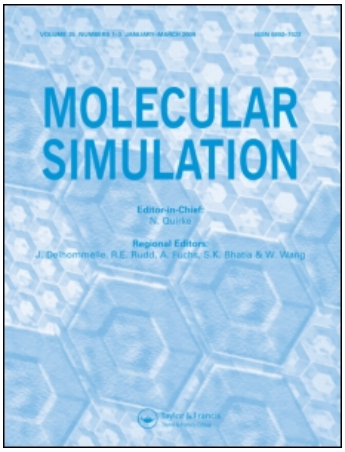

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Can such Long Time Steps Really be used in Dissipative Particle Dynamics Simulations?

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Commonly used time steps in dissipative particle dynamics (DPD) simulations are too large and lead to systematic errors in the computed properties. The main source of errors is the inaccurate integration of the conservative force. This error can be reduced to some extent by constructing a smoother force without any abrupt change at the cut-off distance, but the improvement is marginal. Alternatively, we tried smooth forces that also lead to the same conclusion. It is possible to find combinations of parameters for the random and dissipative forces that make errors cancel, but the combinations will depend on the system's thermodynamic state and on the particular force model. The only safe procedure is to use small time steps, i.e. comparable with those used in MD simulations. Alternatively, an improved integration algorithm should be used for the conservative force.

Keywords: Dissipative particle dynamics; Integration algorithms; Time step; Mesoscale simulation; Water

PACS numbers: 02.70. -C; 02.70. N_s; 05.10. -a

INTRODUCTION

Dissipative particle dynamics (DPD) [1] has become a popular simulation technique for mesoscale soft matter [2]. The basic idea behind DPD is that many important properties of soft matter are determined by the collective properties of clusters of molecules or super-molecular domains rather than by the individual molecules. DPD is used to model such domains with particles subject to a kind of Langevin equation of motion. Despite significant progress [3,4], the relationship between the properties of a dissipative particle and its molecular constituents is still somewhat obscure.

In the classical DP force model, particle i of species a and particle j of species b interact with conservative, dissipative, and random forces according to Ref. [1]

$$\mathbf{f}^C(r_{ij}) = a_{ab} w_{ab}(r_{ij}) \hat{\mathbf{r}}_{ij}, \tag{1a}$$

$$\mathbf{f}^D(r_{ij}) = -\gamma w_{ab}^2(r_{ij})(\mathbf{v}_{ij}\cdot\hat{\mathbf{r}}_{ij})\hat{\mathbf{r}}_{ij}, \text{ and} \tag{1b}$$

$$\mathbf{f}^R(r_{ij}) = \sigma w_{ab}(r_{ij}) \xi_{ij} \hat{\mathbf{r}}_{ij}, \tag{1c}$$

respectively, where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $\hat{\mathbf{r}}_{ij}$ is the unit vector in the direction of $\mathbf{r}_{ij}$, $r_{ij} = |\mathbf{r}_{ij}|$, and $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$. The weight function $w_{ab}(r_{ij})$ limits the range of the forces. It is usually taken to be the same for all three forces. The parameters a_{ab}, γ, σ, and ξ_{ij} will be discussed below, here we only note that $\mathbf{f}^D$ and $\mathbf{f}^R$ act together as a thermostat with set point

$$T_0 = \sigma^2 / 2\gamma k_B, \tag{2}$$

where k_B is Boltzmann's constant [5]. For simplicity, we shall in the following consider a single component.

The classical $w(r_{ij})$ is somewhat arbitrarily chosen according to computational convenience rather than physical realism [1],

$$w(r_{ij}) = \begin{cases} 1 - r_{ij}^* & \text{for } r_{ij}^* < 1 \\ 0 & \text{for } r_{ij}^* \geq 1 \end{cases}, \tag{3}$$

where, $r_{ij}^* = r_{ij}/r_c$, r_c is the range of the force. The potential energy function that corresponds to

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the conservative force, Eqs. (1a) and (3), is

$$u(r_{ij}) = \begin{cases} \frac{1}{2}ar_c\left(1 - r_{ij}^*\right)^2 & \text{for } r_{ij}^* < 1 \\ 0 & \text{for } r_{ij}^* \geq 1 \end{cases} \quad (4)$$

