Dissipative Particle Dynamics (DPD) is a popular simulation model for investigating hydrodynamic behavior of systems with non-negligible equilibrium thermal fluctuations. DPD employs soft core repulsive interactions between the system particles, thus allowing them to overlap. This supposedly permits relatively large integration time steps, which is an important feature for simulations on large temporal scales. In practice, however, an increase in the integration time step leads to increasingly larger systematic errors in the sampling statistics. Here, we demonstrate that the prime origin of these systematic errors is the multiplicative nature of the thermal noise term in Langevin’s equation; i.e., the fact that it depends on the instantaneous coordinates of the particles. This lead to an ambiguity in the interpretation of the stochastic differential Langevin equation, known as the Itô-Stratonovich dilemma. Based on insights from previous studies of the dilemma, we propose a novel algorithm for DPD simulations exhibiting almost an order of magnitude improvement in accuracy, and nearly twice the efficiency of commonly used DPD Langevin thermostats.

where \( r_{ij} = |\vec{r}_i - \vec{r}_j| \) is the pair-distance, \( \hat{v}_{ij} = (\vec{r}_i - \vec{r}_j)/r_{ij} \), and \( \vec{v}_{ij} = \vec{v}_i - \vec{v}_j \) is the relative velocity of the particles. The random force is given by

\[
\vec{f}^R_{ij} = \sqrt{2k_BT\gamma \omega(r_{ij})\theta_{ij}\hat{v}_{ij}},
\]

where \( \theta_{ij} \) is Gaussian white noise satisfying \( \langle \theta_{ij}(t) \rangle = 0 \) and \( \langle \theta_{ij}(t)\theta_{kl}(t') \rangle = \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\delta(t-t') \). The friction and stochastic forces are modulated with a weight function, \( \omega(r_{ij}) \), that determines their range, \( r_c \). The most commonly used weight function is

\[
\omega_{ij} = \left\{ \begin{array}{cc}
1 - \frac{r_{ij}}{r_c} & r_{ij} < r_c \\
0 & r_{ij} \geq r_c,
\end{array} \right.
\]

The total friction and stochastic forces exerted on the \( i \)th particle are given by \( \vec{f}^D = \sum_{j \neq i} \vec{f}^D_{ij} \) and \( \vec{f}^R = \sum_{j \neq i} \vec{f}^R_{ij} \), respectively.

As noted above, the particles in DPD simulations often represent CG groups of atoms and molecules. Coarse-graining is believed to lead to effective soft repulsive pair potentials; but, obviously, one has to keep in mind that due to the softening of the effective interaction potential, some features of the simulated system may change. The conservative force used in DPD simulations is usually given by

\[
\vec{f}^C_{ij} = \left\{ \begin{array}{cc}
a_{ij} \left(1 - \frac{r_{ij}}{r_c} \right) \hat{v}_{ij} & r_{ij} < r_c \\
0 & r_{ij} \geq r_c,
\end{array} \right.
\]

where \( a_{ij} = a_{ji} \) are parameters determining the strength of the repulsion, and the range \( r_c \) is the same as in Eq. (3). The total conservative force acting on the \( i \)th particle is \( \vec{f}^C_i = \sum_{j \neq i} \vec{f}^C_{ij} \). One of the frequently proclaimed advantages of DPD simulations is that the soft-core pair interactions act in a pairwise fashion, and are directed along the line connecting the centers of the particles. This ensures that the total momentum of the system is conserved, which is essential in order to capture the correct hydrodynamic behavior of fluids at large scales.
potential allows the particles to overlap and, therefore, permits relatively large integration time steps $dt$, which speeds up the simulations. In practice, however, it is known that all integration methods for DPD exhibit increasing artificial changes in the sampling statistics as the discretization time step is enlarged [14]. Thus, despite the enhanced numerical stability limit obtained by softening the potentials, this feature imposes severe restrictions on the size of the allowed time steps and, moreover, requires one to validate results in order to assess the statistical errors.

In this paper, we present a novel DPD integrator that, in comparison to other DPD integrators, shows considerably smaller errors in the computed averages of configurational thermodynamic quantities. The new integration method is based on an integrator recently presented by the authors (G-JF Integrator) that exhibits minimal systematic errors in the sampling statistics of conventional LD simulations [13, 16], and on insights gained by implementing the integrator to study LD in systems with spatially varying friction coefficients [17, 18]. In the latter case, an ambiguity, known in the literature as the Itô-Stratonovich dilemma, arises about the integration of the stochastic noise term in Langevin’s equation [13, 19]. DPD belongs to the same class of problems of stochastic dynamics with multiplicative (state-dependent) noise, and it poses several unique complications that we address in what follows.

