Efficient Schmidt number scaling in dissipative particle dynamics

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Dissipative particle dynamics is a widely used mesoscale technique for the simulation of hydrodynamics (as well as immersed particles) utilizing coarse-grained molecular dynamics. While the method is capable of describing any fluid, the typical choice of the friction coefficient γ and dissipative force cutoff r_c yields an unacceptably low Schmidt number Sc for the simulation of liquid water at standard temperature and pressure. There are a variety of ways to raise Sc , such as increasing γ and r_c , but the relative cost of modifying each parameter (and the concomitant impact on numerical accuracy) has heretofore remained undetermined. We perform a detailed search over the parameter space, identifying the optimal strategy for the efficient and accuracy-preserving scaling of Sc , using both numerical simulations and theoretical predictions. The composite results recommend a parameter choice that leads to a speed improvement of a factor of three versus previously utilized strategies. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4930921>]

I. INTRODUCTION

Dissipative particle dynamics (DPD) is a coarse-grained, mesoscale molecular dynamics technique that simulates a fluid as a set of particles, with each particle representing some number of molecules.^{1,2} This coarse-graining leads to a larger time step, which allows one to probe length and time scales that are not feasible for simulations with atomistic detail. However, the underlying thermostat of DPD can be applied to any system, including atomistic simulations, where it has the advantage of preserving hydrodynamic interactions,³ which are not correctly reproduced when using, e.g., a Langevin thermostat.⁴ DPD has been applied to many problems, including electrolyte solutions,⁵ red blood cell suspensions,⁶ cell membrane proteins,⁷ nanoparticle-membrane binding,⁸ DNA flow in a microchannel,⁹ active matter,^{10,11} and colloidal mixtures.¹² It remains an actively developed and utilized technique, as detailed in a recent review.¹³

In order to gain a proper description of angular momentum and torque, one must extend the standard DPD thermostat (which considers only central forces) with perpendicular components.^{14,15} To this end, we adopt the formulation of DPD as detailed by Pan *et al.*¹⁴ This extension does not particularly impact the computational complexity and has the added benefit of enhancing the single-particle hydrodynamics in DPD. Particles have a position $\mathbf{r}_i$, velocity $\mathbf{v}_i$, angular velocity $\boldsymbol{\Omega}_i$, and mass m . Particle pairs have a relative position $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ and relative velocity $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$. Particle i experiences a force and torque given by

$$\begin{aligned}\mathbf{F}_i &= \sum_j \mathbf{F}_{ij}, \\ \mathbf{T}_i &= - \sum_j \frac{\mathbf{r}_{ij}}{2} \times \mathbf{F}_{ij},\end{aligned}\quad (1)$$

with the pairwise force on particle i due to particle j defined by

$$\mathbf{F}_{ij} = \mathbf{F}_{ij}^C + \mathbf{F}_{ij}^T + \mathbf{F}_{ij}^R + \tilde{\mathbf{F}}_{ij}. \quad (2)$$

The associated components are the conservative, translational damping, rotational damping, and random forces, respectively. The conservative force is given by

$$\begin{aligned}\mathbf{F}_{ij}^C &= a(1 - r_{ij}/R)\mathbf{e}_{ij} \quad (r_{ij} \leq R) \\ &= 0 \quad (r_{ij} > R),\end{aligned}\quad (3)$$

where a determines the strength of the repulsion, R is the range of the conservative force, $r_{ij} = |\mathbf{r}_{ij}|$, and $\mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij}$. The parameter a effectively determines the compressibility of the simulated fluid.² The translational damping force is the sum of a central and shear component,

$$\begin{aligned}\mathbf{F}_{ij}^T &= -\gamma_{ij}^C f^2(r_{ij})(\mathbf{v}_{ij} \cdot \mathbf{e}_{ij})\mathbf{e}_{ij} \\ &\quad - \gamma_{ij}^S f^2(r_{ij})[\mathbf{v}_{ij} - (\mathbf{v}_{ij} \cdot \mathbf{e}_{ij})\mathbf{e}_{ij}],\end{aligned}\quad (4)$$

where $\gamma_{ij}^{C,S}$ are the friction coefficients (C and S indicate the central and shear parameters, respectively) and $f(r_{ij})$ is a dimensionless weighting function defined by

$$\begin{aligned}f(r_{ij}) &= (1 - r_{ij}/r_c)^s \quad (r_{ij} \leq r_c) \\ &= 0 \quad (r_{ij} > r_c).\end{aligned}\quad (5)$$

