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DISSIPATIVE PARTICLE DYNAMICS: INTRODUCTION, METHODOLOGY AND COMPLEX FLUID APPLICATIONS — A REVIEW

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The dissipative particle dynamics (DPD) technique is a relatively new mesoscale technique which was initially developed to simulate hydrodynamic behavior in mesoscopic complex fluids. It is essentially a particle technique in which molecules are clustered into the said particles, and this coarse graining is a very important aspect of the DPD as it allows significant computational speed-up. This increased computational efficiency, coupled with the recent advent of high performance computing, has subsequently enabled researchers to numerically study a host of complex fluid applications at a refined level. In this review, we trace the developments of various important aspects of the DPD methodology since it was first proposed in the in the early 1990's. In addition, we review notable published works which employed DPD simulation for complex fluid applications.

Keywords: DPD review; mesoscopic simulation; coarse-graining; boundary models; complex fluid; multiphase flows.

1. Introduction

To bridge the gap between atomistic simulations and macroscopic network simulations, and to overcome the inherent difficulties faced by conventional methods when applied to complex fluid systems, we need an intermediary technique focused at a length scale larger than the atomistic scale, but smaller than the macroscopic connection scale, Groot and Warren [1997], please see Fig. 1. Mesoscopic simulations aim at identifying characteristic physical lengths and times in the system in order to use them for simplification of complex models. In particular, for soft matter and polymeric systems, the hydrodynamic behaviors are captured easily using continuum methods while it is expensive to handle them at atomistic levels.
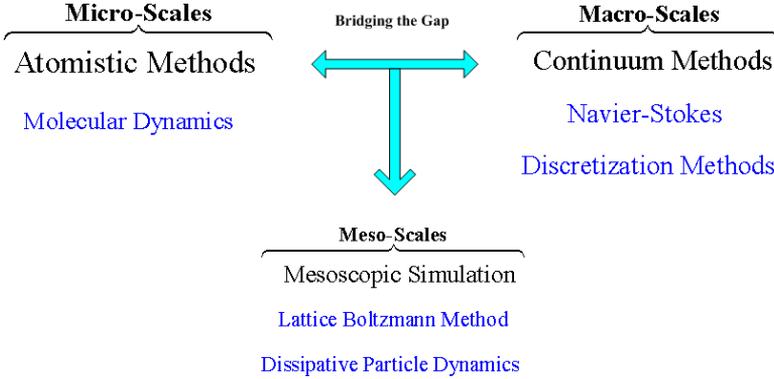

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Micro-Scales   Bridging the Gap   **Macro-Scales**

Atomistic Methods   ⟷ ⟶   Continuum Methods

Molecular Dynamics   Navier-Stokes

                                    Discretization Methods

Meso-Scales

Mesoscopic Simulation

Lattice Boltzmann Method

Dissipative Particle Dynamics

Fig. 1.   Dissipative Particle Dynamics: a mesoscale technique for bridging the gap between the micro- and macro-scales.

Conversely, the interaction between components at the atomistic scale can be taken into account by employing molecular methods, but is not usually straightforward to consider them through continuum methods. Thus, the developments of inter-mediate techniques, which have both features of micro- and macro-scales methods, are essential. Depending on the nature of the problem, several mesoscopic simulation methods have been devised, developed and refined over the years. In the area of mesoscopic complex fluid simulation, several particle-based (off-lattice) methods such as smoothed particle hydrodynamics (SPH), DPD, fluid particle method (FPM), as well as other grid-based techniques such as lattice gas automata (LGA) and lattice Boltzmann (LB) are the more notable techniques found in the literature. For more details on some of these techniques and their applications, please refer to the reviews Monaghan [1992], Koumoutsakos [2005] and Chen and Doolen [1998].

The dissipative particle dynamics (DPD) is a potentially very powerful and simple mesoscopic approach, which facilitates the simulation of the statics and dynamics of complex fluids and soft matter systems at physically interesting length and time scales. Since 1990, when the method was first developed in Europe, DPD has been applied in the study of the dynamical properties of a wide variety of systems and applications, as we shall describe them subsequently in this review. DPD, as an off-lattice technique, does not suffer from some of the restrictions imposed by the lattice as in the LGA or LB methods. We believe that presently, the DPD is arguably one of the best mesoscale simulation techniques, and in the near future, it has the potential to emerge as an even more widely used modeling and simulation technique for many complex fluid systems.