Equation (4) suggests that a dimensionless interaction strength may be defined as

$$a^* = \frac{ar_c}{k_B T_0}. \quad (5)$$

The coarse-graining of the molecular model leads to units of length and time that are larger than in MD simulations for the same system. For instance, in a MD simulation of water, the molecular unit of length is approximately the Lennard–Jones parameter $\sigma \sim 3.2$ Å. In DPD simulations of liquid water, Groot and Rabone [6] used $r_c = 6.46$ Å as the unit of length. Similarly, the unit of time in MD simulations is $t_c = \sigma(m/k_BT)^{1/2}$, which equals 0.86×10^{-12} s for water at 298 K, whereas the corresponding value for a dissipative water particle is $t_c = r_c(m/k_BT)^{1/2} = 3.02 \times 10^{-12}$ s (m is the mass of a molecule or dissipative particle). The coarse-graining in DPD models therefore enables one to simulate a system for a somewhat longer real time compared to MD, given the same number of time steps and particles in the simulations. Moreover, due to the actions of the random and dissipative forces, the system will relax faster towards equilibrium or stationary states.

More important, however, is the fact that the forces used in DPD are soft compared to typical MD [7]. A comparison for water at 298 K is shown in Fig. 1. This allows a much longer time step in reduced units in DPD compared with MD. Groot and Warren recommended that $\delta t^* = \delta t/t_c = 0.04$ (compared to a normal value of 0.005 used in MD) [8].

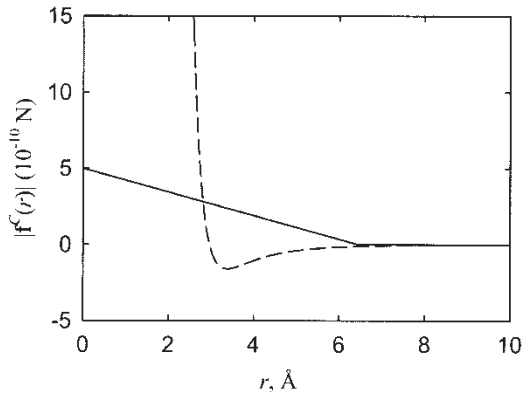

FIGURE 1 The DPD force model for water at 298 K (solid line) compared with a Lennard–Jones model (dashed line).

Apart from the fact that the conservative force has to be repulsive and soft [9], which results from the coarse-graining of the model, little attention has been paid to the details of the functional form of the weight function $w(r_{ij})$. For instance, how does the abrupt change in the force at $r = r_c$ affect the results of the numerical integration of the equations of motion? Secondly, do the weight functions for the conservative force and the random and dissipative forces have the same requirements to the numerical integrator?

It has been shown that the numerical integrator may introduce serious artifacts in the absence of a conservative force (i.e. the ideal gas case) [10–13]. The errors increase with increasing time step. It is believed that these artifacts are less serious if the conservative force dominates the particle interactions [13].

On this background, three features of DPD are explored in this paper:

1. The properties of various soft conservative force models with different smoothnesses,
2. The effect of choosing a smooth function also for the dissipative and random forces, and
3. The effect of using the Lowe–Andersen thermostat instead of the, random and dissipative-forces.

The first question is addressed by studying the energy conservation in the absence of random and dissipative forces. To examine the second and third questions, we consider how the system's temperature and energy depend on the model's parameters for an ideal gas as well as a non-ideal fluid.

FORCE PARAMETERS AND STATE VARIABLES

Groot and Rabone defined r_c as in Ref. [6]:

$$r_c = (v_m N_m \rho^*)^{1/3} \quad (6)$$

where v_m is the molar volume of the real system of interest and N_m is the number of molecules that make up a DP. The reduced density defined as $\rho^* = Nr_c^3/V$ for N dissipative particles in a volume V, is chosen somewhat arbitrarily. Typical values of ρ^* and N_m are in the range 3–5 (the DPD $\mathbf{f}^C$ shown in Fig. 1 is for $N_m = 3$ and $\rho^* = 3$).

