Dissipative Particle Dynamics Modelling of Low Reynolds Number Incompressible Flows

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Synopsis

This paper is concerned with the numerical modelling of a slow (creeping) flow using a particle-based simulation technique, known as dissipative particle dynamics (DPD), in which the particles mass is allowed to approach zero to simultaneously achieve a high sonic speed, a low Reynolds number and a high Schmidt number. This leads to a system of stiff stochastic differential equations, which are solved efficiently by an exponential time differencing (ETD) scheme. The ETD-DPD method is first tested in viscometric flows, where the particle mass is reduced down to 0.001. The method is then applied for the modelling of rigid spheres in a Newtonian fluid by means of two species of DPD particles, one representing the solvent particles and the other, the suspended particle. Calculations are carried out at particle mass of 0.01, with corresponding Mach number of 0.08, Reynolds number of 0.05 and Schmidt number of 6.0×10^3. Stokes results are used to determine the DPD parameters for the solvent-sphere interaction forces. The method obeys equipartition and yields smooth flows around the sphere with quite uniform far-field velocities.

Keywords: DPD, low mass, stiff system, incompressible flow, low Reynolds number

1   Introduction

The Dissipative Particle Dynamics (DPD) method, introduced originally by Hoogerbrugge and Koelman in 1992, is a relatively new simulation technique for fluid flow problems. The method can be regarded as a particle-based flow solver, since the mean quantities extracted from the particles configuration (density, linear momentum, stresses, *etc.*) satisfy the conservation of mass and momentum, irrespective of the potentials chosen (and by implication, irrespective of the length and time scales). The original DPD version of Hoogerbrugge and Koelman was considered as an improvement over the molecular dynamics (MD) [Rapaport and Clementi (1986)] and lattice-gas automata (LGA) [Frisch *et al.* (1986)] simulation methods. The DPD method incorporates dissipation into an MD model to facilitate the simulation of hydrodynamic phenomena, and permits the particles moving freely in continuous space to avoid problems faced by LGA (*i.e.*, the absence of isotropy and Galilean invariance). The DPD method is faster than MD and more flexible than

LGA. Furthermore, in contrast to Brownian Dynamics Simulations (BDS) [Fan *et al.* (1999)], the DPD method conserves both mass and momentum [Español (1995)]. Furthermore, both the flow kinematics and the stress tensor can be found as parts of the solution procedure. Later on, the original DPD model of Hoogerbrugge and Koelman was modified to possess a proper thermal equilibrium state (*i.e.*, satifying a fluctuation-dissipation theorem) [Español and Warren (1995)]. The DPD method can be thought of as a coarse grained version of MD, in addition of its being a particle-based solver. Depending on the purposes of the investigation, we can take either view, or both of DPD. Marsh *et al.* (1997) derived an estimate, based on kinetic theory, for the transport and thermodynamic properties in terms of the model parameters. Useful ranges for the DPD parameters (the repulsion parameter, time step and noise level) for simulations were found and reported in the work of Groot and Warren (1997) and Groot (2004).

The DPD method has emerged as an attractive and powerful tool for the simulation of complex-structure fluids. There have been various DPD applications, for examples, colloidal suspensions [Koelman and Hoogerbrugge (1993); Boek *et al.* (1997); Chen *et al.* (2006); Pan *et al.* (2010)], fluid mixtures [Novik and Coveney (1997); Laradji and Hore (2004)], polymer solutions [Kong *et al.* (1997); Jiang *et al.* (2007)], polymer melts [Nikunen *et al.* (2007)], red blood cell modelling [Pan *et al.* (2010b)] - this list is not meant to be exhaustive. By endowing DPD particles with some forms of connector forces, complex-structure fluids can be handled in a very simple manner. For example, in simulating colloidal suspensions, a colloidal particle can be simply modelled by a set of standard but constrained DPD particles located on a rigid surface [Chen *et al.* (2006)], or by a single DPD particle with a different set of DPD parameters [Pan *et al.* (2008)]. For the former, it is possible to form a colloidal particle of any complex shape. For the latter, parameters for the interaction between the colloidal particle and solvent particles can be determined using Stokes results. As another example, a polymer chain may be simulated by connecting some DPD particles [Kong *et al.* (1997)], in DPD simulations of polymer solutions or melts. In addition, there have been modifications to the standard DPD method [Español (1998); Pan *et al.* (2008)], but we feel that these modifications may not be absolutely necessary for our purposes here.

Incompressibility is a good approximation in many practical flows at low Mach numbers ($M <$ 0.3). Many applications also involve flows that exhibit strongly-viscous behaviour at low fluid

inertia (*i.e.,* low Reynolds number). In a DPD simulation, the fluid is modelled by DPD particles undergoing their Newtonian second law of motion, interacting with each other through a soft repulsive, dissipative and random forces. In the limit of no conservative force, Marsh *et al.* (1997) showed that, in the linearised solution to the first-order Fokker-Planck-Boltzmann equation, the DPD fluid is a *compressible* Newtonian fluid

$$\mathbf{T} = -nk_BT\mathbf{I} + \left(\zeta - \frac{2}{3}\eta\right)\nabla.\mathbf{u}\mathbf{I} + \eta\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right), \tag{1}$$

where $\mathbf{T}$ is the mean field stress tensor, $\mathbf{u}$ the mean field velocity vector, η the shear viscosity, ζ the dilational viscosity, n the number density, k_BT the Boltzmann temperature (mean kinetic energy of the particles), and $\mathbf{I}$ the unit tensor.