The aim of this review is to document the most representative DPD works over the years. This review is organized in the following manner. In the next section, we provide an introduction of the DPD algorithm and summary of the theoretical background, the time integration techniques, and the boundary models which have been used widely in DPD implementations, all in a succinct manner. In Sec. 3, we

extend this review to cover works on other complex fluidic applications in which DPD was employed as the simulation technique. Finally, we provide some concluding remarks, and offer some possible future directions for the implementation of DPD methodology.

2. Dissipative Particle Dynamics: A Coarse-Grained Technique

The dissipative particle dynamics (DPD) technique is an alternative method for mesoscopic complex fluid simulation, which was first devised and developed for simulating hydrodynamic behaviour by Hoogerbrugge and Koelman [1992] and Koelman and Hoogerbrugge [1993]. It was subsequently modified by Español and Warren [1995]. This method can be perceived as the clustering a number of molecules into single particle where the number of molecules per DPD particle is known as the coarse-graining parameter and is usually denoted by N_m, [Español *et al.*, 1997; Flekkøy and Coveney, 1999; Flekkøy *et al.*, 2000; Kinjo and Hyodo, 2007a]. This coarse graining parameter plays a vital role and has significant impact on the speed of simulation, Backer *et al.* [2005a]. For the DPD method, deriving the coarse graining procedure can include finite discretization of the Navier-Stokes equations in a Lagrangian moving Voronoi grid (tessellation) which is relatively easy to implement in two spatial dimensions, [De Fabritiis and Coveney, 2003; De Fabritiis *et al.*, 2002; Serrano *et al.*, 2002; Serrano and Español, 2001]. Español [1996] began from a microscopic description of a harmonic chain and worked out the equations of motion for a coarse-grained chain constructed from groups of clustered atoms. Later, it was noted by Cubero and Yaliraki [2005a, b] that Markovian approximation was not applicable when sound propagation plays an important role in the coarse graining procedure. As indicated in Kinjo and Hyodo [2007b], coarse-graining techniques facilitate simulations of complex systems in larger time spans and with reduced computational work by eliminating some extra degrees of freedom which are deemed unessential in the phenomena of interest. Thus one of the most important issues is to find the upper limit for the coarse-graining parameter by which we could model the physical properties in an efficient manner, and this issue was investigated in significant detail by Pivkin and Karniadakis [2006a]. In Groot and Rabone [2001], they rationalized that the total DPD simulation speed-up with respect to MD can be estimated by $1000 \, N_m^{8/3}$ for a given system volume. Thus, for example if $N_m = 3$ and 7, then the speed-up factors are roughly 2×10^4 and 2×10^5, respectively. Apart from the idea of lumping several atoms together and replacing them by a single bead, the quality and softness of effective interactions between these newly devised clusters also play important function. More specifically, the inclusion of these extremely soft coarse-grained potentials instead of the hard-core Lennard-Jones (LJ) models improves the computational efficiency of the DPD model, Pool and Bolhuis [2006].

The DPD algorithm is essentially a combination of MD, BD and lattice gas automata (LGA), and derives its static and dynamic properties according to the theory in statistical mechanics, Marsh *et al.* [1997b]. Similar to molecular dynamics, the

time evolution of each DPD particle, which represents a cluster of molecules/atoms, can be calculated by Newton's second law

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \quad \frac{d\mathbf{p}_i}{dt} = \sum_{j \neq i} \mathbf{F}_{ij}, \tag{1}$$

where $\mathbf{r}_i$, $\mathbf{v}_i$ and $\mathbf{p}_i$ are respectively the position, velocity and momentum vectors of particle i, and $\mathbf{F}_{ij}$ is the total interparticle force exerted on particle i by particle j. The original interparticle force is defined by three components that lie along their lines of centres and conserves linear and angular momentum, Español [1997b]. Specifically, $\mathbf{F}_{ij} = \mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R$, where a purely repulsive conservative force $\mathbf{F}_{ij}^C$, a dissipative or frictional force $\mathbf{F}_{ij}^D$ which represents the effects of viscosity and slows down the particles motion with respect to each other, and a random (stochastic) force $\mathbf{F}_{ij}^R$ which represents the thermal or vibrational energy of system, are summed to obtain the total force, and these force components can be individually written as