The parameter a^* is determined by matching the compressibility of the DP system to that of the real system of interest. Groot and Warren [8] used the inverse isothermal compressibility for this purpose. From their DP equation of state, the interaction strength is found as

$$a^* = \frac{T^*}{0.202\rho^*}\left(\frac{\kappa_T^{-1} N_m}{\rho_m k_B T_0} - 1\right) \quad (7)$$

for $\rho^* > 2$, where κ_T^{-1} and ρ_m are the experimental inverse compressibility and molecular number density, respectively, of the real system. Typically, $\kappa_T^{-1}/\rho_m k_B T$ equals 16 for liquid water at room temperature, which gives $a^* = 78$ if $N_m = 3$ and $\rho^* = 3$ [6].

The parameter γ is related to the system's viscosity. Once γ is fixed, σ is given by Eq. (2). The random number ξ_{ij} must have zero mean and unit variance; the details of its distribution is thought to be less important [8]. Groot and Warren have given a detailed discussion of how to determine numerical values for the force parameters. A typical value is $\sigma^* = \sigma(r_c^2/k_B^3 T_0^3 m)^{1/4} = 3$. Since the purpose of this paper is to examine the influence of the conservative force in relation to the model's thermodynamic rather than its dynamic properties, we refer the reader to the original papers for a closer look at how these parameters are determined. Here, we simply consider γ and σ^* as parameters.

In this study, we assumed that the underlying purpose was to simulate a given substance in a given state. In the past, parameters corresponding to liquid water at 298 K have often been used, and we will do the same in this work.

Some results for $\rho^* = 3$, $N_m = 3$, $a^* = 78$, $\gamma^* = \gamma r_c/(mk_B T_0)^{1/2} = 4.5$, $\sigma^* = (2\gamma^*)^{1/2} = 3$, and with $N = 500$ are shown in Fig. 2. The time step δt^* was varied between 0.005 and 0.0625. Each run had total length $t^*_{\text{run}} = 20,000$. The expected value of $\langle T^* \rangle$ was 1.0. The numerical integrator was the self-consistent velocity Verlet (SC-VV) integrator proposed by Vattulainen *et al.* [13].

Figure 2 shows that something is wrong with these results. The most obvious flaw is that both $\langle U \rangle$ and $\langle T^* \rangle$ for water increase with increasing δt^* when $\delta t^* \gtrapprox 0.02$. The dependency on δt^* was already pointed out by Groot and Warren [8], who accepted an artificial temperature increase (relative to the thermostat set point) of 2%. In their case, this meant $\delta t^* \leq 0.04$ for $\rho^* = 3$, $N_m = 1$, and $a^* = 25$. The results shown in Fig. 2 are slightly better than that for a higher value of a^* because a better integrator was used.

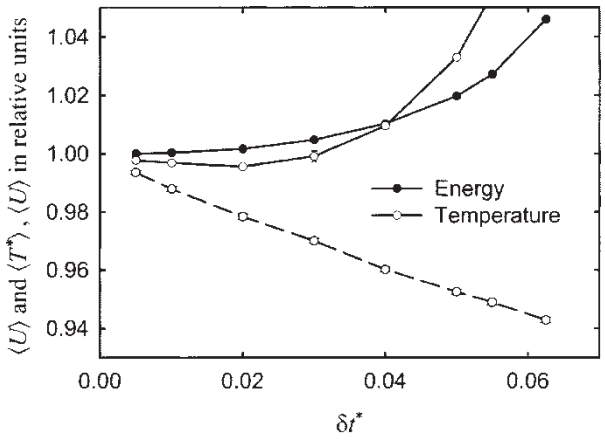

FIGURE 2 $\langle U \rangle$ and $\langle T^* \rangle$ as function of time step. The energy values are relative to the value at $\delta t^* = 0.005$. Parameter values are: $\rho^* = 3$, $N_m = 3$, $\sigma^* = 3$, and $T_0 = 1.0$. Parameter values for the "water" (solid line) and ideal-gas cases (dashed line) are $a^* = 78$ and $a^* = 0$, respectively. The symbol size represents three standard errors in the mean.

In an analysis of several integrators used in DPD simulations, Vattulainen *et al.* showed that the computed system temperature in an ideal gas is lower than the thermostat set point for all integrators [13]. The ideal gas ($a^* = 0$) is considered to be a strong test case because the random and dissipative forces dominate, and they are less suited for the Verlet integration scheme than is the conservative force. The temperature for an ideal gas is included in Fig. 2 for comparison. Some questions arising from these data are:

1. Why does the temperature show a positive deviation for the water model (except at small time steps) and a negative deviation for the ideal gas?
2. Why does the energy of the water model depend on δt^*?