Expressions for the speed of sound, the Reynolds number, and the Schmidt number of the DPD fluid are respectively given by [Español (1995); Groot and Warren (1997)]

$$c_s^2 = \frac{k_BT}{m} + \frac{\lambda anr_c^4}{m}, \ Re = \frac{mnUL}{\eta}, \ Sc = \frac{\eta}{mnD}, \tag{2}$$

where m is the mass of the particle (mn is the density of the fluid), a the repulsion parameter, r_c some radius that limits the range of the conservative force, U and L the characteristic velocity and length, λ a constant, and D the diffusivity. The Mach number, which is defined as $M = U/c_s$, may be used to determine whether a flow can be regarded as an incompressible flow. If $M < 0.3$, compressibility effects may be ignored [Anderson (2010)]. Because of the soft interaction between particles in a DPD system, the speed of momentum transfer is slow and has the same order of particle diffusion, that is, the Schmidt number is about unity. For real fluids of physical properties like those of water, the Schmidt number is $O(10^3)$, and therefore there is the need to improve on the dynamic behaviour of the DPD system. It was observed [Symeonidis *et al.* (2006)] that increasing Sc in DPD simulation leads to a better agreement with experimental data.

This study is concerned with the computational modelling of low Reynolds number flows of a DPD fluid. In regarding the DPD method as a particle-based solver, particles are artificial means of producing fluid density, and linear momentum that satisfy conservation laws. We then need an independent mean of controlling the Reynolds, the Schmidt and the Mach numbers. In published

DPD literature, the particle mass was typically normalised to unity, (*i.e., $m = 1$*). Low values of M and Re were obtained by reducing the velocity U. However, under such conditions, the random forces can be relatively high and therefore may produce large fluctuations in the velocity field. It will be shown later that the effects of compressibility on the flow field may not be negligible for certain situations and can be a complication in the simulation. We propose to reduce the particle mass as an alternative to achieve both low values of M and Re. Furthermore, a physical value of Sc can be reached at the same time. When m is small, the resultant DPD system is stiff and hence special care is needed in order to yield an accurate solution with computational efficiency. A considerable effort has been devoted to developing numerical integrations for stiff problems [Shampine and Gear (1979); Cox and Matthews (2002)]. Examples of such schemes include the backward Euler, the integrating factor and the exponential time differencing (ETD) techniques. They allow relatively-large time steps to be used and therefore provide some computational savings. We adopt the ETD technique here, which is particularly suited to stiff semi-linear differential problems, in the DPD algorithm to handle low mass systems. The present ETD-DPD method is extensively verified through the simulations of Couette and Poiseuille flows with exact analytical solutions and then applied for the modelling of rigid spheres in a Newtonian fluid using two species of DPD particles, one representing the solvent and the other, the suspended particle.

The paper is organised as follows. Section 2 gives a brief review of ETD schemes. We then describe DPD for low mass systems in Section 3. Numerical results are presented in Section 4 for Couette and Poiseuille flows and in Section 5 for flow past a sphere. Section 6 gives some concluding remarks.

2 Exponential time differencing (ETD) schemes

The following ordinary differential equation (ODE)

$$\frac{d\phi(t)}{dt} = c\phi(t) + A(t), \tag{3}$$

where the parameter c is either large and negative or large and imaginary, with A representing forcing terms, is said to be stiff. This equation may have a solution that evolves on vastly different time scales, all occurring simultaneously. It is known that classical integration methods do not handle stiff problems very effectively. They require many small time steps that produce significant roundoff errors, which may invalidate the solution [Shampine and Gear (1979)].

We multiply (3) by the integrating factor e^{-ct}, and then integrate the equation over a single time step from t to $t + \Delta t$ to get

$$\phi(t + \Delta t) = \phi(t)e^{c\Delta t} + e^{c\Delta t} \int_0^{\Delta t} e^{-c\tau} A(t + \tau)d\tau. \tag{4}$$

This result is exact, and the basis of the ETD method lies in the derivation of approximations to the integral on the right side of (4). In the simplest approximation (A is treated a constant within this time step), one arrives at the first-order ETD scheme

$$\phi(t + \Delta t) = \phi(t)e^{c\Delta t} + \frac{1}{c} \left(e^{c\Delta t} - 1 \right) A(t). \tag{5}$$

If we apply the following higher-order approximation

$$A(t + \tau) = A(t) + \frac{\tau(A(t) - A(t - \Delta t))}{\Delta t}, \tag{6}$$

then the second-order ETD scheme is obtained

$$\phi(t + \Delta t) = \phi(t)e^{c\Delta t} + \frac{1}{c^2 \Delta t} \left[\left((c\Delta t + 1)e^{c\Delta t} - 2c\Delta t - 1 \right) A(t) + \left(-e^{c\Delta t} + c\Delta t + 1 \right) A(t - \Delta t) \right]. \tag{7}$$

It should be emphasised that the above scheme is designed for a deterministic system so that the approximate solutions do not contain unwanted fast time scales.