The parameter r_c is the cutoff radius for dissipative and fluctuating forces, and the exponent s determines the structure of the weighting function (i.e., how quickly it transitions from 1 to 0 with r_{ij}). We note that this definition of s is equivalent to $s/2$ as defined by Groot and Warren.² The rotational damping force is

$$\mathbf{F}_{ij}^R = -\gamma_{ij}^S f^2(r_{ij}) \left[\frac{\mathbf{r}_{ij}}{2} \times (\boldsymbol{\Omega}_i + \boldsymbol{\Omega}_j) \right]. \quad (6)$$

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Finally, the fluctuating random force is given by

$$\tilde{F}_{ij} = f(r_{ij}) \left[\frac{1}{\sqrt{3}} \sigma_{ij}^C \text{tr}(\mathbf{W}_{ij}) \mathbf{1} + \sqrt{2} \sigma_{ij}^S \mathbf{W}_{ij}^A \right] \cdot \mathbf{e}_{ij}, \quad (7)$$

where $\sigma_{ij}^{C,S} = \sqrt{2k_B T \gamma_{ij}^{C,S} / \Delta t}$, Δt is the time step, and $\mathbf{W}_{ij}$ is a $d \times d$ matrix of Gaussian distributed random numbers with zero mean and unit variance for d spatial dimensions. The temperature is determined by $k_B T$, where k_B is the Boltzmann constant. The matrix $\mathbf{W}_{ij}^{A\mu\nu} = \frac{1}{2}(\mathbf{W}_{ij}^{\mu\nu} - \mathbf{W}_{ij}^{\nu\mu})$ is the antisymmetric matrix corresponding to $\mathbf{W}_{ij}$. Traditional DPD is recovered by setting $\gamma^S = 0$. Hereafter, we take $\gamma^C = \gamma^S = \gamma$.

The parameters of a DPD fluid, namely, γ , a , r_c , and s , must be modified to produce the proper hydrodynamic numbers and properties for a given system. It has been determined^{9,16} that the Schmidt number Sc of a DPD simulation must be $O(10^3)$ (as in water) in order to give expected results, despite the typically chosen parameters yielding $Sc \sim O(1)$. Since $Sc = \nu/D$, where ν is the (kinematic) viscosity and D is the diffusion, parameter changes that increase ν and decrease D are sought. This can be accomplished by increasing either γ or r_c , with $Sc \propto \gamma^2 r_c^8$.² Additionally, reducing the weighting function exponent s also leads to an increase of Sc .⁹ Despite the necessity to reach adequate values of Sc , and the multiple parameters that can be manipulated, a detailed study of an optimal strategy for parameter selection has not been performed to our knowledge. We present a detailed exploration of DPD parameter space, determining Sc for various values of $\{\gamma, r_c, s\}$ and examining the associated computational cost for each parameter selection, as well as considering the associated theoretical predictions. We find that the conventional strategy⁹ of modifying r_c is actually less efficient than modifying γ alone, when all aspects of the simulation (e.g., time step, accurate temperature representation, and neighbor searching) are considered. The impact of the parameter s on the efficiency was determined to be insignificant.

II. PROCEDURE

The equations of motion are integrated using a standard leapfrog algorithm, with the addition of a predicted velocity for force calculation (since the forces depend on velocity). Thus, the position and velocity of particle i are updated along time t as follows:

$$\begin{aligned} \mathbf{F}_i(t + \Delta t/2) &= \mathbf{F}_i(\mathbf{r}(t + \Delta t/2), \tilde{\mathbf{v}}(t + \Delta t/2)), \\ \mathbf{v}_i(t + \Delta t) &= \mathbf{v}_i(t) + \mathbf{F}_i(t + \Delta t/2) \Delta t / m, \\ \tilde{\mathbf{v}}_i(t + 3\Delta t/2) &= \mathbf{v}_i(t + \Delta t) + \lambda \mathbf{F}_i(t + \Delta t/2) \Delta t / m, \\ \mathbf{r}_i(t + 3\Delta t/2) &= \mathbf{r}_i(t + \Delta t/2) + \mathbf{v}_i(t + \Delta t) \Delta t, \\ \mathbf{T}_i(t + \Delta t/2) &= \mathbf{T}_i(\tilde{\mathbf{\Omega}}(t + \Delta t/2)), \\ \mathbf{\Omega}_i(t + \Delta t) &= \mathbf{\Omega}_i(t) + \mathbf{T}_i(t + \Delta t/2) \Delta t / I, \\ \tilde{\mathbf{\Omega}}_i(t + 3\Delta t/2) &= \mathbf{\Omega}_i(t + \Delta t) + \lambda \mathbf{T}_i(t + \Delta t/2) \Delta t / I, \end{aligned} \quad (8)$$