In order to understand the origin of the problems in numerical integration of DPD, we start by writing Langevin’s equation of motion

$$m_i d\vec{v}_i = \left( \vec{f}_i^C + \vec{f}_i^D + \vec{f}_i^R \right) dt,$$

where $m_i$ is the mass of the $i$th particle. The G-JF integrator preserves the fluctuation-dissipation theorem in discrete time by using the exact relationships:

$$\int_{t_n}^{t_{n+1}} \vec{f}_i^D dt = -\int_{t_n}^{t_{n+1}} \gamma \vec{v}_i dt = -\gamma (\vec{r}_{i+1}^n - \vec{r}_i^n),$$

$$\int_{t_n}^{t_{n+1}} \vec{f}_i^R dt = \sqrt{2k_BT} \gamma \int_{t_n}^{t_{n+1}} \vec{R}_i(t) dt = \sqrt{2k_BT} \gamma dt \vec{R}_i^{n+1},$$

where $t_{n+1} = t_n + dt$ denotes discrete time, $\vec{r}_i^n = \vec{r}_i(t_n)$, and $\vec{R}_i^{n+1}$ is a vector whose coordinates are Gaussian random numbers of zero mean and unity variance. Combining Eqs. (5) and (6) with the (second order in $dt$) approximations used in the derivation of the Verlet algorithm [21] for Molecular Dynamics simulations in microcanonical ensembles, one arrives at the G-JF algorithm for constant-temperature LD simulations, which (after some rearrangement) reads

$$\vec{r}_{i+1} = \vec{r}_i + b \left( \vec{v}_i dt + \frac{dt^2}{2m_i} \vec{f}_i^C + \frac{dt}{2m_i} \vec{R}_i^{n+1} \right),$$

$$\vec{v}_{i+1} = a \vec{v}_i + \frac{dt}{2m_i} \left( a \vec{f}_i^C + \vec{f}_i^{n+1} \right) + \frac{b}{m_i} \vec{R}_i^{n+1},$$

where $\vec{r}_i^n = \vec{r}_i(t_n)$, $\vec{f}_i^n = \vec{f}_i^C(t_n)$ is the conservative force, and the constants

$$b = \left( 1 + \frac{\gamma dt}{2m_i} \right)^{-1}; a = \left( 1 - \frac{\gamma dt}{2m_i} \right) b.$$

It has been demonstrated that, unlike other integrators, the G-JF algorithm exhibits minimal changes in the configurational sampling statistics as $dt$ is varied, up to the stability limit of the integrator [15, 16, 21].

When $\gamma = \gamma(\vec{r}_i)$ depends on the coordinate of the particle, one needs to specify where along the path from $\vec{r}_i^n$ to $\vec{r}_i^{n+1}$, the friction coefficient used in Eqs. (7) and (10) is evaluated. This ambiguity leads to the problem known as the Itô-Stratonovich dilemma, after the conventions $\gamma_{i(I)}^{n+1} = \gamma(\vec{r}_i^n)$ of Itô [22], and $\gamma_{i(S)}^{n+1} = \left[ \gamma(\vec{r}_i^n) + \gamma(\vec{r}_i^{n+1}) \right]/2$ of Stratonovich [23]. The vast majority of the literature on this topic focuses on the overdamped (strictly non-inertial) limit of Langevin’s equation $|m_i \equiv 0$ in Eq. (5)], where different conventions lead to different statistical ensembles even for infinitesimally small integration steps, $dt \to 0$. In the case of full (inertial) dynamics (i.e., when the l.h.s. of Langevin’s equation does not vanish completely), the different conventions lead to the same statistical sampling when $dt \to 0$.