3 DPD for low mass systems

The DPD system consists of a set of N particles that can move freely; its evolution algorithm can be written as

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \tag{8}$$

$$m_i \frac{d\mathbf{v}_i}{dt} = \mathbf{F}_i, \tag{9}$$

where m_i, $\mathbf{r}_i$ and $\mathbf{v}_i$ represent the mass, position and velocity vector of a particle i, respectively; and $\mathbf{F}_i$ is the total force vector exerted on it, containing three parts

$$\mathbf{F}_i = \sum_{j=1,j\neq i}^{N} \left(\mathbf{F}_{ij,C} + \mathbf{F}_{ij,D} + \mathbf{F}_{ij,R} \right), \tag{10}$$

in which the sum runs over all other particles, denoted by j, within a certain cutoff radius r_c. The first term on the right is referred to as conservative force (subscript C), the second dissipative force (subscript D) and the third random force (subscript R). These forces are usually given in the forms

$$\mathbf{F}_{ij,C} = a_{ij} w_C \mathbf{e}_{ij}, \tag{11}$$

$$\mathbf{F}_{ij,D} = -\gamma w_D \left(\mathbf{e}_{ij} \cdot \mathbf{v}_{ij} \right) \mathbf{e}_{ij}, \tag{12}$$

$$\mathbf{F}_{ij,R} = \sigma w_R \theta_{ij} \mathbf{e}_{ij}, \tag{13}$$

where a_{ij}, γ and σ are constants reflecting the strength of the forces; w_C, w_D and w_R the distance-dependent weighting functions; $\mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij}$ a unit vector from particle j to particle i ($\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $r_{ij} = |\mathbf{r}_{ij}|$); $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ the relative velocity vector, and θ_{ij} a Gaussian white noise ($\theta_{ij} = \theta_{ji}$) with stochastic properties

$$\langle \theta_{ij} \rangle = 0, \tag{14}$$

$$\langle \theta_{ij}(t) \theta_{kl}(t') \rangle = \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} \right) \delta \left(t - t' \right), \text{with } i \neq k \text{ and } j \neq l. \tag{15}$$

It is noted that the cutoff radius r_c can be different for different types of forces. In incremental form, the random force takes the form

$$\Delta \mathbf{F}_{ij,R} = \sigma w_R(r_{ij})\Delta \xi_{ij}\mathbf{e}_{ij}\sqrt{\Delta t}, \tag{16}$$

where $\Delta \xi_{ij}$ is a random number with zero mean and unit variance, chosen independently for each pair of particles and each time step in the numerical integration process. All forces act along the line joining the pair of particles and the DPD method thus conserves momentum.

It was shown [Español and Warren (1995)] that the equilibrium and detailed balance of the system lead to the following constraints

$$w_D(r_{ij}) = (w_R(r_{ij}))^2, \tag{17}$$

$$k_B T = \frac{\sigma^2}{2\gamma}, \tag{18}$$

which relate the strength of the dissipative force to the strength of the random force through the definition of the thermodynamic temperature (the equipartition principle or fluctuation-dissipation theorem).

The standard form of the weighting functions is [Groot and Warren (1997)]

$$w_C(r_{ij}) = 1 - \frac{r_{ij}}{r_c}, \tag{19}$$

$$w_D(r_{ij}) = \left(1 - \frac{r_{ij}}{r_c}\right)^2. \tag{20}$$

To increase the Schmidt number, which governs the dynamic response of a fluid, Fan *et al.* (2006) proposed a generalised form for the dissipative weighting function

$$w_D(r_{ij}) = \left(1 - \frac{r_{ij}}{r_c}\right)^s, \tag{21}$$

where s is a constant - typically $s = 1/2$ is used. In this work, we consider reducing the particle mass to further increase the Schmidt number. Using the approximate analysis of Marsh *et al.* (1997), for any value of s, one can arrive at approximate expressions for the viscosity, diffusivity

and Schmidt number in terms of the system parameters. For $s = 1/2$, which is used in this study, we obtain

$$\eta = \frac{315mk_BT}{128\pi\gamma r_c^3} + \frac{512\pi\gamma n^2 r_c^5}{51975}, \tag{22}$$

$$D = \frac{315k_BT}{64\pi n\gamma r_c^3}, \tag{23}$$

$$Sc = \frac{1}{2} + \frac{32768}{16372125}\frac{\pi^2\gamma^2 n^2 r_c^8}{mk_BT}. \tag{24}$$

The equation of state for the pressure has been shown to be [Groot and Warren (1997)]

$$p = nk_BT + \frac{2\pi}{3}n^2 \int_0^{r_c} rF_C(r)g(r)r^2 dr, \tag{25}$$

where $g(r)$ is the radial distribution function. If one assumes $g(r) \sim 1$, the above expression reduces to

$$p = nk_BT + \frac{\pi}{30}an^2 r_c^4, \tag{26}$$

from which the speed of sound is computed as

$$c_s^2 = \frac{\partial p}{\partial \rho} = \frac{k_BT}{m} + \frac{\pi}{15}\frac{anr_c^4}{m}, \tag{27}$$

where $\rho = mn$ is the mass density of the DPD fluid.