$$\mathbf{F}_{ij}^C = w^C(r_{ij})\mathbf{e}_{ij}, \tag{2}$$

$$\mathbf{F}_{ij}^D = -\gamma w^D(r_{ij})[\mathbf{v}_{ij} \cdot \mathbf{e}_{ij}]\mathbf{e}_{ij}, \tag{3}$$

$$\mathbf{F}_{ij}^R = \sigma w^R(r_{ij})\theta_{ij}\mathbf{e}_{ij}, \tag{4}$$

where $\mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij}$, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ and $\mathbf{v}_{ij} = (\mathbf{v}_i - \mathbf{v}_j)$. w^C, w^D and w^R are the conservative dissipative and random r dependent weight functions. The θ_{ij} term is a Gaussian white noise function with symmetry property $\theta_{ij} = \theta_{ji}$ to ensure the total conservation of momentum and has the following stochastic properties

$$\langle \theta_{ij}(t) \rangle = 0, \langle \theta_{ij}(t)\theta_{kl}(t') \rangle = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \delta(t - t') \tag{5}$$

All of the above forces are acting within a sphere of interaction or cut-off radius $\mathbf{r}_c$, which is the length scale parameter of the system. The symbols γ and σ are the coefficients of the dissipative and random forces, respectively. The extension of DPD forces to include coloured noise instead of Gaussian white noise was reported in Cotter and Reich [2003]. Similar to the fluctuation-dissipation theorem of Kubo [1966] but adapted for DPD, Español and Warren [1995] obtained the detailed balance condition which is sufficient condition guaranteeing that the system has a Gibbsian equilibrium

$$w^D(r) = [w^R(r)]^2, \sigma^2 = 2\gamma k_B T/m, \tag{6}$$

where k_B is the Boltzmann constant and T the equilibrium temperature. This condition makes the DPD equations act like as a thermostat and because the algorithm depends on relative velocities and the interactions between particles are symmetric, it is an isotropic Galilean invariant thermostat which preserves the hydrodynamics, [Allen and Schmid, 2007; Groot, 2006; Stoyanov and Groot, 2005]. Later the ergodicity of the DPD dynamics in one dimension was proved by Shardlow and Yan [2006]. Recently an extended version of the DPD interactions (transverse DPD

thermostat) which includes the damping of the perpendicular components of the relative velocity was reported by Junghans *et al.* [2007]. The conservative force weight function can be defined as a simple decaying function of distance as

$$w^C(r_{ij}) = \begin{cases} a_{ij}\left(1 - \dfrac{r_{ij}}{r_c}\right) & r_{ij} \leq r_c \\ 0 & r_{ij} > r_c \end{cases} \tag{7}$$

where a_{ij} is the repulsion parameter between particle i and particle j. Defining the conservative weight function and especially the repulsion parameter is one the most important aspects of DPD simulations. The definition of soft repulsive potential facilitates accessibility of much larger length and time scales, [Klapp *et al.*, 2004; Vattulainen *et al.*, 2002]. For the same types of solvent particles, Groot and Warren [1997], Groot and Rabone [2001] and Keaveny *et al.* [2005] matched the compressibility condition and determined the repulsion parameters as a function of DPD number density ρ and system temperature. The central and most cited work in the DPD area is that of Groot and Warren [1997] who specified the repulsion parameter between different types of particles. In order to consider interaction between components in the solution, they related the DPD parameters to the χ-parameters in Flory-Huggins theory for polymers, and subsequently obtained the relation between the χ-parameters and the repulsion parameters for unequal particles, [Groot and Warren, 1997; Groot and Rabone, 2001; Keaveny *et al.*, 2005]. In order to address the relation of bead-bead interaction parameters to bead-size, solubility parameter, and surface tension authors of Maiti and McGrother [2004] re-visited the work of Groot and Warren [1997]. Later, Wijmans *et al.* [2001] extended the methodology of Groot and Warren [1997] for Gibbs ensemble Monte Carlo simulations. To predict the lower critical solution temperature (LCST) and to model pressure-induced phase separation of polymer-solvent mixtures, Van Vliet *et al.* [2000, 2003] extended the Flory-Huggins theory and introduced a pressure and temperature dependent repulsion parameter for DPD simulations. Following this, the polymer branching effects and its influences on the LCST curve was investigated in Van Vliet *et al.* [2002]. The dissipative and random weight functions take the general form

$$w^D(r_{ij}) = [w^R(r_{ij})]^2 = \begin{cases} \left(1 - \dfrac{r_{ij}}{r_c}\right)^s & r_{ij} \leq r_c \\ 0 & r_{ij} > r_c, \end{cases} \tag{8}$$

where the exponent $s = 1$ in the original DPD algorithm and other values for s can be chosen to adjust the fluid viscosity, Fan *et al.* [2006], Symeonidis *et al.* [2006]. The random force transforms to $\mathbf{F}_{ij}^R = \sigma w^R(r_{ij})\varsigma_{ij}/\sqrt{dt}\mathbf{e}_{ij}$, where ς_{ij} represents an independent increment in a stochastic process, which is represented by a uniform distribution of random numbers with zero and unit variance, and is chosen independently for different pairs of particles at each time step.