However, in numerical simulations with non-vanishing time steps, the error caused by employing different conventions varies considerably from one choice to another, and this error adds to the general error caused by the integrator itself. In a previous study [17, 18, 25, 26], we used the accurate G-JF integrator to study LD of a single particle in a medium with space-dependent friction coefficient. We demonstrated that both Itô and Stratonovich interpretations lead to noticeable deviations that scale linearly with $dt$ from the equilibrium Boltzmann distribution. We proposed a new interpretation that produces markedly smaller discrepancies between the computed and the correct distributions and which, moreover, shows very little sensitivity to $dt$ (and, thus, enables larger integration time steps). The newly proposed convention for choosing the value of $\gamma_{i}^{n+1}$ is based on the recognition that the random collision forces between the Brownian particle and the molecules of the heat bath (which are not accounted for explicitly at molecular resolution) are decomposed in Langevin’s equation into two contributions. The friction term represents the mean change in the momentum of the particle due to the collisions, while the noise accounts for the Gaussian statistical fluctuations around the mean value $\vec{s}_i^n$. We, therefore, consider the deterministic part of Langevin’s equation without the random component, and define $\vec{s}_i^{n+1} = \vec{r}_i^n + \vec{v}_i dt + \left( \vec{f}_i^n - \gamma(\vec{r}_i^n) \vec{v}_i^n \right) (dt^2/2m_i)$ that satisfies $\langle \vec{s}_i^{n+1} \rangle \sim \vec{s}_i^{n+1} + O(dt^2)$. Our new convention for $\gamma_{i}^{n+1}$ reads: $\gamma_{i(G-JF)}^{n+1} = \left[ \gamma(\vec{r}_i^n) + \gamma(\vec{s}_i^{n+1}) \right]/2$. This definition resembles the Stratonovich interpretation for $\gamma_{i}^{n+1}$; yet it does not create spurious drift. For a detailed discussion on the spurious drift problem, we refer to refs. [17, 18, 25, 26] (and references therein). In short,
the fact that the noise term in Eq. [5] generates the distribution of momentum changes around the mean value, implies that the r.h.s. of Eq. [7] must satisfy
\[ \langle \sqrt{2k_B T \gamma_i^{n+1} dt \hat{R}_i^{n+1}} \rangle = 0. \] (11)

However, because \( \hat{R}_i^{n+1} \) is a Gaussian random number with zero mean, condition (11) can only be fulfilled if \( \gamma_i^{n+1} \) and \( \hat{R}_i^{n+1} \) are independent of each other, which is not the case with the seemingly physical Stratonovich interpretation, where \( \gamma_i^{n+1} \) depends on \( \hat{r}_i^{n+1} \), which itself depends on \( \hat{R}_i^{n+1} \). Itô’s interpretation satisfies Eq. (11); however, it uses a poor estimation for \( \gamma_i^{n+1} \) (the initial value - completely ignoring the path of the particle) and, therefore, also fails to produce accurate statistical sampling for large dt. The new G-JF interpretation satisfies condition (11)(like Itô), but with a value of \( \gamma_i^{n+1} \) representing a spatial average over the ensemble of trajectories of the particle during the time step (like Stratonovich).

DPD simulations present an even more challenging task of handling multiplicative (state-dependent) noise. The complexity is mainly linked to the fact that friction and noise forces act in a pairwise fashion, and that they must be weighted in a manner that on the one hand represents an average over the time step (like Stratonovich), and on the other hand independent of each pair act along the same direction, as well as the values of the friction coefficients. We, thus, continue with calculating the random forces acting on the particles
\[ f_i^{n+1} dt = \sum_{i \neq j} \sqrt{2k_B T \gamma_i^{n+1} s_{ij}^{n+1} dt} \theta_i^{n+1} s_{ij}^{n+1/2}, \] (13)

where \( s_{ij} = |\vec{s}_{ij} - \vec{s}_j| \) and \( \theta_i^{n+1} s_{ij}^{n+1/2} \) are the new coordinates of the particles at their new coordinates, \( \vec{s}_{ij}^{n+1} \), and then compute the averages
\[ s_i^{n+1/2} \equiv \left( \vec{s}_i^n + \vec{s}_i^{n+1} \right) / 2 \]

\[ = \vec{s}_i^n + \vec{s}_i^n dt / 2 + \left[ F_i^C (\vec{r}_i^n) + F_i^D (\vec{v}_i^n, \vec{s}_i^n) \right] dt^2 / 4m_i, \] (12)

where \( \vec{r} \) and \( \vec{v} \) (to be distinguished from \( \hat{r}_i \) and \( \hat{v}_i \)) denote dependence on coordinates \( r \) and velocities \( v \) of all the particles. The coordinates \( s_i^{n+1/2} \) define the directions of the friction and noise forces within the time step, as well as the values of the friction coefficients. We, thus, continue with calculating the random forces acting on the particles

\[ \vec{f}_i^{n+1} = \vec{f}_i^C (\vec{r}_i^{n+1}) + \vec{f}_i^D (\vec{v}_i^{n+1}, \vec{s}_i^{n+1}), \] (16)