where $\tilde{\mathbf{v}}$ is the predicted velocity, $\tilde{\mathbf{\Omega}}$ is the predicted angular velocity, and the moment of inertia is $I = 2mr^2/5$, with particle radius $r = 0.27R$.¹⁴ The value of λ can be tuned to improve the accuracy of the integration scheme with respect to temperature reproduction² and has been set to $\lambda = 1/2$ for all simulations in this paper.

For the duration of this paper, reduced units will be used: the DPD particle mass $m = 1$, the temperature $k_B T = 1$, and the conservative force range $R = 1$. Each simulation takes place in a periodic cubic box of side length $L = 10$, at a density of $\rho = 3$, and in $d = 3$ spatial dimensions. The parameter $a = 25$ is set to satisfy the proper compressibility of water ($a = 75k_B T / \rho$) at the given density.² The default values of the other parameters (which will be varied) are $\gamma = \gamma_0 = 4.5$, $r_c = R = 1$, and $s = 1/4$, the latter of which yields better accuracy than the typical value of $s = 1$.¹⁴ In order to definitively determine the cost of a given $\{\gamma, r_c, s\}$ choice, the time step Δt is not fixed, but independently determined for each position of parameter space. As the viscosity ν increases, the time step required to keep the same level of numerical accuracy decreases. This can be seen as the result of more numerous (r_c) or stronger (γ, s) fluctuations and greater friction (γ, r_c, s). The measured temperature in DPD will differ from the input value due to a finite time step in the integration scheme. If the time step allows for excess temperatures of 3% or more, clear departures from the Maxwell-Boltzmann distribution begin to appear. It was found² that a departure of 2% or less is satisfactory to maintain numerical accuracy, and this standard has been used to select the time step for each parameter set. One additional input parameter exists for the implementation of DPD, namely, the neighbor cutoff r_N . Neighbor searching reduces the amount of particle pairs that must be examined at each step in order to determine the forces (i.e., which pairs are within the cutoff distance r_c). The value of r_N was also optimized for each $\{\gamma, r_c, s\}$ choice, since the diffusion D changes the number of different neighbors a particle can interact with on a given time scale. This involves taking the minimum value of r_N that does not cause a deviation from the result for $r_N = \infty$. The effect this has on the simulation cost will be examined below.

To determine the Schmidt number Sc , the viscosity and diffusion must be measured. The diffusion is given by

$$D = \lim_{t \rightarrow \infty} \frac{\langle (\mathbf{r}(t_0 + t) - \mathbf{r}(t_0))^2 \rangle}{2dt}, \quad (9)$$

where the angle brackets indicate an average over time and over all particles. This value was calculated for each set $\{\gamma, r_c, s\}$ from a simulation of length 10^3 (ranging from 3.8×10^5 to 1.5×10^7 steps), using a limiting value of $t = 100$ (yielding a convergence of D with respect to time). The viscosity was determined using the periodic Poiseuille flow method¹⁷ with a simulation length of 1.5×10^3 , after which time there was no significant change to the measured values.