In the case of low mass, we recast the velocity equation of particle i (9) as

$$\frac{d(v_i)_\alpha}{dt} = (c_i)_\alpha (v_i)_\alpha + (A_i)_\alpha + (B_i)_\alpha \theta_{ij}, \tag{28}$$

where the subscript $\alpha(= 1, 2, 3)$ is used to denote the αth component of the vectors in parentheses,

$$(c_i)_\alpha = -\frac{1}{m_i}\sum_{j \neq i}\gamma w_D \left(\frac{(r_i)_\alpha - (r_j)_\alpha}{r_{ij}}\right)^2, \tag{29}$$

$$(A_i)_\alpha = -\frac{1}{m_i} \sum_{\beta=1,\beta\neq\alpha}^{3} \sum_{j\neq i} \gamma w_D \left(\frac{(r_i)_\beta - (r_j)_\beta}{r_{ij}}\right) \left(\frac{(r_i)_\alpha - (r_j)_\alpha}{r_{ij}}\right) (v_i)_\beta$$

$$+ \frac{1}{m_i} \sum_{j\neq i} \gamma w_D (\mathbf{e}_{ij} \cdot \mathbf{v}_j) \left(\frac{(r_i)_\alpha - (r_j)_\alpha}{r_{ij}}\right) + \frac{1}{m_i} \sum_{j\neq i} F_{ij,C} \left(\frac{(r_i)_\alpha - (r_j)_\alpha}{r_{ij}}\right),$$

and

$$(B_i)_\alpha = \frac{1}{m_i} \sum_{j\neq i} \gamma w_D \left(\frac{(r_i)_\alpha - (r_j)_\alpha}{r_{ij}}\right). \tag{30}$$

Here, the value of $(c_i)_\alpha$ is always large and negative, when m is small, leading to stiff stochastic differential equations. An efficient numerical solution to (28) can be found using the first-order ETD scheme in which $(A_i)_\alpha$ and $(B_i)_\alpha$ are regarded as constants in the interval $(t, t + \Delta t)$

$$(v_i)_\alpha (t + \Delta t) = (v_i)_\alpha (t) e^{(c_i)_\alpha \Delta t} + \frac{\left(e^{(c_i)_\alpha \Delta t} - 1\right) \left[(A_i)_\alpha (t) + (\Delta\xi_{ij}/\sqrt{\Delta t}) (B_i)_\alpha (t)\right]}{(c_i)_\alpha}, \tag{31}$$

where the fluctuating part is handled according to the Ornstein-Uhlenbech process [Uhlenbeck and Ornstein (1930)], with a slight modification of its autocorrelation.

For each time step, the solution procedure can be summarised as follows

- $(r_i)_\alpha \leftarrow (r_i)_\alpha + (v_i)_\alpha \Delta t$;

- Apply the boundary conditions;

- Calculate the conservative force $F_{ij,C}$, the random force $F_{ij,R}$, the dissipative part involving $\mathbf{v}_i$ (i.e., $\gamma w_D (e_{ij})_1 (v_i)_1$, $\gamma w_D (e_{ij})_2 (v_i)_2$ and $\gamma w_D (e_{ij})_3 (v_i)_3$), and the dissipative part involving $\mathbf{v}_j$ (i.e., $\gamma w_D \mathbf{e}_{ij} \cdot \mathbf{v}_j$);

- Calculate the x, y and z components of $\mathbf{c}_i$, $\mathbf{A}_i$ and $\mathbf{B}_i$;

- $(v_i)_\alpha \leftarrow (v_i)_\alpha e^{(c_i)_\alpha \Delta t} + \left(e^{(c_i)_\alpha \Delta t} - 1\right) \left[(A_i)_\alpha (t) + (\Delta\xi_{ij}/\sqrt{\Delta t}) (B_i)_\alpha (t)\right] / (c_i)_\alpha$;

- Evaluate physical properties of the DPD fluid.

Hereafter, we assume identical mass $m_i = m$.