and the associated friction forces

\[ \vec{f}_i^{Dn+1/2} = -\sum_{i \neq j} \gamma_i ( \vec{s}_{ij}^{n+1/2} - \vec{u}_{ij}^{n+1/2} ) \vec{s}_{ij}^{n+1/2} / 2m_i, \] (15)

where \( \vec{u}_{ij} = \vec{u}_i - \vec{u}_j \). The new coordinates of the particles can now be computed using

\[ \vec{r}_i^{n+1} = \vec{r}_i^n + \vec{v}_i^n dt + \left[ \vec{f}_i^C (\vec{r}_i^n) + \vec{f}_i^D (\vec{v}_i^n, \vec{s}_i^n) \right] dt^2 / 4m_i, \] (17)

where \( s_{ij} = |\vec{s}_{ij} - \vec{s}_j| \) and \( \theta_i^{n+1} s_{ij}^{n+1/2} \) are the new coordinates of the particles at their new coordinates, \( \vec{s}_{ij}^{n+1} \), and then compute the averages

\[ s_i^{n+1/2} \equiv \left( \vec{s}_i^n + \vec{s}_i^{n+1} \right) / 2 \]

\[ = \vec{s}_i^n + \vec{s}_i^n dt / 2 + \left[ F_i^C (\vec{r}_i^n) + F_i^D (\vec{v}_i^n, \vec{s}_i^n) \right] dt^2 / 4m_i, \] (12)

We also compute the new deterministic forces, \( \vec{f}_i^C (\vec{r}_i^{n+1}) \), and then evaluate the new velocities via

\[ \vec{v}_i^{n+1} = \vec{v}_i^n + \left[ \vec{f}_i^C (\vec{r}_i^n) + \vec{f}_i^D (\vec{r}_i^{n+1}) + \vec{f}_i^{Dn+1/2} + \vec{f}_i^{Dn+1} \right] dt. \] (18)

We “close the loop” by calculating the friction forces \( \vec{f}_i^{Dn+1/2} (\vec{r}_i^{n+1}, \vec{v}_i^{n+1}) \) to be used at the next application of Eq. (12).

The sequence of Eqs. (12)–(18) constitutes our proposed new DPD integrator, which we term DPD-DE after the “deterministic estimation” of \( s_{ij}^{n+1} \) in Eq. (12). To test the algorithm, we simulate a system of \( N = 500 \) identical particles in a cubic box of length \( L = 5 \) with the parameter set \( r_v = 1, k_B T = 1, m_i = 1, a_{ij} = 25, \) and \( \gamma = 4.5 \). This system, with the same set of parameters,
has recently been used in ref. [27] for comparison between several DPD integrators. As a benchmark, we use the DPD Velocity-Verlet (DPD-VV) method of Besold et al. [28], which is implemented in several popular simulation packages. We note that in the simulations of the very same system in ref. [27], the accuracy and efficiency of the DPD-VV algorithm was found to be almost identical to other commonly used DPD Langevin integrators such as Shardlow’s splitting method [29, 30]. Therefore, the DPD-VV results also allow comparison with other integration schemes for constant-temperature DPD. We also note that methods for DPD simulations with energy conservation exist (e.g., [31, 32]), but the discussion of constant-energy DPD is beyond the scope of this paper.

The performance of the integrator is evaluated by measuring the mean and standard deviation of the potential energy of the system in simulations with increasing time steps. These quantities characterize the quality of configurational sampling. For each time step, ranging from \( dt = 0.01 \) and up to a time step showing significant deviations from the asymptotic \( dt \to 0 \) limit, we simulated the system for \( 1.44 \times 10^6 \) time units, and sampled the energy at intervals of 1.2 time units. Our results for the mean (\( \langle E \rangle \)) and standard deviation (\( \sigma_E \)) of the potential energy (normalized per particle) are plotted, respectively, in Fig. 1. We observe that both methods exhibit an increase in the measured \( \langle E \rangle \) and \( \sigma_E \) with \( dt \) indicating unwanted changes in the sampling statistics. However, per \( dt \), the results of the DPD-DE integrator of this work appear to be about 6–7 times more accurate (i.e., exhibiting smaller relative errors) than the results of the DPD-VV method. A similar degree of improvement in accuracy has been found in simulations of both denser and more dilute systems, and for different values of the the parameter \( a_{ij} \) representing stronger/weaker repulsion between the particles.