THE PROBLEM WITH THE CONSERVATIVE FORCE

The reason why $\langle T^* \rangle$ decreases with increasing δt^* when $a^* = 0$ (ideal gas) is related to the numerical integrator's inadequate handling of $\mathbf{f}^D(r_{ij})$ and/or $\mathbf{f}^R(r_{ij})$ [13]. However, the increase in $\langle T^* \rangle$ and $\langle U \rangle$ when $a^* > 0$ must stem from $\mathbf{f}^C(r_{ij})$. The system appears to be artificially heated when $a^* > 0$ in a way the thermostatting function of the random and dissipative forces is not able to correct.

The heating must also appear as a lack of energy conservation when $\mathbf{f}^D(r_{ij})$ and $\mathbf{f}^R(r_{ij})$ are absent (i.e. in a MD simulation). We therefore checked the energy conservation, setting $\sigma^* = 0$. This is like switching off the thermostat in a *NVT* MD simulation, turning it into a *NVE* simulation. In MD, we would then require the energy to be conserved within an acceptable limit. If not, the time step should be reduced or the integrator improved.

The drift in the system's energy during a MD run of length $t^* = 10,000$, using the velocity Verlet (VV) algorithm (which is normally used for the conservative force in DPD simulations), is shown in Table I. The classical model showed very poor energy conservation except perhaps for $\delta t^* = 0.005$. We suspected the source of this problem to be the discontinuity in $\partial w(r_{ij})/\partial r_{ij}$ at $r_{ij} = r_c$ and modified the classical model with a smooth

TABLE I Increase (in %) of $\langle U^*/Nk_BT_0\rangle$ during a MD simulation for the classical DPD conservative force model with different truncation schemes. The total simulation time was $t^* = 10,000$ in all cases. The dashes show cases when the energy diverged after a few time steps

	Classical model with smooth truncation (Eq. (8))		
δt^*	*Eq. (3)*	$\Delta = 0.1$	$\Delta = 0.2$
0.005	0.1	0.0	0.0
0.01	2.1	0.0	0.0
0.02	50	0.2	0.0
0.03	–	4.4	0.7
0.04	–	–	6.7
0.05	–	–	–

truncation of $w(r_{ij})$ around r_c. A spline function was used for this purpose[¶]:

$$w(r_{ij}) = \begin{cases} 1 - r_{ij}^* & \text{for } r_{ij}^* < 1 - \Delta \\ \frac{1}{4\Delta}(1 - r_{ij}^* + \Delta)^2 & \text{for } 1 - \Delta \le r_{ij}^* \le 1 + \Delta \\ 0 & \text{for } r_{ij}^* > 1 + \Delta \end{cases} \tag{8}$$

The results obtained with this model are given in Table I.

When the weight function is truncated in a smooth way, energy is better conserved, although not for the values of δt^* that are normally used in DPD simulations. Clearly, the classical conservative force model gives rise to a stochastic energy contribution that heats the system up. One may expect that the thermostat will suppress this heating when $\sigma^* > 0$ in DPD, but the consequence may still be systematic errors in the system's properties.

In order to further investigate the properties of the weight function, we designed the following class of models:

$$w(r_{ij}) = \begin{cases} [1 - \left(r_{ij}^*\right)^n]^m & \text{for } r_{ij}^* < 1 \\ 0 & \text{for } r_{ij}^* \ge 1 \end{cases} \tag{9}$$

These models allow us to control discontinuities in higher order derivatives, the curvature of $w(r_{ij})$ around $r_{ij} = r_c$ and the behavior at $r_{ij} = 0$. The classical weight function is the special case with $n = m = 1$.

Table II shows results for $(n, m) = (1, 2)$, (2,2), and (2,3). All these models have a smooth truncation at $r_{ij} = r_c$, smoother for higher values of m. The difference between $n = 1$ and $n = 2$ is that $w(r_{ij})$ has a non-zero derivative at $r_{ij} = 0$ for $n = 1$, but zero derivative for $n = 2$. The equation of state depends on the conservative force, and in order to compare the results for different (n, m)-combinations, we chose to let all models represent water at 298 K through a match of the compressibility. This gives different values for a^*, and the values we used are included in Table II.