2.1. *Theoretical aspects*

Extracting the DPD Fokker-Planck equation, which is analogous to MD Liouville equation, demonstrates the theoretical connection between dissipative particle dynamics and continuum fluid mechanics and is the essential formalism for the derivation of the kinetic and hydrodynamic equations, [Español, 1995; Coveney and Español, 1997]. The Fokker-Planck equation governs the N-particle distribution function that provides the probability density of the microscopic variables of the system, which are the positions and momentums of all the particles. It is related to DPD by the corresponding Langevin equations, which are the stochastic differential equations for the dynamics of the particles subjected to conservative, dissipative, and random forces. Using standard projection operator techniques, Español [1995] obtained the DPD macroscopic hydrodynamic equations. The derivation of more general equation of motion for coarse-grained particles was recently reported by Kinjo and Hyodo [2007b]. Español and Serrano [1999] and Serrano *et al.* [1999] investigated the behavior of the velocity autocorrelation function and found the importance of collective hydrodynamic effects for high values of friction. Marsh *et al.* [1997a, 1997b] formulated the kinetic theory for DPD such that the transport coefficients, namely the self-diffusion coefficient and shear viscosity, in the hydrodynamic equations, were related to the DPD model parameters, [Evans, 1999; Masters and Warren, 1999; Noguchi and Gompper, 2007; Satoh and Majima, 2005].

The equilibrium solution is not obtained by solving the Fokker-Planck equation directly, but it is a natural outcome of proving the H-theorem and demonstrating that the Gibbs distribution is the stationary solution of the Fokker-Planck equation. Proof of an H-theorem is the fundamental result in statistical mechanics for a dynamical system and shows that DPD particles tend to migrate towards the equilibrium state, which yields the Gibbs distribution as the equilibrium solution, [Coveney and Español, 1997; Marsh *et al.*, 1997a, 1997b]. The H-theorem yields stability of the solution and guarantees that all states in phase space lead to equilibrium. Detailed balance condition for DPD, equation (6), which is the same condition as the one in conventional Brownian motion, is the basic requirement in deriving the H-theorem. If this condition is violated, the H-theorem cannot be derived, and the Gibbs distribution is not a stationary solution of the Fokker-Planck equation.

In addition to central pairwise forces, Español [1997b, 1998] and Español and Revenga [2003] proposed the fluid particle model (FPM) in order to consider the noncentral shear forces between dissipative particles. This model can be considered as both the thermodynamically consistent version of smoothed particle hydrodynamics (SPH), Español *et al.* [1999], and the generalized DPD method that includes torques and angular velocities of the particles. Furthermore, it is not straightforward to determine the transport coefficients from the original DPD algorithm and the physical scales in DPD simulations are undefined, Español and Revenga [2003]. Therefore, the introduction of FMP improves some of these inherent deficiencies in original DPD technique.

Willemsen *et al.* [1998] proposed the combination of DPD with the Monte Carlo technique to compute thermodynamic properties in a more efficient manner. More recently, Goicochea [2007] predicted absorption and disjoining pressure isotherms of confined polymers using this combined model. Also, combining the basic elements of DPD with reaction Monte Carlo method enabled Lísal *et al.* [2006] to introduce a new method termed the reaction ensemble DPD in order to evaluate the reaction equilibria of polymer systems and to calculate the polydispersity under various conditions.

