Delta t/\tau_c) - \exp\Big(-\frac{\gamma}{m}\Delta t\Big)\Big]\Big\}\varepsilon(t) + \frac{1}{\gamma\tau_c}\bar{g}(x(t))\omega_2, \tag{8}$$

$$v(t+\Delta t) = \exp\Big(-\frac{\gamma}{m}\Delta t\Big)v(t) + F_v + \frac{1}{m}\bar{g}(x(t))\Big\{\frac{m\tau_c}{\gamma\tau_c - m}\Big[\exp(-\Delta t/\tau_c) - \exp\Big(-\frac{\gamma}{m}\Delta t\Big)\Big]\Big\}\varepsilon(t) + \frac{1}{m\tau_c}\bar{g}(x(t))\omega_1, \tag{9}$$

$$\varepsilon(t+\Delta t) = \exp\Big(-\frac{\Delta t}{\tau_c}\Big)\varepsilon(t) + \frac{1}{\tau_c}\omega_0, \tag{10}$$

with

$$\{F_x, F_v\} = \int_t^{t+\Delta t}\Big\{\Big[1-\mathrm{e}^{-\frac{\gamma}{m}(t+\Delta t-s)}\Big], \mathrm{e}^{-\frac{\gamma}{m}(t+\Delta t-s)}\Big\}f(x(s))\,\mathrm{d}s. \tag{11}$$

In Eqs. (8)–(10), ω_i ($i = 0, 1, 2$) are given by

$$\begin{aligned}
\omega_0 &= \int_t^{t+\Delta t} \exp\left[-\frac{1}{\tau_c}(t+\Delta t-s)\right]\eta(s)\,\mathrm{d}s,\\
\omega_1 &= \int_t^{t+\Delta t} \exp\left[-\frac{\gamma}{m}(t+\Delta t-t')\right]\mathrm{d}t'\int_t^{t'} \exp\left[-\frac{1}{\tau_c}(t'-s)\right]\eta(s)\,\mathrm{d}s,\\
\omega_2 &= \int_t^{t+\Delta t} \left\{1-\exp\left[-\frac{\gamma}{m}(t+\Delta t-t')\right]\right\}\mathrm{d}t'\int_t^{t'} \exp\left[-\frac{1}{\tau_c}(t'-s)\right]\eta(s)\,\mathrm{d}s.
\end{aligned} \tag{12}$$

They are independent Gaussian random variables with zero mean, and the standard deviations and cross correlations are given in Appendix A. It is noticed that ω_0 and ω_1 used in the next three steps are the same as the first one, however, following the same pattern of Honeycutt [17], it requires two sets of random numbers instead of one for ω_2. So the present algorithm requires four evaluations of both the force and the noise intensity, as well as four independent Gaussian random numbers per updating step, which is computationally very easily and avoids evaluating derivative of $f(x)$ and $g(x)$.

3. Solving generalized Langevin equation

To further illustrate the versatility of our damping-integration algorithm, we apply this approach to a GLE with an exponential memory friction. The GLE reads

$$m\ddot{x}(t) + \int_0^t \gamma_e(t-t')\dot{x}(t')\,\mathrm{d}t' = f(x) + \xi(t), \tag{13}$$

with

$$\langle \xi(t)\xi(t')\rangle = T\gamma_e(|t-t'|) = T\frac{\alpha}{\tau_D}\exp\left[-\frac{|t-t'|}{\tau_D}\right], \tag{14}$$

where T is the temperature, α is the zero-frequency damping coefficient, and τ_D the memory time.

Eq. (13) can be rewritten as a three-dimensional Markovian LE, i.e.

$$\begin{aligned}
\dot{x}(t) &= v,\\
\dot{v}(t) &= \frac{1}{m}z + \frac{1}{m}f(x),\\
\dot{z}(t) &= -\frac{1}{\tau_D}z - \frac{\alpha}{\tau_D}v + \frac{\sqrt{2\alpha T}}{\tau_D}\eta(t).
\end{aligned} \tag{15}$$