TABLE II Same as Table I, but with (n, m) conservative force models (Eq. (9)). The values of a^* are given in parenthesis the heading

	(n, m)		
δt^*	*(1,2) (a^*=225)*	*(2,2) (a^*=90)*	*(2,3) (a^*=150)*
0.005	0.0	0.0	0.0
0.01	0.0	0.0	0.0
0.02	0.1	0.4	0.0
0.03	2.1	5.7	0.4
0.04	–	–	22
0.05	–	–	–

There is indeed an improved energy conservation for the smoother functions at $r_{ij} = r_c$ whereas the slope at $r_{ij} = 0$ has little effect. There is little difference between the (n, m)-forms and the classical form with a smooth truncation at r_c. The value of a^* seems to have little effect on the energy conservation (compare, e.g. the (1,2) and (2,2) cases). In principle, combination of the (2,3) model or the smooth truncated (1,1) model with a good integrator of dissipative-random forces should allow us to get the right $\langle T^*\rangle$ and $\langle U^*\rangle$ at least up to $\delta t^* = 0.02$.

THE RANDOM AND DISSIPATIVE FORCES

The role of the weight function for the random and dissipative forces was tested by comparing the classical model with the smooth model defined by Eq. (8) with $\Delta = 0.2$, keeping $a^* = 0$, $\sigma^* = 3$, and varying δt^*. The results from this test are shown in Fig. 3. The conclusion here is that the weight function smoothness has virtually no impact on the computed temperature for this particular integrator (the SC-VV algorithm).

To find out if this was true also for other functional forms and other integrators, we tested the (n, m)-weight functions listed in Table II with the SC-VV algorithm. We also tested the modified VV algorithm [8] for the $(n, m) = (2, 3)$ case ($\lambda = 0.65$) and the more recent algorithm by Lowe [14]. It should be noted that the Lowe algorithm does not use the dissipative and random forces. Instead, the system is thermalized in such a way that, for all pairs of particles for which $r_{ij} < r_c$, a new relative velocity is drawn from the Maxwell distribution with a probability $\Gamma\delta t^*$. Nikunen *et al.* [15] recently found that the Lowe

[¶]Introducing a smooth truncation will change the equation of state. The change is small, and we have used the same a^*-values, determined from Eq. (7) for both models.

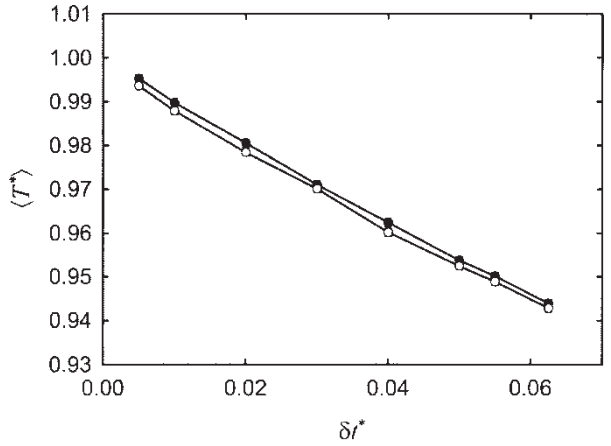

FIGURE 3 $\langle T^* \rangle$ as function of time step for the ideal gas. The two plots are for the classical model (white circles) and the model with smooth truncation with $\Delta = 0.2$ (black circles). Parameter values are: $\rho^* = 3$, $N_m = 3$, $\sigma^* = 3$, $a^* = 0$, and $T_0 = 1.0$. The symbol size represents three standard errors in the mean.

algorithm performs extremely well for time steps as large as $\delta t^* = 0.1$ in the ideal-gas case with the classical weight function. Our results are shown in Fig. 4, where data for the classical weight function and the SC-VV algorithm are included for comparison. The results confirm previous findings [13,15] for the various integrators. They also show little difference between the different weight functions. We can apparently draw the general conclusion that the smoothness of the weight function has little consequence for performance of the different integrators in the ideal-gas case. We can also confirm the findings of Nikunen *et al.* that the Lowe integrator performs extremely well for the ideal gas.

THE COUPLING BETWEEN THE FORCES

In the previous sections, we showed that the classical weight function for the conservative force heats the system up and that various integration schemes for the random and dissipative forces may give either heating or cooling, depending on the integrator. The Lowe integrator is especially attractive because of good thermostatting ability and computational simplicity. In this section, we will consider the case when all three forces are active.

