Computer Physics Communications 221 (2017) 290–298

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Imposition of physical parameters in dissipative particle dynamics

N. Mai-Duy [a,*], N. Phan-Thien [b], T. Tran-Cong [a]

[a] Computational Engineering and Science Research Centre, School of Mechanical and Electrical Engineering, University of Southern Queensland, Toowoomba, QLD 4350, Australia

[b] Department of Mechanical Engineering, Faculty of Engineering, National University of Singapore, 9 Engineering Drive 1, 117575, Singapore

ARTICLE INFO

Article history:
Received 3 February 2017
Received in revised form 5 August 2017
Accepted 1 September 2017
Available online 9 September 2017

Keywords:
Dissipative particle dynamics
Physical/dimensionless parameters
Weighting functions
Inertia and relaxation time scales
Compressibility
Viscosity
Dynamic response

ABSTRACT

In the mesoscale simulations by the dissipative particle dynamics (DPD), the motion of a fluid is modelled by a set of particles interacting in a pairwise manner, and it has been shown to be governed by the Navier–Stokes equation, with its physical properties, such as viscosity, Schmidt number, isothermal compressibility, relaxation and inertia time scales, in fact its whole rheology resulted from the choice of the DPD model parameters. In this work, we will explore the response of a DPD fluid with respect to its parameter space, where the model input parameters can be chosen in advance so that (i) the ratio between the relaxation and inertia time scales is fixed; (ii) the isothermal compressibility of water at room temperature is enforced; and (iii) the viscosity and Schmidt number can be specified as inputs. These impositions are possible with some extra degrees of freedom in the weighting functions for the conservative and dissipative forces. Numerical experiments show an improvement in the solution quality over conventional DPD parameters/weighting functions, particularly for the number density distribution and computed stresses.

1. Introduction

Dissipative particle dynamics (DPD) has become a popular numerical tool for probing the behaviour of complex fluids at a mesoscopic length scale (e.g. polymeric/colloidal fluids), (see, e.g., [1–7]). In DPD, the fluid is replaced by a set of particles (called DPD particles) undergoing Newton's 2nd law of motion while interacting in a pairwise manner. There are three typical types of interaction forces between DPD particles, a conservative force used to model local thermodynamics, a dissipative force used to model viscous actions, and a random force to provide a balance to the dissipative force, to maintain a constant specific kinetic energy (defined as the Boltzmann temperature). All forces are pairwise and centre-to-centre. DPD has a sound statistical foundation: it is shown to satisfy conservations of mass and momentum in the mean [8,9]. The input parameters of DPD include a noise level σ, Boltzmann temperature k_BT, repulsion strength a_{ij}, number density n, particle's mass m and cut-off radius r_c (which may be different for conservative and dissipative forces). It is noted that a friction coefficient γ is derived from the noise level through the fluctuation–dissipation theorem; it is not an independent input. For the scaling in DPD, a physical system represented by N_{phys} "molecular particles" can be scaled (coarse-grained) at different levels ν so that one deals with a smaller number of particles $N = N_{phys}/\nu$ in which ν is referred to as the coarse-grained level [10]. Let ν (modelled by $\{N, k_BT, n, m, r_c, a_{ij}, \gamma\}$) and ν' ($\{N', k_BT', n', m', r_c', a_{ij}', \gamma'\}$) be two different coarse-grained levels; both represent the same physical fluid. By constraining the compressibility of the coarse-grained level fluids, it was shown that if two different coarse-grained levels are related by (ϕ is the scaling)

$$N' = \phi^{-1}N, \quad k_BT' = \phi k_BT, \quad n' = \phi^{-1}n, \tag{1}$$

then

$$\begin{aligned} m' &= \phi m, & r_c' &= \phi^{1/3} r_c, & \tau' &= \phi^{1/3}\tau, \\ a_{ij}' &= \phi^{2/3} a_{ij}, & \gamma' &= \phi^{2/3}\gamma, & \sigma' &= \phi^{5/6}\sigma, \end{aligned} \tag{2}$$