III. RESULTS

All the raw data presented in this article are tabulated in the supplementary material.¹⁸ We initially restrict ourselves to the $\{\gamma, r_c, \frac{1}{4}\}$ plane for the sake of clarity and will return to the s parameter later on. A total of 72 pairs $\{\gamma, r_c\}$ were analyzed in the range $1.0 \leq r_c \leq 1.7$ (where the range of γ was varied in order to look at the relevant values of Sc). We can estimate the cost χ_t of a simulation (with units of laboratory seconds/system time) due to the necessary time step using the inverse viscosity, since this represents the time scale that must

FIG. 1. Optimized time step (red points) compared to inverse viscosity (blue dashed line). The error bars are based on a $\pm 10\%$ range in Δt , due to the method of optimization. While temperature control was always within 2% of the target value, this number varies in sensitivity to the time step. Thus, each point does not have the exact same temperature accuracy, which leads to being above (less accurate) or below (more accurate) the fit line. Δt_0 is the value of Δt at $\{\gamma_0, R, \frac{1}{4}\}$.

be resolved by the integrator. The theoretical estimate for the viscosity is $\nu \propto \gamma r_c^5$,² so we expect the optimized time step to be $\Delta t \propto \gamma^{-1} r_c^{-5}$. This relationship is confirmed in Fig. 1, where Δt_0 is the value of Δt at $\{\gamma_0, R, \frac{1}{4}\}$. This cost must be multiplied by the number of interacting pairs in DPD (i.e., r_c^3) in order to get the full cost, yielding $\chi \propto \gamma r_c^8$. The data given in Fig. 2 agree quite well with this relationship, although the data are not exactly linear (here, χ_0 is a parameter of the fit). In reality, the effect of neighbor searching reduces the powers of γ and r_c due to the reduced diffusion of DPD particles: a lower diffusion means a smaller neighbor cutoff r_N may be used, which reduces the number of distances computed in each step. A proper fit yields $\chi \propto \gamma^{0.9} r_c^{7.4}$. We note that the previously reported result⁹ of $\chi \propto r_c^{2.4}$ shows this same effect but neglects the factor of r_c^5 coming from time step optimization. Finally, we compare the measured values of Sc

FIG. 2. Simulation cost (red points) compared to the expected value (blue dashed line). χ_0 is a parameter of the linear regression. While the results match relatively well with the expectation, a more accurate fit yields $\chi \propto \gamma^{0.9} r_c^{7.4}$. This is because increasing γ and r_c leads to reduced diffusion, which in turn leads to a shorter neighbor searching cutoff. Fewer neighbors means fewer distance calculations in each time step, which reduces χ more for points further to the right in the figure.

FIG. 3. Measured Schmidt number (red points) compared to theoretical value (blue dashed line). While the expected trend is well represented, the measured values are spread out due to the mismatch between ideal and actual diffusion, as discussed in the text. Sc_0 is a parameter of the linear regression.

to the theoretical prediction² of $Sc \propto \gamma^2 r_c^8$ in Fig. 3, showing good agreement (here, Sc_0 is a parameter of the fit). The spread of the points around the anticipated value is primarily due to the diffusion D , which deviates from the ideal case. While we expect² $D \propto \gamma^{-1} r_c^{-3}$, the measured value has an extra reduction owing to r_c . This is because the formula assumes an ideal gas (i.e., constant) radial distribution function. As the cutoff radius increases, the relative velocity force from Eq. (4) leads to further departures from the theoretical value of the diffusion, making the error in the assumption more prominent.

Comparing the Schmidt number Sc to the cost χ , we can define a Schmidt number efficiency $\eta_{Sc} = Sc/\chi$, where a larger η_{Sc} at a given value of Sc indicates greater computational efficiency. We plot this efficiency as a function of Sc in Fig. 4, for cutoff radii from 1.0 to 1.7. Each line represents a different value of r_c , where the points along the line follow increasing values of γ (from lower-left to upper-right). Evidently, at a given value of Sc , the highest efficiency is obtained by taking

FIG. 4. Schmidt number efficiency $\eta_{Sc} = Sc/\chi$ as a function of Sc for all data points on the $\{\gamma, r_c, \frac{1}{4}\}$ plane. Each line is a different value of r_c , as indicated. Points along a line from left to right follow increasing values of γ . At every value of Sc , the greatest efficiency is obtained by using the shortest value of r_c . Thus, it is best to keep $r_c = R$ and vary γ when adjusting Sc for a run. The window around $Sc = 10^3$, a typical value needed for simulations of liquid water, is fully characterized.

the lowest value of r_c . Additionally, for a constant r_c , increasing γ further increases the efficiency. This naturally follows from the fits obtained previously, i.e.,

$$\eta_{Sc} = Sc/\chi \propto \gamma^2 r_c^8 / \gamma^{0.9} r_c^{7.4} \propto \gamma^{1.1} r_c^{0.6}. \quad (10)$$