The smooth weight functions show much better energy conservation for the water case with $\sigma^* = 0$ compared with the classical model. If the conservative force causes a drift in energy, we might expect that the thermostat is able to suppress this, at least to some extent. We could argue that if the two models give the same result (i.e. agree within the combined errors), the energy conservation problem is insignificant. This would give a range of δt^*-values where the results are not affected by the energy conservation problem. Alternatively, we could follow Groot and Warren [8] and accept a temperature deviation from the set point of max. 2%.

Figure 5 compares results from the classical and smoothed classical model for the water case, using the SC-VV algorithm. Three features should be commented. First, the deviation from the thermostat set point is significant for time steps larger than $\delta t^* > 0.04$. This can be attributed to the thermostat's inability to control the large temperature increase stemming from the conservative force. Second, the smoothed weight function gives a somewhat better temperature control for large time steps. This is due to the conservative force's better behavior in the integration algorithm. Third, after an initial temperature decline for small time steps, the temperature goes through a minimum and then increases. The decline for small time steps is the same effect as shown in Fig. 3, whereas the effect shown in Fig. 2 becomes dominant at large time steps. By the Groot–Warren criteria, the situation is unacceptable for $\delta t^* > 0.04$ with the classical model and for $\delta t^* > 0.05$ for the smooth classical model.

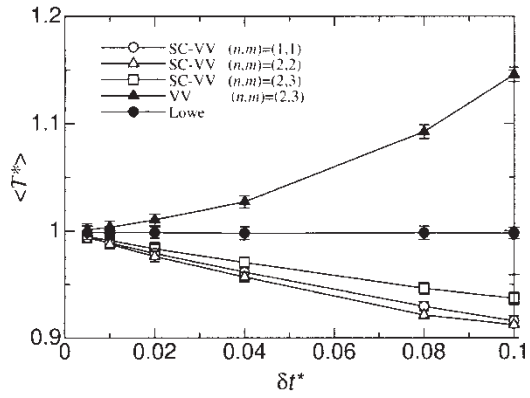

FIGURE 4 Same as in Fig. 3, but with different weight functions and integration algorithms. The labels are explained in the text. The Lowe algorithm was used with $\Gamma = 0.74$.

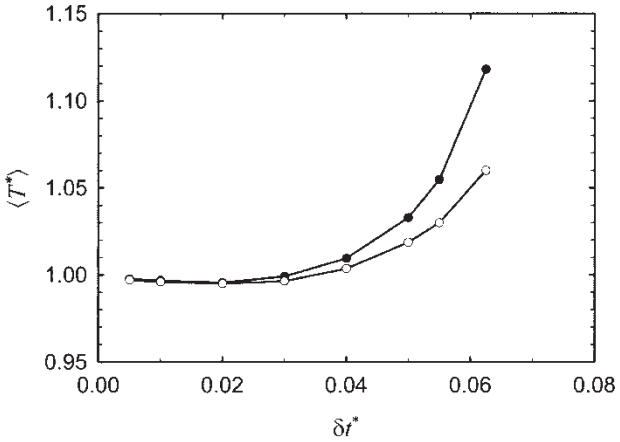

FIGURE 5 The water model's temperature as function of time step. Black circles represent the classical model and white circles the smooth classical model with $\Delta = 0.2$. The parameter values are the same as in Fig. 2.

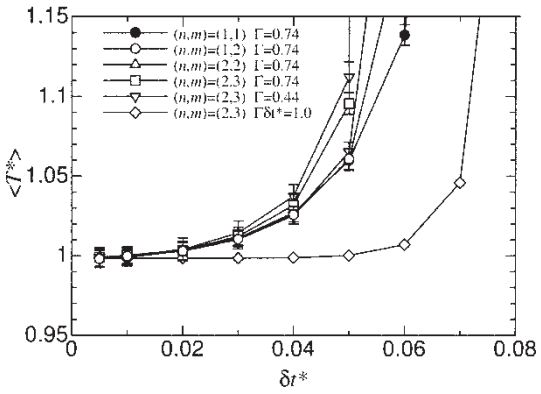

FIGURE 6 Same as in Fig. 5, but with different weight functions for the conservative force and with the Lowe integration algorithm. The labels are explained in the text.