Consequently, the damping-integration algorithm for solving the above three-dimensional LE is suggested as

$$x(t+\Delta t) = x(t) + \frac{1}{r_1-r_2}\left\{\frac{r_1}{r_2}[\exp(r_2\Delta t)-1] - \frac{r_2}{r_1}[\exp(r_1\Delta t)-1]\right\}v(t) + F_x + \frac{\sqrt{2\alpha T}}{m\tau_D(r_1-r_2)}Y_3, \tag{16}$$

$$v(t+\Delta t) = \frac{[r_1\exp(r_2\Delta t) - r_2\exp(r_1\Delta t)]}{r_1-r_2}v(t) + \frac{[\exp(r_1\Delta t)-\exp(r_2\Delta t)]}{m(r_1-r_2)}z(t) + F_v + \frac{\sqrt{2\alpha T}}{m\tau_D(r_1-r_2)}Y_2, \tag{17}$$

$$z(t+\Delta t) = \frac{mr_1r_2}{r_1-r_2}[\exp(r_2\Delta t) - \exp(r_1\Delta t)]v(t) + \frac{1}{r_1-r_2}[r_1\exp(r_1\Delta t) - r_2\exp(r_2\Delta t)]z(t) + F_z + \frac{\sqrt{2\alpha T}}{\tau_D(r_1-r_2)}Y_1, \quad (18)$$

where r_1 and r_2 are the roots of the equation: $m\tau_D r^2 + mr + \alpha = 0$, and

$$F_x = \frac{1}{m(r_1-r_2)}\int_t^{t+\Delta t}\left(\frac{r_2}{r_1}\{1-\exp[r_1(t+\Delta t-s)]\} - \frac{r_1}{r_2}\{1-\exp[r_2(t+\Delta t-s)]\}\right)f(x(s))\,\mathrm{d}s,$$
$$F_v = \frac{1}{m(r_1-r_2)}\int_t^{t+\Delta t}\{r_1\exp[r_2(t+\Delta t-s)] - r_2\exp[r_1(t+\Delta t-s)]\}\cdot f(x(s))\,\mathrm{d}s, \quad (19)$$
$$F_z = \frac{r_1r_2}{r_1-r_2}\int_t^{t+\Delta t}\{\exp[r_2(t+\Delta t-s)] - \exp[r_1(t+\Delta t-s)]\}\cdot f(x(s))\,\mathrm{d}s.$$

The above three quantities are numerically calculated by using the fourth-order S-R-K algorithm [17]. As well as Y_i $(i=1,2,3)$ in Eqs. (16)–(18) are given by

$$Y_1 = \int_t^{t+\Delta t}\{r_1\exp[r_1(t+\Delta t-s)] - r_2\exp[r_2(t+\Delta t-s)]\}\eta(s)\,\mathrm{d}s,$$
$$Y_2 = \int_t^{t+\Delta t}\{\exp[r_1(t+\Delta t-s)] - \exp[r_2(t+\Delta t-s)]\}\eta(s)\,\mathrm{d}s, \quad (20)$$
$$Y_3 = \int_t^{t+\Delta t}\left(\frac{1}{r_2}\{1-\exp[r_2(t+\Delta t-s)]\} - \frac{1}{r_1}\{1-\exp[r_1(t+\Delta t-s)]\}\right)\eta(s)\,\mathrm{d}s.$$

Here, Y_1, Y_2, and Y_3 are also three independent Gaussian random variables with zero-mean, their standard deviations and cross correlations are given in Appendix B.

It should like to remark that the real parts of both r_1 and r_2 are negative, so that the iterations of Eqs. (16)–(18) are always stability. In the limit of $\Delta t \to 0$ $(\Delta t/\tau_D \to 0)$, we have $\lim_{\Delta t\to 0} Y_1 = O(\Delta t^{1/2})$, $\lim_{\Delta t\to 0} Y_2 = O(\Delta t^{3/2})$, and $\lim_{\Delta t\to 0} Y_3 = O(\Delta t^{5/2})$, thus the present algorithm can reduce to a multi-variable S-R-K algorithm developed by Honeycutt in [17]. Moreover, our algorithm is also valid in the limit of $\tau_D \to 0$ (i.e., $r_1 = -\alpha/m$ and $r_2 \to -\infty$).