Although the classical DPD model can successfully simulate the hydrodynamics, it is not able to reproduce the thermodynamic behaviour of a real system accurately. To overcome this limitation and to obtain the correct dynamics of nonideal fluids, Pagonabarraga and Frenkel [2000, 2001] introduced the "many body" DPD approach. In this model, the amplitude of the soft repulsions is dependent on the local excess free energy, which provides a wider range of possibilities for the equation of state (a density dependent conservative force approach). Following this, Trofimov *et al.* [2002] refined this model for strongly nonideal systems and generalized it to multicomponent mixtures, and later they extended it for a constant pressure ensemble in Trofimov *et al.* [2005]. Warren [2003a] and Klapp *et al.* [2004] noted that the density dependent pair potentials and "many body" effects are very important considerations for achieving correct physical properties. This is especially so in applications with vapor-liquid coexistence, and other works involving many-body DPD include those by Warren [2003b] and Tiwari and Abraham [2006, 2008].

2.2. *Dissipative particle dynamics with energy conservation*

The existence of non-isothermal phenomena and heat flow will inevitably intensify the complication of simulating complex systems, as can be observed in the works of Han *et al.* [2008], He and Qiao [2008] and Qiao and He [2008]. As the original DPD model was isothermal and could not incorporate energy transport, Español [1997a] and Avalos and Mackie [1997] independently proposed a generalization of DPD algorithm that incorporated the conservation of the total energy in particle-particle interactions in addition to conserving the total momentum, such that the thermal conduction and temperature gradients could be modelled. The related detailed balance and H-theorem were proved for this energy conserving DPD algorithm (EDPD) by Marsh and Coveney [1998]. In Ripoll *et al.* [1998], heat conduction was simulated with this model and the correct equilibrium fluctuations and reproduction of Fourier law were observed. Later, Ripoll *et al.* [2001] analytically calculated the wave number dependent transport properties of the DPD fluid and more recently, Ripoll and Ernst [2005] extended the kinetic theory for the generalized hydrodynamic regime to incorporate the heat conduction.

Mackie *et al.* [1999] refined the energy model of DPD for every time step and derived the macroscopic equilibrium probability distribution and equations of state. Subsequently, in Avalos and Mackie [1999] and Mackie *et al.* [1999], they analyzed

the transport properties of this model and conducted some heat transport and thermal convection simulations to confirm the consistency of the model. To facilitate the study of complex fluids in the (N,V,E) ensemble, Pastewka *et al.* [2006] proved that the energy conserving Peters thermostat, Peters [2004], is equivalent to the EDPD in the limit of vanishing time-step.

In Willemsen *et al.* [2000b], a consistent boundary condition to model phase change of materials with EDPD was developed. More recently Qiao and He [2007] employed the EDPD method to model heat conduction in nanocomposites which can be interpreted as a model for thermal transport in heterogeneous materials. They were able to account for the interfacial thermal resistance, which is an atomistic phenomenon, by using the EDPD model. Moreover, they estimated the thermal conductivity of heterogeneous nanocomposite and it was found that the embedding of high thermal conductivity nanoparticles enhances the thermal conductivity of the matrix materials. Based on the DPD model with conserved energy, Stoltz [2006] proposed an interesting mesoscopic model for the simulation of shock waves and he successfully simulated the shock waves in a crystalline polymer. Later this reduced model was refined by Maillet *et al.* [2007] to handle chemical reactions.

2.3. *Time integration schemes*

An extra degree of difficulty arises in the time integration of the DPD algorithm because unlike MD, the DPD equations are stochastic and there is thus no guarantee for time reversibility of the integration process. Moreover, the dissipative force depends on the velocity, which in turn depends on the force, and so there exists a nonlinear coupling. Typically the simple Euler and velocity-Verlet algorithms can be used to integrate the DPD equations, [Español and Warren, 1995; Groot and Warren, 1997; Warren, 1998; Gibson *et al.*, 1999a; Hafskjold *et al.*, 2004]. In order to follow the phase space path of the particles more accurately and for better representation of the stochastic differential equations, various finite time-step implementations of DPD which are often based on analogies to higher-order solvers for conservative systems have been proposed. These include the Verlet or leap-frog algorithms that would be expected to follow the evolution up to the second-order in the time-step. However, care must be taken in the implementation to take account of the stochastic nature of the underlying equations, and an analysis of these methods for DPD can be found in Novik and Coveney [1998]. Correspondingly, other complex integration schemes such as the Lowe's approach, Lowe [1999], self consistent Verlet, [Besold *et al.*, 2000; Pagonabarraga *et al.*, 1998], and Shardlow's splitting method, Shardlow [2003], have been proposed. A detailed comparison of the performance of these integrators is given in Nikunen *et al.* [2003] and Vattulainen *et al.* [2002]. Vattulainen *et al.* [2002] found that the integrators in which the velocities and dissipative forces are estimated self-consistently, as in Besold *et al.* [2000] and Pagonabarraga *et al.* [1998], demonstrated better performance. More recently, the applicability of the stochastic Trotter integration scheme (a common MD integrator)

as an alternative updating algorithm for DPD was investigated by De Fabritiis *et al.* [2006], Serrano *et al.* [2006] and Thalmann and Farago [2007].