One conclusion from tests on ideal gas (Fig. 4 and Ref. [15]) was that the Lowe integrator shows promising properties. We therefore tried it on the water model. The parameter Γ in the Lowe algorithm controls the coupling between the particles and the heat reservoir. If $\Gamma\delta t^* \approx 0$ or $\Gamma\delta t^* \approx 1$, the coupling is weak or strong, respectively.

Results for the temperature, using various weight functions and Γ-values are shown in Fig. 6. Compared to using the SC-VV integrator, we find the same increasing trend with increasing time step. With the Lowe integrator, the initial decline in $\langle T^* \rangle$ has disappeared because the Lowe algorithm does not show the negative deviation for the non-conservative forces that the SC-VV algorithm does. Moreover, one has to use Γ-values close to maximum in order to control the temperature up to $\delta t^* = 0.05$.

From Fig. 6 it seems that the classical weight function does not differ significantly from the (n, m) type. When we consider the energy, however, this picture is changed. Figure 7 shows that the system's energy (for the same cases as in Fig. 6) is rather poor even for time steps as small as $\delta t^* = 0.03$. It does not help much to increase the coupling to the heat reservoir. Unexpectedly, the classical weight function is better than the smooth ones. This trend must be closely related with the stochastic thermalization procedure of the Lowe algorithm. In the Lowe algorithm, all pairs of particles have the same probability to be thermalized as long as the particles are within the interaction range, i.e. the thermostat works independently of the interparticle distance. On the other hand, the weight function of the conservative force does depend on the distance. The derivative of the weight function is constant for the (1,1), model, but not for the other (n, m) models for which there is a range of rapidly changing force. Therefore, in the case of the (1,1) model, the impact of the stochastic thermostat on the conservative force is constant and modest. This is a possible reason that the Lowe algorithm works reasonably well in combination with the classical weight function.

With the somewhat confusing picture drawn up to this point, one may wonder why DPD seems to work for such long time steps that have been used in the past. The reason is a fortuitous cancellation of errors. Results from a series of simulations with the SC-VV algorithm, the smooth model defined by Eq. (8) with $\Delta = 0.2$, keeping $a^* = 78$, and varying σ^* and δt^*, are shown in Fig. 8. For large time steps, the temperature cannot be controlled well. It appears that good performance (say, $|\langle T^* \rangle - T_0|T_0 < 0.02$) is obtained only within a range of δt^* and σ^*. The combination recommended by Groot and Warren [8] ($\sigma^* = 3$, $\delta t^* = 0.04$) happens to be within this range. Using the Lowe integrator, which is clearly a better integrator, would lead to a worse situation in the sense that the system's temperature would be greater

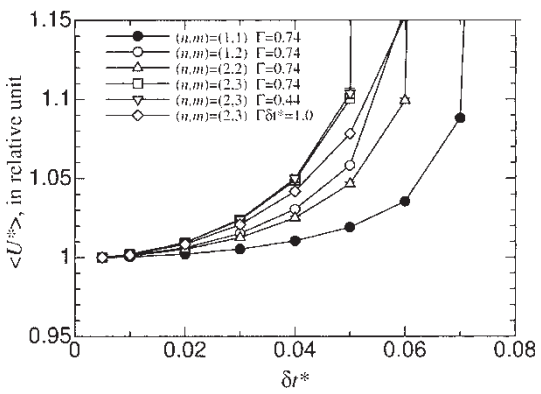

FIGURE 7 Same as in Fig. 6, but for the system's energy instead of temperature.

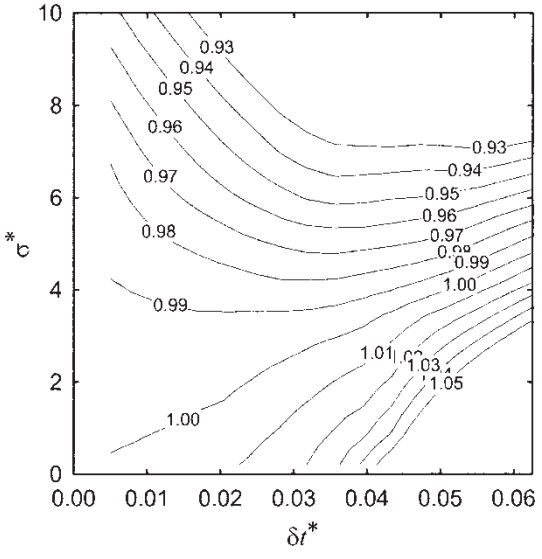

FIGURE 8 $\langle T^* \rangle$ as function of time step and σ^* for the smooth classical model with $\Delta = 0.2$. The other parameter values are the same as in Fig. 2.

than the thermostat set point for all values of δt^* except the smaller ones.