4. Numerical examples

4.1. Example 1: directed flux in a periodic potential

As an example for the effort of the proposed algorithm, we consider state-dependent diffusion of an overdamped particle, where the potential and the diffusion coefficient [11] are taken to be

$$U(x) = U_0[1-\cos(x)], \quad D^{-1}(x) = D_0^{-1}[1-\lambda\cos(x-\phi)], \quad (21)$$

where λ $(0 \leqslant \lambda < 1)$ is the amplitude of the modulation, the phase ϕ plays a role of determining the direction of flow. It is appreciated a long time ago that the Boltzmann distribution which governs system subjected to the state-dependent diffusion, thus one must have [11]

$$f(x) = -U'(x) + \frac{1}{2}\frac{\mathrm{d}D(x)}{\mathrm{d}x}, \quad g(x) = \sqrt{D(x)}. \quad (22)$$

The simulation of the transport process of a particle is done starting from $x(0) = 0$, $v(0) = 0$, and sampling $\varepsilon(0)$ from a Gaussian distribution [18–20] with averaging over $N = 5 \times 10^4$ stochastic realizations. The parameters used are $U_0 = 1.0$, $\gamma = 1.0$, and $\phi = \pi/2$.

In Fig. 1, we evaluate time evolution of the mean velocity of the particle $\langle v(t) \rangle$ by using two kinds of time steps $\Delta t = 0.002$ and 0.0002. Three kinds of algorithms are applied: the overdamped white-noise algorithm [Eq. (1)]; the proposed massive white-noise algorithm [Eqs. (2) and (3) with $\tau_c = 0$]; and the colored-noise algorithm of Fox [Eqs. (2)–(4) with $m = 0$]. The results obtained by the first method show that the error increases with decreasing time step due to the effect of the spurious drift. Thus, it is demonstrated that the overdamped multiplicative white-noise algorithm is fail in the calculation of the temporal velocity of the particle, namely, it does not allow to provide very small time steps.

The average steady velocity as a function of the control parameters m or τ_c is shown in Fig. 2. In order to eliminate fluctuation drift of the calculated results [20], the time-averaged velocity is numerically evaluated by

$$\langle v \rangle = \frac{1}{t_b - t_a} \int_{t_a}^{t_b} \langle \dot{x}(s) \rangle \, ds = \frac{1}{N} \sum_{n=1}^{N} \frac{x_n(t_b) - x_n(t_a)}{t_b - t_a}, \tag{23}$$

where $t_b > t_a$, $t_a \gg m/\gamma$ and τ_c, $\Delta t = 5 \times 10^{-4}$, $t_a = 3.0$, and $t_b = 8.0$. The realistic value of the steady velocity is $\bar{v} = 0.3365$ in the limits of both $m \to 0$ and $\tau_c \to 0$. It is observed that our massive white-noise algorithm is more stable than that of the colored-noise scheme [10], and the former can approach the realistic value of the steady velocity. On the basis of Eq. (23), one concludes that the expectation value $\bar{v}$ computed via various algorithms can converge flatly, thus without fundamentally curing the convergence failure of the algorithm.

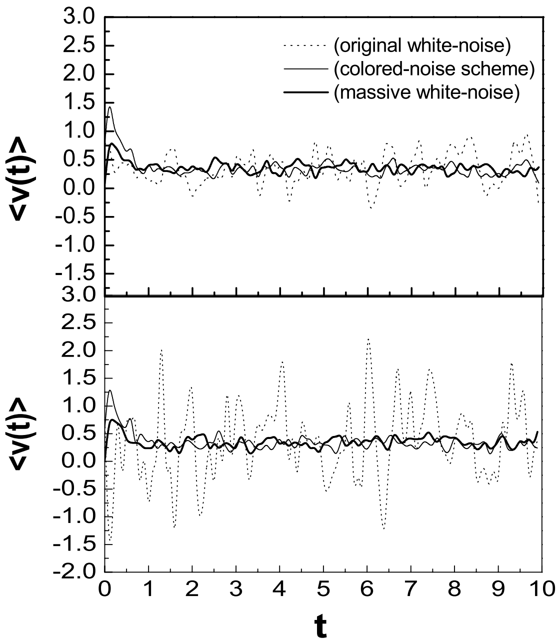

Fig. 1. Comparison of temporal velocity using three kinds of algorithms. The parameter values are $D_0 = 2.0$, $\lambda = 0.7$, $\gamma = 1.0$, $m = 0.01$, and $\tau_c = 0.01$. The step size for the first case is $\Delta t = 0.002$ and for the second case $\Delta t = 0.0002$.