4 Viscometric flow verifications

We simulate Couette and Poiseuille flows on the domain $L_x \times L_y \times L_z = 40 \times 10 \times 30$ for four values of m, namely 1.0, 0.1, 0.01 and 0.001. Other parameters used are $r_c = 1.0$, $n = 4$, $a_{ij} = 18.75$, $\sigma = 3.0$, $s = 1/2$ and $k_B T = 1.0$. Using (22), the viscosity is estimated as $\eta = 2.4059$ for $m = 1$, $\eta = 2.2494$ for $m = 0.1$, $\eta = 2.2337$ for $m = 0.01$ and $\eta = 2.2322$ for $m = 0.001$. We impose $\mathbf{U} = (7.5, 0, 0)^T$ on the two walls $z = -15$ and $z = 15$ (to simulate Couette flow) and apply a body force $\mathbf{F} = (0.1, 0, 0)^T$ to each particle (to simulate Poiseuille flow). For the latter, a parabolic velocity profile is expected to be

$$u_x = \frac{nF_x}{2\eta} \left(\frac{L_z}{2} - z \right) \left(\frac{L_z}{2} + z \right). \tag{32}$$

In our simulation, the wall boundary is constructed using three layers of frozen particles. In addition, we assume that there is a thin layer near the wall, in which a random velocity distribution with zero mean corresponding to a given temperature is generated to maintain the no-slip boundary condition [Fan *et al.* (2003)]. In order to prevent particles from penetrating the walls, we further require that the particles in this layer always leave the wall according to the reflection law reported in [Revenga *et al.* (1998)].

Initially, a FCC arrangement of particles is formed and is allowed to equilibrate before the simulation is started. The central flow region across the z direction is divided into 300 bins (for the averaging purpose), and the averaging is done in each bin over every 10,000 time steps.

Variations of the diffusivity and the Schmidt number versus the particle mass are given in Table 1. The former is numerically estimated using the mean square displacement (MSD) approach

$$D = \frac{1}{6} \lim_{t \to \infty} \frac{d}{dt} \langle |\mathbf{r}_i(t) - \mathbf{r}_i(0)|^2 \rangle, \tag{33}$$

and the velocity autocorrelation function (VACF) through the Green-Kubo integral

$$D = \frac{1}{3} \int_0^\infty \langle \mathbf{v}_i(t) \cdot \mathbf{v}_i(0) \rangle dt. \tag{34}$$

Table 1: DPD fluid, $r_c = 1.0$, $n = 4$, $a_{ij} = 18.75$, $\sigma = 3.0$, $s = 1/2$ and $k_B T = 1.0$: the diffusivity and the Schmidt number for several values of m using the mean square displacement (MSD) and velocity autocorrelation function (VACF) approaches.

m	D	Sc
1.0	0.10 (MSD)	6.0
	0.12 (VACF)	5.0
0.1	0.12 (MSD)	46.9
	0.13 (VACF)	43.3
0.01	0.15 (MSD)	372.3
	0.14 (VACF)	398.9
0.001	0.15 (MSD)	3720.3
	0.14 (VACF)	3986.1

It can be seen from the table that both approaches produce similar numerical results. When m is reduced from 1.0 to 0.001, there are a slight variation in the self-diffusion coefficient and a significant increase in the Schmidt number. It is noted that the present numerical values for D, $D = 0.10 - 0.15$, are somewhat larger than the kinetic estimate (23), $D = 0.09$, and a Schmidt number of $O(10^3)$ is achieved at $m = 0.001$.

Table 2: Couette flow: Comparison of the mean equilibrium temperature of the ETD and velocity-Verlet algorithms for the case of $m = 0.1$. The velocity-Verlet algorithm fails to converge at $\Delta t \gtrapprox 0.009$.

	$\overline{k_B T}$	
Δt	ETD	velocity-Verlet
0.01	1.003	-
0.009	1.002	-
0.007	1.002	0.9538
0.005	1.002	0.9386
0.003	1.002	0.9607
0.001	1.002	0.9869
0.0009	1.002	0.9884

The equilibrium temperature is measured from the calculated velocity field

$$k_B T = \frac{1}{3} m V^2. \tag{35}$$

Table 3: Couette flow: Comparison of the mean equilibrium temperature of the ETD and velocity-Verlet algorithms for the case of $m = 0.01$. The velocity-Verlet algorithm fails to converge at $\Delta t \gtrapprox 0.0009$.

Δt	ETD		velocity-Verlet	
	$\overline{k_B T}$	Error(%)	$\overline{k_B T}$	Error(%)
0.007	0.5680	43.19	-	-
0.005	0.7633	23.66	-	-
0.003	0.9356	6.44	-	-
0.001	0.9835	1.64	-	-
0.0009	0.9863	1.36	-	-
0.0007	0.9916	0.83	0.9187	8.12
0.0005	0.9958	0.41	0.9322	6.77
0.0003	0.9987	0.12	0.9576	4.23
0.0001	0.9992	0.07	0.9840	1.60

where V is the peculiar velocity (*i.e.*, the fluctuation of the velocity of particle with respect to the mean field velocity). Tables 2, 3 and 4 show the behaviour of the temperature against the time step for $m = 0.1$, $m = 0.01$ and $m = 0.001$, respectively. Results by the velocity-Verlet algorithm [Groot and Warren (1997)] are also included. It can be seen that the ETD algorithm works effectively for relatively-large time steps. Furthermore, for a given small time step, the ETD algorithm is much more accurate than the velocity-Verlet algorithm. In the case of $m = 0.1$, the ETD algorithm produces the equilibrium temperature that is accurate up to 3 significant digits. In the case of $m = 0.01$ and $m = 0.001$, equipartition is consistently improved as the time step is reduced. The velocity-Verlet algorithm fails to converge except at small time steps, and the associated errors are much larger than those produced by the ETD algorithm.