in which $\tau = r_c\sqrt{m/k_BT}$ and $\tau' = r_c'\sqrt{m'/k_BT'}$ are time scalings. Under these scalings, one can show that the two coarse-grained systems are equivalent (i.e. the scale free property). There are several issues in the classical DPD method. The physical parameters of the fluid to be modelled are not inputs of the DPD system, making its parametric study difficult. Any change in the input model parameters (e.g. the cut-off radius and Boltzmann temperature) may result in a different fluid. Although the scheme defined by (1) and (2) allows of the use of ν larger than 1, it does not provide an appropriate link between the scaling and thermal fluctuations to ensure that the fluctuations will reduce their magnitude when the coarse-grained level increases. Also, the method always produces a local pressure as a quadratic function of the number density

* Corresponding author.
E-mail address: nam.mai-duy@usq.edu.au (N. Mai-Duy).

http://dx.doi.org/10.1016/j.cpc.2017.09.003
0010-4655/

(i.e. a fixed equation of state), and does not inherit the feature of "mesh/grid convergence" from conventional discretisation methods. There is still no formal way of deriving DPD from an atomistic system for simple fluids (unbonded atoms). On the other hand, DPD possesses an algorithmic simplicity and has the ability to model many different complex fluids. Indeed, objects suspended in the fluid can also be represented by DPD particles with appropriate forms of interactions. For example, a solid particle can be modelled by a single DPD particle [5] or by a few constrained basic DPD particles [7], allowing efficient simulations of particulate suspensions [5,7,11], and of thixotropic materials exhibiting pseudo yield stress behaviour [12] to be carried out. When the atoms are bonded (e.g. complex molecules like proteins), the coarse-grained mapping can be well defined and there have been many attempts in DPD modelling to explore flows of such fluids [13,14]; here the DPD method can be regarded as a bottom-up approach. In contrast to DPD, the smoothed DPD (sDPD) method [15] is directly derived from the Navier–Stokes equation with the inclusion of thermal fluctuations (i.e. a top-down approach). Its formulation thus combines the advantages of the Navier–Stokes equation (i.e. an arbitrary equation of state, specified viscosity and convergence property) and the DPD (i.e. mesoscopic description). Each sDPD particle is defined with an explicit volume. For the scaling in sDPD, it was shown in [16] that the deterministic part is scale invariant and the thermal fluctuation part has a consistent scaling with the volume of fluid particles. The reader is referred to [17] for a recent comprehensive review of the field.

In DPDs, the compressibility of the model fluid is set to match the compressibility of water at room temperature, resulting in a constraint to the repulsion strength [18]

$$a_{ij} = \frac{71.54 k_B T}{n r_c^4} \quad \text{for 3D case,} \tag{3}$$

$$a_{ij} = \frac{57.23 k_B T}{n r_c^3} \quad \text{for 2D case,} \tag{4}$$

revealing the dependence of a_{ij} on k_BT, n and r_c. In [15], it was shown that the friction coefficient can be chosen to fix the viscosity of the system. In [18–22], the dynamic response of a DPD fluid, measured by the Schmidt number (the ratio between momentum diffusion (viscosity) and mass diffusivity) was discussed. In this study, apart from the physical parameters just mentioned, another dimensionless parameter, i.e. the ratio between the inertia and relaxation time scales of the DPD equations, will also be considered. This parameter provides a direct link between the conservative and dissipative forces; it governs how fast the system approaches the statistical equilibrium state, together with the clustering of particles, and therefore an appropriate value of this ratio helps stabilise the density distribution of DPD particles in the flow domain.

We will examine the response of a DPD fluid to a flow condition in the following two forms. In the first, there are two dimensionless quantities (time-scale ratio and isothermal compressibility) to be imposed. The method here is basically the same as conventional DPDs, except that its conservative force involves two free parameters (instead of one). In the second, three dimensionless quantities (time-scale ratio, isothermal compressibility and Schmidt number), and the viscosity are to be enforced. These simultaneous impositions are possible by modifying both the weighting functions of the conservative and dissipative forces. Some simulations are carried out in viscometric flows to illustrate the advantages of the proposed DPD fluid.