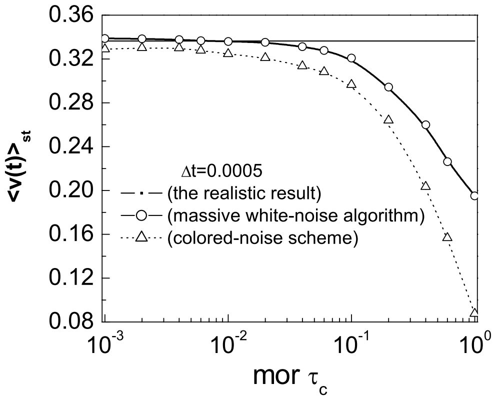

Fig. 2. The average steady velocity as a function of the introduced parameters m and τ_c. The time step used is $\Delta t = 0.0005$ and the other parameters are the same as Fig. 1.

The comparison of temporal velocity is performed here by using three kinds of algorithms. The parameters used are $D_0 = 2.0$, $\lambda = 0.7$, $\gamma = 1.0$, $m = 0.01$, and $\tau_c = 0.01$. The step size for the first case is $\Delta t = 0.002$ and for the second case $\Delta t = 0.0002$. A further demonstration of the inefficiency of the over-damped multiplicative white-noise algorithm is observed in calculating the correlation function of velocity as

$$C(t_d) = \langle \delta v(t - t_d)\delta v(t) \rangle, \quad \delta v(t) = v(t) - \langle v(t) \rangle. \tag{24}$$

In Fig. 3, the correlation function of velocity is plotted as a function of time. Here, two step sizes are $\Delta t = 0.002$ and 0.0002, respectively. It is seen that, the fluctuation in the correlation function of velocity is

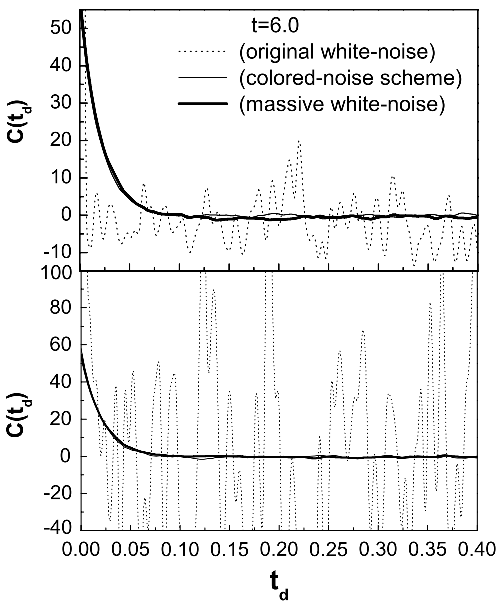

Fig. 3. Comparison of velocity correlation function using three kinds of algorithms. The parameter values are $D_0 = 2.0$, $\lambda = 0.5$, $\gamma = 1.0$, $m = 0.02$, and $\tau_c = 0.02$. The step size for the first case is $\Delta t = 0.002$ and for the second case $\Delta t = 0.0002$.

stronger than that of the velocity itself, and increases with decreasing time step if one uses directly numerical integration of Eq. (1). This is due to the fact that the term $(\Delta t)^{-1/2}$ appears in the calculated quantity. However, both the colored-noise scheme [10] and our massive white-noise algorithm can give the accepted results.

Dependence of the diffusion rate constant D^* of the particle on the control parameters m or τ_c is shown in Fig. 4. Here, the diffusion rate constant is evaluated from $D^* = \frac{1}{2}\lim_{t\to\infty}\frac{1}{t}\langle[x(t) - \langle x(t)\rangle]^2\rangle$ [15], and its realistic value can be determined by this expression from Eq. (1). The calculated result by using two indirect algorithms approaches asymptotically to D^* of Eq. (1). Indeed, it is observed that the present massive white-noise algorithm gives the best accurate result and converges flatly in comparison with the weak colored-noise scheme.