The strong dependence of the DPD equilibrium kinetic temperature to the time-step was explored in Marsh and Yeomans [1997]. Based on Andersen's thermostat, Andersen [1980], Lowe [1999] formulated an alternative DPD approach in which the interaction potential does not include dissipative or random forces. The relative velocities of the proposed Lowe-Andersen thermostat are taken from the Maxwellian distribution which maintains rigorous temperature control. More importantly, higher viscosities and consequently higher Schmidt numbers, which are the characteristics of liquid dynamics, can be achieved by adjusting related parameters in this scheme. Later, to control temperature fluctuations, Den Otter and Clarke [2000, 2001] proposed another method in which the coefficients of the random and dissipative forces are tuned according to the size of the time-step. Chen et al. [2005] employed the Lowe-Andersen thermostat to simulate polymeric systems, and in particular to examine the efficiency of this method for modelling microphase separation of diblock copolymers. It should be pointed out that one most efficient algorithms, based on both computational cost and degree of accuracy, is the modified velocity-Verlet scheme

$$
\begin{aligned}
\mathbf{r}_i^{t+dt} &= \mathbf{r}_i^t + dt\mathbf{v}_i^t + \frac{1}{2}dt^2\mathbf{f}_i^t \\
\widetilde{\mathbf{v}}_i^{t+dt} &= \mathbf{v}_i^t + \lambda dt\mathbf{f}_i^t \\
\mathbf{f}_i^{t+dt} &= \mathbf{f}_i(\mathbf{r}_i^{t+dt}, \widetilde{\mathbf{v}}_i^{t+dt}) \\
\mathbf{v}_i^{t+dt} &= \mathbf{v}_i^t + \frac{1}{2}dt(\mathbf{f}_i^t + \mathbf{f}_i^{t+dt}),
\end{aligned}
\tag{9}
$$

where the actual velocity-Verlet algorithm would be recovered for $\lambda = 1/2$. This modified integration scheme was first devised by Groot and Warren [1997] and subsequently used by many researchers in the area of DPD simulations. Due to the stochastic nature of the process, the order of the algorithm becomes indistinct, and the variable factor λ, introduced empirically, appears to account for some of the additional effects of the stochastic interactions.

In addition to the difficulties of finding appropriate time integrating scheme arising from the stochastic nature of the DPD algorithm, other problems may be encountered when simulating complex soft matter systems. In particular, the use of the Lennard-Jones (LJ) potential for each bead pair of polymers requires smaller time-step compared to soft repulsion of typical DPD particles, Soddemann *et al.* [2003]. Due to the presence of both soft and hard potentials, Symeonidis *et al.* [2005] and Symeonidis and Karniadakis [2006] proposed the use of time-staggered algorithms to study the polymeric physical quantities (such as end-to-end distance or radius of gyration) efficiently. For DPD simulations of lipid bilayers in water, Jakobsen *et al.* [2005] investigated the sensitivity of the pressure profiles and the kinetic bead temperatures to the artifacts caused by varying the integration time step and

the thermostat. Subsequently, to speed up the DPD simulations, Jakobsen *et al.* [2006] introduced a multiple time-step integrating scheme based on the velocity-Verlet algorithm, whereby the solvent particles are updated at lower frequencies than the bounded interactions within the solute. In addition, Allen [2006] pointed out the necessity of examination and measurement of the configurational temperature besides the typical kinetic temperature, for determining the optimum time-step values in multicomponent systems.

2.4. *Boundary models*

Defining the correct boundary conditions, especially at solid boundaries, is one of the main issues in DPD simulations involving wall-bounded geometries. In DPD, it is possible to employ the general implementation of boundary conditions that is usually used in the lattice Boltzmann method (LBM) and molecular dynamics (MD) formulations. However, due to the soft repulsion between the DPD particles, the fluid particles are not naturally prevented from penetrating solid boundaries. This is unlike the MD method, and appropriate mechanisms thus have to be developed and implemented at the walls. In addition to impenetrability, the boundary should impose the correct velocity profile through in the general flow field and also at the boundaries (no slip condition) while having consistency to macroscopic system properties; i.e. the temperature and density profiles should obey the thermal and continuum limits, especially near the boundaries. A full description and classification of DPD boundary models can be found in Moeendarbary *et al.* [2008], and here we shall briefly review most of works related to DPD boundary models.