Since the random force has only well-defined statistical properties, the velocity equation (9) is understood as a stochastic differential equation. Based on the interaction zone and the peculiar velocity, one can define the following time scale [Español and Warren (1995)]

$$t_c = \frac{r_c}{V} = \frac{\sqrt{m} r_c}{\sqrt{3 k_B T}}. \tag{36}$$

For the present DPD fluid, $t_c = 0.1826$ for $m = 0.1$, $t_c = 0.0577$ for $m = 0.01$, and $t_c = 0.0183$ for $m = 0.001$. The time step used should be much smaller than t_c. Otherwise, the motion of

Table 4: Couette flow: Comparison of the mean equilibrium temperature of the ETD and velocity-Verlet algorithms for the case of $m = 0.001$. The velocity-Verlet algorithm fails to converge at $\Delta t \gtrsim 0.00007$.

	ETD		velocity-Verlet	
Δt	$\overline{k_B T}$	Error(%)	$\overline{k_B T}$	Error(%)
0.0002	0.9501	4.98	-	-
0.0001	0.9805	1.94	-	-
0.00009	0.9837	1.62	-	-
0.00008	0.9865	1.34	-	-
0.00007	0.9891	1.08	-	-
0.00006	0.9916	0.83	0.9127	8.72
0.00005	0.9934	0.65	0.9235	7.64
0.00004	0.9951	0.48	0.9365	6.34
0.00003	0.9958	0.41	0.9502	4.97

DPD particles, where their displacements can approach the range of the interaction in one time step, may no longer follow that predicted by the velocity equation [Español and Warren (1995)]. From Tables 2, 3 and 4, relatively large time steps can be employed here, 0.01 for $m = 0.1$, 0.007 for $m = 0.01$ and 0.0002 for $m = 0.001$. They are a decreasing function of the particle mass as expected.

Results concerning velocity, temperature and number density are presented in Figure 1 for the case of Couette flow and in Figure 2 for the case of Poiseuille flow. We obtain a linear/parabolic velocity profile in the x direction, and uniform temperature and density using a time step $\Delta t = 0.02$ for $m = 1.0$, $\Delta t = 0.005$ for $m = 0.1$, $\Delta t = 0.001$ for $m = 0.01$ and $\Delta t = 0.0002$ for $m = 0.001$. In the case of Poiseuille flow, by fitting the obtained parabolic velocity profiles to equation (32), the viscosity is numerically estimated as $\eta = 2.6354$ for $m = 1$ ($\Delta t = 0.01$), $\eta = 1.9914$ for $m = 0.1$ ($\Delta t = 0.0009$), $\eta = 1.9649$ for $m = 0.01$ ($\Delta t = 0.0001$), and $\Delta t = 1.9230$ for $m = 0.001$ ($\Delta t = 0.00003$). The percentage differences (relative to kinetic theory estimate (22)) of the calculated viscosity are 9.53% for $m = 1$ and 13.85% for $m = 0.001$.

5   Modelling rigid spheres in a Newtonian fluid

Consider a steady uniform flow of a Newtonian fluid past a stationary sphere. We choose the dimensions of the domain as $L_x = 40$, $L_y = 30$ and $L_z = 30$ and place the sphere at the centre of the domain. Periodic boundary conditions are applied in the x and y directions, while the velocity vectors $\mathbf{U} = (3.0, 0, 0)^T$ are imposed on the two planes $z = -15$ and $z = 15$. We choose the particle mass as 0.01 and conduct the simulations using $\Delta t = 0.001$, unless otherwise stated.

We employ DPD particles to represent the fluid (solvent) phase with the following parameters: $n = 4$, $a_{ij}^{SS} = 18.75$, $r_{c,C}^{SS} = r_{c,D}^{SS} = 1.0$, $w_C^{SS} = (1 - r_{ij}/r_{c,C}^{SS})$, $w_D^{SS} = (1 - r_{ij}/r_{c,C}^{SS})^{1/2}$, $\sigma^{SS} = 2.0$ and $k_B T = 0.25$. It is noted that (i) the superscript SS is used to denote the solvent-solvent interaction; and (ii) $r_{c,C}$ and $r_{c,D}$ represent the cut-off radius used for the conservative and dissipative forces, respectively. Such parameters constitute a Newtonian fluid of $\eta = 3.9682$, using the estimated viscosity (equation (22)), and $Sc = 6012.4$, using the VACF approach (equation (34)). Although a DPD particle is a point mass, it is endowed with a soft repulsive potential, and therefore has an "effective" size, which is the exclusion zone of the particle. To estimate the effective radius of a DPD particle, we utilise the radial distribution function [Reichl (1980)]