It is clear from Figs. 1 and 3 that the fluctuation in the velocity of particle and its correlation function is excessively large if one uses the overdamped multiplicative white-noise algorithm with a small Δt. The question is, when is such a small time step essential in any calculation? and one wants to know whether the spurious drift is due simply to the small value of Δt used. In order to answer these questions, here, we plot instead in Fig. 5, for a small value of m or τ_c, the average velocity $\bar{v}$ [Eq. (23)] and its fluctuation width determined by

$$\sigma_v = \left\{\frac{1}{t_b - t_a}\int_{t_a}^{t_b}\left\langle[\dot{x}(s) - \bar{v}]^2\right\rangle \mathrm{d}s\right\}^{1/2},$$

as a function of Δt. It is shown that the fluctuation width of velocity decreases with the increase of time step, however, the mean velocity is diverged from the correct value as the time step used is increased. If one uses a large step size, the calculated results will be instability because of the numerical error of evaluating the force evaluation. Moreover, in order to evaluate the velocity correction function between a short time difference τ_d, the time step needs to be chosen: $\Delta t \ll t_d$. It is remarkably that the time step should be also decreased for the cases of large noise intensity and higher non-linearity of force filed.

4.2. Example 2: relaxation with a weak memory friction

Another example for the usefulness of the damping-integration algorithm is the calculation of the energy relaxation for a week non-Markovian process. The potential is taken to be [5,6]

$$U(x) = x^4 - 2x^2. \tag{25}$$

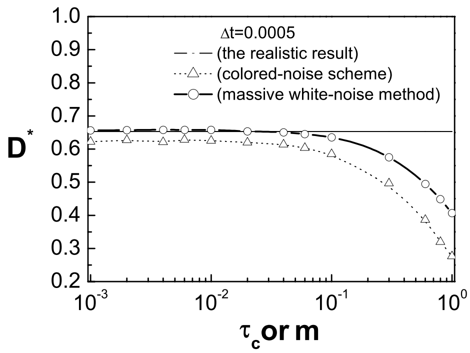

Fig. 4. The diffusion rate constant as a function of the introduced parameters m or τ_c. The diffusive time corresponds to $t = 80.0$, the step size to $\Delta t = 5\times10^{-4}$, as well as the other parameters are the same as Fig. 3.

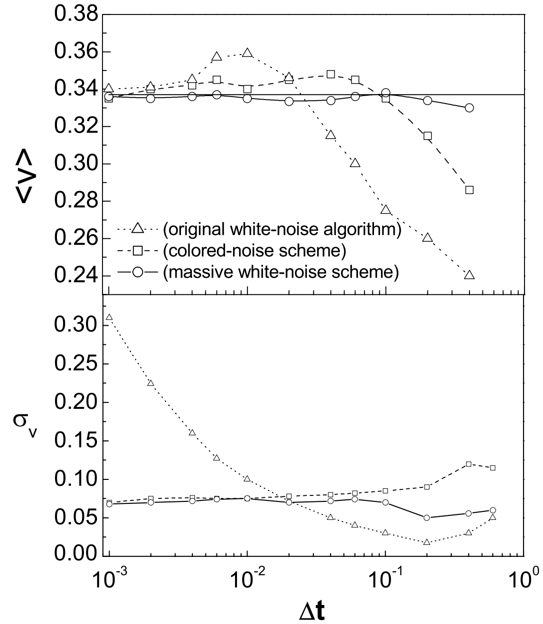

Fig. 5. The average steady velocity and its fluctuation width as functions of time step. The parameters sued are $D_0 = 2.0$, $\lambda = 0.7$, $m = \tau_c = 0.01$, $t_a = 2.0$, and $t_b = 6.0$. The thin straight line is the realistic result.

By use of parameters $\alpha = 1$, $T = 0.2$, and for a small memory time τ_D, we simulate the relaxation of a particle starting from $x(0) = 0$ and $v(0) = 0$ evolving to a finite time of $t = 6$. The temporal energy is

$$\langle E(t)\rangle = \frac{1}{2}\langle v(t)^2\rangle + \langle U(x(t))\rangle. \tag{26}$$

For comparison, the result obtained by Forbert and Chin [6] is $\langle E(t=6)\rangle = -0.773$ for the Markovian white noise case ($\tau_D \to 0$).