The structure of the paper is organised as follows. In Section 2, brief overviews of the DPD equations and their associated standard input values are given. In Section 3, numerical issues concerning the time scales in the DPD equations are discussed. In Section 4, the response of the DPD system under constraints of satisfying some given physical/dimensionless parameters of the fluid concerned is examined. Section 5 gives some concluding remarks.

2. DPD model

2.1. Equations

In DPD, the fluid is modelled by a system of particles undergoing Newton's 2nd law of motion:

$$m_i \ddot{\mathbf{r}}_i = m_i \dot{\mathbf{v}}_i = \sum_{j=1, j\neq i}^{N} \left(\mathbf{F}_{ij,C} + \mathbf{F}_{ij,D} + \mathbf{F}_{ij,R} \right), \tag{5}$$

where m_i, $\mathbf{r}_i$ and $\mathbf{v}_i$ represent the mass, position vector and velocity vector of a particle $i = 1, \ldots, N$, respectively, N is the total number of particles, the superposed dot denotes a time derivative, and the three forces on the right side of (5) represent the conservative force (subscript C), the dissipative force (subscript D) and the random force (subscript R):

$$\mathbf{F}_{ij,C} = a_{ij} w_C \mathbf{e}_{ij}, \tag{6}$$

$$\mathbf{F}_{ij,D} = -\gamma w_D \left(\mathbf{e}_{ij} \cdot \mathbf{v}_{ij} \right) \mathbf{e}_{ij}, \tag{7}$$

$$\mathbf{F}_{ij,R} = \sigma w_R \theta_{ij} \mathbf{e}_{ij}, \quad w_R = \sqrt{w_D}, \quad \sigma = \sqrt{2\gamma k_B T}, \tag{8}$$

where a_{ij}, γ and σ are constants reflecting the strengths of these forces, w_C, w_D and w_R configuration-dependent weighting functions, $\mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij}$ a unit vector from particle j to particle i ($\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $r_{ij} = |\mathbf{r}_{ij}|$), $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ a relative velocity vector, and θ_{ij} a Gaussian white noise. It is noted that the random force is introduced in a way that satisfies the fluctuation–dissipation theorem.

2.2. Standard input values

Groot and Warren [18] suggested that the noise level σ can be chosen as a balance between a fast simulation and a good satisfaction of the specified Boltzmann temperature — a value of 3 was recommended (for $k_BT = 1$, the corresponding γ is 4.5). They also recommended that the repulsion strength a_{ij} is chosen such that a DPD fluid has the same compressibility as water at room temperature. This results in the constraints (3) and (4). As discussed in Section 1, a relatively small number of particles can be chosen to represent the fluid. In practice, the number density $n = 4$ has been widely used.

For conventional DPDs, the weighting functions are given by

$$w_C = 1 - \frac{r_{ij}}{r_c}, \tag{9}$$

$$w_D = \left(1 - \frac{r_{ij}}{r_c} \right)^2. \tag{10}$$

It is noted that the exponent in w_D is also often taken as 1/2 (rather than 2), with a resulting improvement in the response of the fluid. In this study, the value of 1/2 is employed for the conventional DPD.

3. Time scales

Let us focus on a tagged, but otherwise arbitrary DPD particle in the system, and let τ be its relaxation time scale, τ_I its inertia time scale and α the ratio of the two time scales.

$$\tau = O\left(\frac{\gamma}{H} \right) = O\left(\frac{\gamma r_c}{a_{ij}} \right), \tag{11}$$

$$\tau_I = O\left(\frac{m}{\gamma} \right), \tag{12}$$

$$\alpha = \frac{\tau}{\tau_I} = O\left(\frac{\gamma^2 r_c}{m a_{ij}} \right), \tag{13}$$