$$g(q) = \frac{1}{N/V} \frac{\langle s \rangle}{4\pi q^2 \Delta q}, \tag{37}$$

where V is the volume of the domain of interest and $\langle s \rangle$ is the average number of particles in a spherical shell of width $q \to (q + \Delta q)$ at a distance q from any particle in the fluid. As opposed to the Stokes-Einstein relation, equation (37) does not involve the estimated viscosity and diffusivity. The present procedure is a direct determination and thus has the ability to give a better estimation. Figure 3 shows the variation of $g(q)$, where Δq is chosen as 0.05, for the present DPD fluid. Let $\bar{q}$ be the value of q at which $g(q)$ becomes non-zero, say at $g(q) > 0.05$. The effective radius of the solvent particles can be estimated as $a_{eff}^S = \bar{q}/2 = 0.32/2 = 0.16$ (taking half because $\bar{q}$ is the distance between the two particles centres). Making use of this function g, one can compute the sound speed and the Mach number for the present fluid in a more precise way. The equation of state (25) reduces to $p = nk_B T + 0.0968an^2 r_c^4$ from which, through (27), one acquires $c_s = 38.43$. It leads to a Mach number of $M = U/c_s = 3.0/38.43 = 0.078$.

We model a rigid suspended sphere using a single DPD particle. It can be seen that parameters associated with this rigid (colloidal) particle should not be the same as those with the solvent particles. We use the superscript CS to denote the colloidal-solvent interaction. Parameters are chosen as $r_{c,C}^{CS} = 1.0$, $r_{c,D}^{CS} = 1.5$, $w_C^{CS} = (1 - r_{ij}/r_{c,C}^{CS})^{1/2}$, $w_D^{CS} = (1 - r_{ij}/r_{c,D}^{CS})^{1/4}$, $a_{ij}^{CS} = 1750$, and $\sigma^{CS} = 3.2$.

We also utilise the radial distribution function to determine the radius of the colloidal particle. The quantity $ng4\pi q^2 \Delta q$ is the number of particles in a spherical sell of width Δq at a distance q from the centre of the colloidal particle. Let $\bar{q}$ be the value of q at which $g(q)$ becomes non-zero, at $g(q) > 0.05$. The effective radius of the colloidal particle can be estimated as (Figure 4)

$$\bar{q} - a_{eff}^S \leq a_{eff}^C \leq \bar{q} + \Delta q - a_{eff}^S. \tag{38}$$

Figure 5 shows the variation of $g(q)$ against q. The value of $\bar{q}$ is measured to be 0.95. With $a_{eff}^S = 0.16$, we arrive at $0.79 \leq a_{eff}^C \leq 0.84$. It leads to $0.0478 \leq Re = 2a_{eff}^C U\rho/\eta \leq 0.0508$. Using Stokes results [Happel and Brenner (1973)], the corresponding drag force is in the range

$$177.27 \leq F = 6\pi\eta a_{eff}^C U \leq 188.49. \tag{39}$$

We plot the drag and its conservative, dissipative and random parts against the time in Figure 6. As expected, the total force is larger in the x direction than in the y and z directions. Furthermore, after a certain time, the mean values of the total, dissipative and conservative forces in the x direction appear to be stable, showing that the flow reaches a steady state condition. The obtained total force, which is measured in an average sense for the chosen period of $60 \leq t \leq 150$, is 178.36, in the range of 177.27 to 188.49 as given by (39).

Figures 7, 8 and 9 display distributions of the temperature, x-component velocity and velocity vector on the middle plane $y = 0$, respectively. It can be seen that the method obeys equipartition (Figure 7) and produces a smooth flow field around the sphere (Figure 9). Velocity in the x direction appears to be constant on the two boundary lines $x = -19.83$ and $x = 19.83$ (Figures

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8 and 9). Making use of Stokes solution for a sphere moving with a velocity $\mathbf{U} = (U, 0, 0)^T$ in a stationary fluid [Batchelor (1967)] and then superimposing on this for a stationary sphere, one can obtain the x-component velocity of the fluid at the distance $x = \mp L a_s$ (a_s is the radius of the sphere) as

$$\frac{u_x}{U} = 1 - \frac{3}{4L} + \frac{1}{4L^3} \tag{40}$$

Substitution of $U = 3$ and $L = 19.83/0.8 = 24.79$ into (40) yields $u_x = 2.9093$. From our DPD calculations, the average values of the x-component velocity at the upstream and downstream (*i.e.*, $x = \mp 19.83$ and $y = 0$) are 2.8651 and 2.8323, and their percentage errors (relative to Stokes solution (40)) are thus 1.51% and 2.64%, respectively.

Figure 10 is a plot of the drag coefficient, defined as $C_d = \overline{F}/(0.5\pi(a_{eff}^C)^2\rho U^2)$, versus the Reynolds number. Re is changed by means of the particle mass. We use $m = 0.005 \to 0.1$, which leads to $0.02 \leq Re \leq 0.48$ and $0.05 \leq M \leq 0.24$. The corresponding flows can thus be considered as low Reynolds number quasi-incompressible flows. It can be seen from the figure that the obtained drag coefficient is very close to that predicted by Stokes' law. It is noted that if $m = 1$ is used, one has $Re = 4.80$ and $M = 0.78$ and hence, the effects of compressibility on the flow field may be noticeable. As shown in Figure 11, values of u_x are readily smaller than U in the regions close to the centreline at the upstream and downstream planes, indicating that compressibility effects may be already significant.