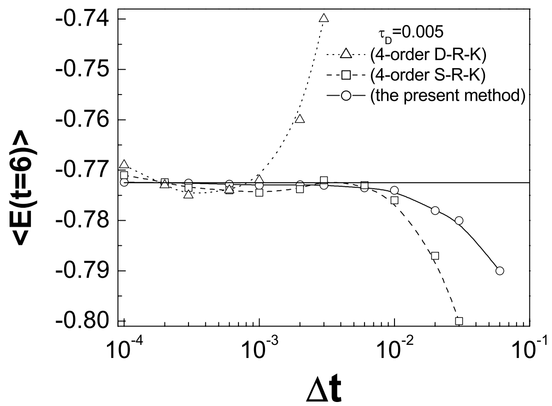

Fig. 6. The convergence of various algorithms for solving the stiff GLE. The energy calculated is at a finite time of $t = 6$ with parameters $T = 0.2$, $\alpha = 1$, and $\tau_D = 0.005$. The thin straight line is the realistic result.

In Fig. 6, dependence of the damping-integration algorithm on time step is remarkably flat, and this algorithm yields convergent result. A strong point of favor for our algorithm is that the integration time step can keep a constant for any memory times, namely, the limit of $\tau_D \to 0$ and Δt finite ($\Delta t/\tau_D \to \infty$) can be safely taken. In other words, for $\tau_D \to 0$ (which corresponds to the limit of white noise), the proposed algorithm [Eqs. (16)–(18)] yields exactly the Markovian Lengevin algorithm at order $(\Delta t)^4$ for the integration of force. Let us also notice the results calculated by the fourth-order deterministic R-K algorithm (D-R-K) of Hershkovitz [4] and the S-R-K of Honeycutt [17]. The former occurs numerical overflow when $\Delta t > 0.003$, and the step sizes larger than 0.03 will be avoided in the latter run. Clearly, our damping-integration algorithm is the most stable when the time step changes. It suggests that the better convergent of the present algorithm for larger Δt is not only due to the finite value of the ratio $\Delta t/\tau_D$, but also to the fact that the value of Δt can be considered to probably large to even precise integrate the force function via the fourth-order S-R-K method.

5. Summary

In this paper, the proposed algorithm makes the maximum use of analytical knowledge of the SDEs, and the time step of integration can be chosen to meet the required precision for the deterministic parts. We make two kinds of suggestions that an inertial term is added into usual overdamped multiplicative SDEs and a weak Ornstein–Uhlenbeck with a small correlation time is used to mimic the white noise. Thus intrinsic fluctuation in the velocity at small time steps can be reduced and "spurious" drift from expectation value can be removed. It is shown that the massive white-noise scheme not only avoids the spurious drift, but it also provides us with highly accurate time-averaged quantities. Any parameters of the model can be considered and the stiff difficult has been avoided. Computing the mean energy of a particle in a bistable potential with an exponential memory friction, we have shown that even for a much weak non-Markovian process, a finite time step size can be safely taken. It is also seen that the present algorithm has got a very flat convergent curve. One should therefore explore the effect of using the damping-integration algorithm rather than the other methods in implementing stiff stochastic differential equations.

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Appendix A. Noise moments in massive colored-noise algorithm

$$\langle \omega_0^2 \rangle = \frac{\tau_c}{2}\left[1 - \exp\left(-\frac{2}{\tau_c}\Delta t\right)\right], \tag{A.1}$$

$$\langle \omega_0 \omega_1 \rangle = \frac{\tau_c^2}{2}\left\{\frac{1 - \exp\left[-\left(\tau_c^{-1} + \frac{\gamma}{m}\right)\Delta t\right]}{1 + \frac{\gamma}{m}\tau_c} + \frac{\exp\left(-\frac{2}{\tau_c}\Delta t\right) - \exp\left[-\left(\tau_c^{-1} + \frac{\gamma}{m}\right)\Delta t\right]}{1 - \frac{\gamma}{m}\tau_c}\right\}, \tag{A.2}$$

$$\langle\omega_1^2\rangle = \frac{\tau_c^2}{1+\frac{\gamma}{m}\tau_c}\left\{\frac{m}{2\gamma}\left[1-\exp\left(-2\frac{\gamma}{m}\Delta t\right)\right] + \frac{\tau_c\exp\left(-2\frac{\gamma}{m}\Delta t\right)}{1-\frac{\gamma}{m}\tau_c}\left[\exp\left(-\frac{\Delta t}{\tau_c}+\frac{\gamma}{m}\Delta t\right)-1\right]\right\} - \frac{\tau_c^3}{2}\exp\left(-2\frac{\gamma}{m}\Delta t\right)\left\{\frac{1-\exp\left[-\frac{\Delta t}{\tau_c}+\frac{\gamma}{m}\Delta t\right]}{1-\frac{\gamma}{m}\tau_c}\right\}^2, \tag{A.3}$$