To see the scaling for a given Sc , we hold Sc constant (so that $\gamma \sim r_c^{-4}$) and obtain

$$\eta_{Sc}(Sc = \text{const}) \propto r_c^{-3.4} \propto \gamma^{0.95}. \quad (11)$$

While this prediction yields the correct trends, it does not perfectly match with the data. This is because, while the data given in Fig. 3 seem to match quite well, the ideal diffusion² $D \propto \gamma^{-1} r_c^{-3}$ deviates with respect to its r_c dependence, as described above. For instance, the point $\{7\gamma_0, 1.0, \frac{1}{4}\}$ has $Sc = 886$ and $\chi = 103$, and the point $\{\gamma_0, 1.5, \frac{1}{4}\}$ has $Sc = 855$ and $\chi = 330$, yielding an efficiency ratio of 3.3 despite the prediction of $1.5^{3.4} \approx 4.0$. Nevertheless, there is clear evidence that modifying γ and not r_c is the more practical way to reach $Sc = O(10^3)$ in DPD.

Four values of s ($\frac{1}{8}$, $\frac{1}{4}$, $\frac{1}{2}$, and 1) were additionally examined, in order to determine what effect the weighting function exponent has on the value of η_{Sc} . These analyses were restricted to the $\{\gamma, R, s\}$ plane since the previous results indicated only negative effects from increasing r_c . Surprisingly, varying the value of s (while keeping Sc constant) does not significantly affect the efficiency, as seen in Fig. 5. While Sc and χ do not have the simple power law scaling with s that they do with γ and r_c , we can nevertheless obtain some insight into theory. The viscosity and diffusion (considering only relevant factors) are given by^{2,19}

$$\begin{aligned} \nu &\propto \gamma[(2s+1)(2s+2)(2s+3)(2s+4)(2s+5)]^{-1}, \\ D &\propto \gamma^{-1}[(2s+1)(2s+2)(2s+3)], \end{aligned} \quad (12)$$

yielding a Schmidt number of

$$Sc = \nu/D \propto \frac{\gamma^2}{[(2s+1)(2s+2)(2s+3)]^2(2s+4)(2s+5)}. \quad (13)$$

If we decrease s from 1 to $\frac{1}{4}$, Sc increases by a factor of 35.5. To examine the constant- Sc efficiency, we must reduce γ by

FIG. 5. Schmidt number efficiency $\eta_{Sc} = Sc/\chi$ as a function of Sc for all data points on the $\{\gamma, R, s\}$ plane. As opposed to γ and r_c , s does not have a significant impact on efficiency, although $s = \frac{1}{2}$, $\frac{1}{4}$ appears to give a slight advantage.

a factor of 6. Since χ is proportional to ν , we can determine the efficiency change by comparing the viscosity with $\gamma/6$ and $s = \frac{1}{4}$ to the value with γ and $s = 1$. This yields a 30% theoretical increase in χ , which is small compared to the effects of changing γ alone. This is also offset by the same reduction in neighbor cutoff examined above, resulting in the reduced impact of s on η_{Sc} .

IV. CONCLUSIONS

While there has been some discussion as to whether or not the Schmidt number is a relevant physical quantity in DPD,²⁰ past analyses nonetheless indicate^{9,16} that large values are necessary to achieve physically accurate results. Thus, we have examined the scaling and efficiency of the Schmidt number as a function of the DPD parameters γ , r_c , and s , across three orders of magnitude of Sc , considering both theoretical predictions and the results from numerical simulations. In both cases, we see (for constant Sc) that the efficiency η_{Sc} increases with γ , decreases with r_c , and remains relatively constant for alternate values of s . Therefore, despite the apparent, preferable scaling of $Sc \propto r_c^8$, it is more beneficial to leave $r_c = R$ and increase γ alone in order to reach a Schmidt number consistent with liquid water. This is the result of maintaining equivalent temperature reproduction and numerical accuracy for every set of input parameters (which results in a modification of the time step and neighbor searching cutoff). The values of η_{Sc} indicate a factor of 3–4 speed improvement when manipulating γ instead of increasing r_c for $Sc = O(10^3)$. While the single-particle hydrodynamics extension of Karniadakis¹⁴ was used for the simulations, the theoretical predictions apply equally well to standard DPD.

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