Fig. 2 depicts the results for the simulated kinetic temperature, \( T_k = (2/3)\langle K \rangle / (N - 1) \) (where \( K \) is the kinetic energy), as a function of \( dt \). One may erroneously conclude from the results for \( T_k \) that DPD-VV performs better than DPD-DE. This impression, however, is incorrect. It has been now well established (see numerous discussions on this point in, e.g., [15, 16, 21, 27, 33]) that in contrast to the potential energy, the simulated kinetic energy is not very important and cannot be taken as a reliable measure for the accuracy of a simulation method. This feature of numerical integrators does not originate from the discretization of the friction and noise forces. This is an inherent property of the classic Verlet algorithm where the discrete-time momentum \( \vec{p}_n^i \) is not exactly conjugated to the coordinate \( \vec{r}_n^i \). For this reason, one should not attempt to use (with any integrator) quantities, such as momentum autocorrelations, for precise measures, unless very small integration time steps are applied.

To ensure that the new integrator is useful for DPD simulations, it is necessary to also demonstrate that it produces the correct dynamics, at least as accurately as other algorithms. As a measure for the dynamical
evolution of the system, we consider the diffusion coefficient \[ D = \lim_{t \to \infty} \frac{1}{6Nt} \sum_{i=1}^{N} [\vec{r}_i(t) - \vec{r}_i(0)]^2, \] (19)
whose value depends only on the discrete-time coordinates \( \{\vec{r}_i^n\} \), but not on the discrete-time momenta \( \{\vec{v}_i^n\} \). Results for \( D \) as a function of \( dt \) are shown in Fig. 3. As expected, the results of both integrators converge to the same limit when \( dt \to 0 \), indicating convergence to the correct dynamical behavior. Interestingly, the trends in the variations of \( D \) resembles the trends in \( T_k \) (Fig. 2). Also noticeable, the discretization time errors of the DPD-DE algorithm are always smaller the errors of the DPD-VV algorithm. The last observation suggests that the new DPD-DE method improves not only configurational sampling, but also provide a better dynamical description of DPD systems.

The improvement by a factor of 6-7 in configurational sampling accuracy is outstanding considering that, per \( dt \), all currently available Langevin thermostats for DPD simulations exhibit relative errors essentially identical to the one of the DPD-VV method \[27\]. This property suggests that the main source of numerical error in Langevin DPD thermostats is the application of Itô’s interpretation to the friction coefficients, which is the common feature of all of these methods. The DPD-DE integrator of this work uses a different convention, which is based on spatial averaging of the friction along the trajectory that the particle would follow had the random noise force been turned off \[32\]. This new convention differs from the seemingly more physical Stratonovich convention that is based on the actual trajectory of the particle, and which also takes into account the influence of the random force along the trajectory. The Stratonovich interpretation represents an incorrect reading of Langevin’s differential equation. In Langevin’s equation, the friction force represents the mean change in the momentum of a particle, while the noise term accounts for the statistical distribution around the mean value. The Stratonovich interpretation “mixes” the two terms and, therefore, it leads to spurious drift \[17,18\].

We close by noting that in order to assess the computational efficiency of integrators, one also needs to take into account the CPU time required to perform a single time step. For that purpose, we adopt the criterion suggested in ref. \[27\], which defines the numerical efficiency as the step size giving the same relative accuracy as the DPD-VV method with step size \( dt = 0.05 \), divided by the CPU time. From Fig. 1 we read that the DPD-DE method with \( dt = 0.1 \) has the same accuracy as the DPD-VV method with \( dt = 0.05 \). Simulations on several different machines also reveal that the run time of DPD-DE is about 1.15-1.3 larger than that of DPD-VV \[36\]. Thus, the scaled efficiency of DPD-DE is about 155% − 175%, placing it second in the list of integrators examined in ref. \[27\] in terms of computational efficiency, just an inch behind the method that came first with scaled efficiency of 187%. However, the latter method, as well as all other integration methods ranked at the top places of the list, are based on a Nosé-Hoover thermostat. Such methods are more complicated for implementation, and their optimization requires fine-tuning of additional friction parameters. In contrast, DPD-DE is a pure Langevin thermostat having only a single tunable friction parameter \( \gamma \) [see Eqs. (1) and (2)]. It, thus, offers both ease of implementation and benefit of accuracy.

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For practical reasons, the algorithm is based on a forward approximation of the trajectory. The run time depends on many factors including the type of processor used, the compiler of the code, and the computing skills of the programmer.

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