A different conclusion for the numerical values would be drawn if we consider a different value of a^*, a different system, or indeed a different property. For instance, the values of acceptable time steps are slightly changed if we instead consider the energy. An error in the energy of, say, max. 2% can be achieved with $\delta t^* < 0.05$ for the classical (1,1) model and with $\delta t^* < 0.03$ for the other (n, m) models with the Lowe algorithm. With the SC-VV algorithm, the limit would be $\delta t^* < 0.05$ for the (1,1) model (see Fig. 3).

CONCLUSION

In conclusion, we have shown that recommended values for the potential parameters and time steps in DPD [6,8] give systematic errors in the computed properties of a water model. In agreement with Vattulainen *et al*. [11,13], we also found that there is a strong dependency on the time step due to the dissipative force in the ideal-gas case, For the conservative force, however, there is an opposite effect due to numerical truncation errors for large time steps. When applied to a water model, the errors partly cancel each other, but only for specific combination of the simulation parameters. Using a smooth weight function or the Lowe algorithm does not improve the situation significantly.

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References

[1] Hoogerbrugge, P.J. and Koelman, J.M.V.A. (1992) "Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics", *Europhys. Lett.* **19**, 155.
[2] Frenkel, D. and Smit, B. (2002) *Understanding Molecular Simulation*, 2nd. ed. (Academic Press, San Diego).
[3] Flekkoy, E.G. and Coveney, P.V. (1999) "From molecular dynamics to dissipative particle dynamics", *Phys. Rev. Lett.* **83**, 1775.
[4] Flekkoy, E.G., Coveney, P.V. and De Fabriths, G. (2000) "Foundations of dissipative particle dynamics", *Phys. Rev. E* **62**, 2140.
[5] Espanõl, P. and Warren, P. (1995) "Statistical mechanics of dissipative particle dynamics", *Europhys. Lett.* **30**, 191.
[6] Groot, R.D. and Rabone, K.L. (2001) "Mesoscopic simulation of cell membrane damage, morphology change and rupture by nonionic surfacetants", *Biophys. J.* **81**, 725.
[7] Spenley, N.A. (2000) "Scaling laws for polymers in dissipative particle dynamics", *Europhys. Lett.* **49**, 534.
[8] Groot, R.D. and Warren, P.B. (1997) "Dissipative particle dynamics: bridging the gap between atomistic and mesoscopic simulation", *J. Chem. Phys.* **107**, 4423.
[9] Forrest, B.M. and Suter, U.W. (1995) "Accelerated equilibration of polymer melts by time-coarse-graining", *J. Chem. Phys.* **102**, 7256.
[10] Pagonabarraga, I., Hagen, M.H.J. and Frenkel, D. (1998) "Self-consistent dissipative particle dynamics", *Europhys. Lett.* **42**, 377.
[11] Besold, G., Vattulainen, I., Karttunen, M. and Polson, J.M. (2000) "Towards better integrators for dissipative particle dynamics simulations", *Phys. Rev. E* **62**, R7611.
[12] den Otter, W.K. and Clarke, J.H.R. (2001) "A new algorithm for dissipative particle dynamics", *Europhys. Lett.* **53**, 426.
[13] Vattulainen, I., Karttunen, M., Besold, G. and Polson, J.M. (2002) "Integration schemes for dissipative particle dynamics simulations: from softly interacting systems towards hybrid models", *J. Chem. Phys.* **116**, 3967.
[14] Lowe, C.P. (1999) "An alternative approach to dissipative particle dynamics", *Europhys. Lett.* **47**, 145.
[15] Nikunen, P., Karttunen, M. and Vattulainen, I. (2003) "How would you integrate the equations of motion in dissipative particle dynamics simulations?", *Comput. Phys. Commun.* **153**, 407.