$$\langle\omega_0\omega_2\rangle = \tau_c^2\left[1-\exp\left(-\frac{\Delta t}{\tau_c}\right)\right] - \tau_c\langle\omega_0^2\rangle - \langle\omega_0\omega_1\rangle, \tag{A.4}$$

$$\langle\omega_1\omega_2\rangle = \tau_c^2\left\{\frac{m}{\gamma}\left[1-\exp\left(-\frac{\gamma}{m}\Delta t\right)\right] + \frac{\tau_c m}{\gamma\tau_c - m}\left[\exp\left(-\frac{\gamma}{m}\Delta t\right)-\exp\left(-\frac{\Delta t}{\tau_c}\right)\right]\right\} - \tau_c\langle\omega_0\omega_1\rangle - \langle\omega_1^2\rangle, \tag{A.5}$$

$$\langle\omega_2^2\rangle = \tau_c^2\left\{\Delta t - \tau_c\left[1-\exp\left(-\frac{\Delta t}{\tau_c}\right)\right] - \frac{m}{\gamma}\left[1-\exp\left(-\frac{\gamma}{m}\Delta t\right)\right] + \frac{\tau_c m}{\gamma\tau_c - m}\left[\exp\left(-\frac{\Delta t}{\tau_c}\right)-\exp\left(-\frac{\gamma}{m}\Delta t\right)\right]\right\} - \tau_c\langle\omega_0\omega_2\rangle - \langle\omega_1\omega_2\rangle. \tag{A.6}$$

Now, ω_0, ω_1, and ω_2 can be produced by a linear combination of three uncorrelated Gaussian random numbers with zero-mean and standard deviation one [18].

Appendix B. Noise moments in GLE algorithm

$$\langle Y_1^2\rangle = \frac{r_1}{2}[\exp(2r_1\Delta t)-1] + \frac{r_2}{2}[\exp(2r_2\Delta t)-1] - \frac{2r_1r_2}{r_1+r_2}\{\exp[(r_1+r_2)\Delta t]-1\}, \tag{B.1}$$

$$\langle Y_2^2\rangle = \frac{1}{2r_1}[\exp(2r_1\Delta t)-1] + \frac{1}{2r_2}[\exp(2r_2\Delta t)-1] - \frac{2}{r_1+r_2}\{\exp[(r_1+r_2)\Delta t]-1\}, \tag{B.2}$$

$$\langle Y_3^2\rangle = \left(\frac{r_1-r_2}{r_1r_2}\right)^2\Delta t + \frac{r_1-r_2}{r_1+r_2}\left\{\frac{1}{r_2^3}[1-\exp(r_2\Delta t)] - \frac{1}{r_1^3}[1-\exp(r_1\Delta t)]\right\} + \frac{1}{2r_1^3}[1-\exp(r_1\Delta t)]^2 + \frac{1}{2r_2^3}[1-\exp(r_2\Delta t)]^2 - \frac{2}{r_1r_2(r_1+r_2)}\{\exp[(r_1+r_2)\Delta t]-\exp(r_1\Delta t)-\exp(r_2\Delta t)+1\}, \tag{B.3}$$

$$\langle Y_1Y_2\rangle = \frac{1}{2}[\exp(r_1\Delta t)-\exp(r_2\Delta t)]^2, \tag{B.4}$$

$$\langle Y_1Y_3\rangle = \frac{1}{2r_1}[1-\exp(r_1\Delta t)]^2 + \frac{1}{2r_2}[1-\exp(r_2\Delta t)]^2 - \frac{2}{r_1+r_2}\{1-\exp(r_1\Delta t) - \exp(r_2\Delta t) + \exp[(r_1+r_2)\Delta t]\}, \tag{B.5}$$

$$\langle Y_2Y_3\rangle = \frac{1}{2r_1^2}[1-\exp(r_1\Delta t)]^2 + \frac{1}{2r_2^2}[1-\exp(r_2\Delta t)]^2 - \frac{1}{r_1r_2}\{1-\exp(r_1\Delta t) - \exp(r_2\Delta t) + \exp[(r_1+r_2)\Delta t]\}. \tag{B.6}$$

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