Table 5: Flow around a sphere, $r_{c,C}^{CS} = 1$, $r_{c,D}^{CS} = 1.5$, $a_{ij}^{CS} = 1750$: Effects of σ^{CS} on the forces and the size of the sphere. It is noted that the obtained forces acting on the sphere are shown in the mean for the period of $60 \leq t \leq 150$.

σ^{CS}	$\overline{F}$	$\overline{F}_C$	$\overline{F}_D$	$\overline{F}_R$	$\overline{q}$
2.8	166.44	54.99	110.46	0.98	0.95
3.2	178.36	47.53	130.73	0.10	0.95
3.6	187.97	39.96	148.03	-0.01	0.95
4.0	197.47	33.40	163.14	0.92	0.95
4.4	203.65	26.68	178.79	-1.82	0.95

Some implementation notes:

Table 6: Flow around a sphere, $r_{c,C}^{CS} = 1$, $r_{c,D}^{CS} = 1.5$, $\sigma^{CS} = 3.2$: Effects of a_{ij}^{CS} on the forces and the size of the sphere. It is noted that the obtained forces acting on the sphere are shown in the mean for the period of $60 \leq t \leq 150$.

a_{ij}^{CS}	$\overline{F}$	$\overline{F}_C$	$\overline{F}_D$	$\overline{F}_R$	$\overline{q}$
1000	177.74	46.34	129.81	1.57	0.95
1250	177.15	45.66	130.82	0.67	0.95
1500	177.88	48.52	129.95	-0.59	0.95
1750	178.36	47.53	130.73	0.10	0.95
2000	176.70	46.94	129.23	0.52	0.95
2250	177.23	46.30	129.69	1.24	0.95

Table 7: Flow around a sphere, $r_{c,C}^{CS} = 1.0$, $r_{c,D}^{CS} = 1.0$, $a_{ij}^{CS} = 1750$: Effects of σ^{CS} on the forces and the size of the sphere. It is noted that the obtained forces acting on the sphere are shown in the mean for the period of $60 \leq t \leq 150$.

σ^{CS}	$\overline{F}$	$\overline{F}_C$	$\overline{F}_D$	$\overline{F}_R$	$\overline{q}$
3.0	113.34	100.27	13.20	-0.14	0.95
4.0	124.37	100.63	23.59	0.14	0.95
5.0	133.84	97.80	35.99	0.04	0.95
6.0	147.75	96.54	51.00	0.20	0.95
7.0	164.22	95.28	68.69	0.25	1.00
8.0	183.35	94.70	88.52	0.11	0.95

- Effects of σ^{CS} on the drag force and the size of the sphere are presented in Table 5. Increasing σ^{CS} leads to a decrease in the conservative component and an increase in the dissipative component. Furthermore, the radius of the sphere remains unchanged. For all values of σ^{CS} employed, the dissipative force is dominant. The parameter σ^{CS} has a strong influence on the drag force, which can be helped to tune in the correct value of the drag force on the sphere.

- Effects of a_{ij}^{CS} on the drag force and the size of the sphere are presented in Table 6. The parameter a_{ij}^{CS} does not greatly affect the forces exerted on the sphere. As a_{ij}^{CS} increases, the radius of the sphere remains unchanged. It appears that the size of the sphere is mainly decided by $r_{c,C}^{CS}$ and a_{eff}^{S}, which is different from that reported in [Pan *et al.* (2010)] (they reported that the size of a colloidal particle can be controlled by adjusting the value of a_{ij}^{CS},

which we do not find here).

- In the case of $r_{c,C}^{CS} = r_{c,D}^{CS}$, one needs to employ relatively-large values of σ^{CS} (about 8.0) to fit the drag force and the radius of the sphere in the model predicted by Stokes' law ($177.27 \leq F = 6\pi\eta a_{eff}^{C} U \leq 188.49$) (Table 7). For all values of σ^{CS} employed, the conservative force is larger than the dissipative force.

6   Concluding remarks

We have reduced the mass of DPD particles to induce an incompressible slow viscous flow in a DPD fluid and to enhance its dynamic response. This approach appears effective as the simplicity of the DPD algorithm still retains and an efficient solution is still achieved with the help of an ETD algorithm. Numerical simulations for the Couette flow have showed that the present method works effectively for relatively-large time steps and, for a given a small time step for which the velocity-Verlet algorithm works, the ETD algorithm produces more accurate results than the velocity-Verlet algorithm. We have also investigated the use of a single DPD particle to represent a rigid sphere suspended in a Newtonian fluid. Detailed results show that (i) the cut-off radius for the conservative force and the effective radius of solvent particles are the key factors in deciding the size of the suspended sphere, and (ii) the strength and the cut-off radius of the dissipative force are instrumental in fitting the computed drag force and the size of the sphere into the Stokes drag model. Extension of the method to colloidal suspensions is underway and results will be reported in future work.

Acknowledgement

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