In Revenga *et al.* [1998], the boundary is modelled as layer of fixed DPD particles, and taking the continuum limit of this layer, the dissipative and stochastic forces on the DPD fluid particles are determined analytically. In Revenga *et al.* [1999], the effects of specular, Maxwellian, and bounce back reflections on sticking boundary conditions and temperature distributions, were examined. A similar method to Revenga *et al.* [1998], (i.e. obtaining effective forces for planar geometries), but adapted for cylindrical and spherical geometries, was used by Colmenares and Rousse [2006] to obtain explicit expressions for the effective random and dissipative forces for a point DPD particle. For the DPD simulation of the shearing of a liquid drop on a solid surface, Jones *et al.* [1999] used similar densities for the solid and liquid, but with a strong repulsive interaction between both phases to keep them separated. Also, in an attempt to avoid slip at wall boundaries, they imposed a certain velocity on all particles within a close distance from the wall. Willemsen *et al.* [2000a] proposed a scheme which intrinsically imposes no-slip boundary conditions in DPD without having to artificially use high wall densities to achieve the same. By adjusting the distance between the layers of wall particles, a new implementation was reported by Duong-Hong *et al.* [2004], for achieving no slip boundary condition with low density distortion. In order to reduce the undesirable effects on macroscopic properties, Visser *et al.* [2005] developed a notable method whereby

impenetrable flat and cylindrical solid walls were devised via a wall construction technique that employs parallel twin systems which set up the wall through back-to-back placement.

In order to measure the viscosity of flow in a particle method like the DPD, Backer *et al.* [2005b] introduced a novel type of periodic boundary conditions to simulate counter-flowing Poiseuille flows without the use of explicit boundaries. Based on an equivalent force between wall and DPD particles, Pivkin and Karniadakis [2005] developed a method to obtain the no slip boundary condition. Subsequently, Pivkin and Karniadakis [2006b] also proposed a general adaptive method to prevent the density fluctuations. Haber *et al.* [2006] employed DPD simulations in flow generated by two rotating concentric cylinders and used this model to examine some of the earlier proposed boundary conditions for analyzing the velocity, density and temperature profiles. For treating DPD simulations with higher dissipation rates, simple modifications to the Lees-Edward periodic boundary condition was made in by Chatterjee [2007]. Employing a stochastic boundary forcing technique for a number of benchmark DPD problems, Altenhoff *et al.* [2007] obtained the accurate no slip boundary condition while minimizing other spurious fluctuations. Another method for the treatment of solid-liquid interfaces was reported recently in Henrich *et al.* [2007], in which the solid representation is that of an amorphous, thermally rough ensemble of particles.

3. Complex Fluid Applications

Elliott and Windle [2000] constructed a model for the geometrical packing of irregularly shaped filler particles in composite materials within the DPD framework. Following this, Rahatekar *et al.* [2005] simulated the packed assemblies of oriented fibres suspended in a viscous medium and the DPD assembled structures were used in Monte Carlo simulations to estimate the network impedance. More recently, the modification of the molecular dynamics package (DL_POLY) to handle mesoscale modelling of fibre networks was reported by Elliott *et al.* [2006]. The well-known attributes of carbon nanotubes (CNTs) which include excellent mechanical, thermal, and electrical properties, finds promising applications in nanocomposites, and designing their dispersion within polymeric matrices is a very important aspect in this emerging area of nanotechnology. By improving the Flory-Huggins theory for DPD parameters, Maiti *et al.* [2005] were able to obtain the equilibrium morphology of the polymer-nanotube composites. Later, Wescott *et al.* [2007] mapped the DPD calculated mesoscale morphology of these composites onto a finite-element grid and the electrical conductivity of the films was estimated. In order to predict the structure of polymer-clay nanocomposites (PCN), nanotube–polymer composites and polymer blends (PCN), Fermeglia and Pricl [2007] and Scocchi *et al.* [2007a, b] reported a hierarchical procedure which bridges the atomistic and mesoscopic simulations. They calculated the interaction parameters of mesoscopic DPD model by mapping the corresponding energy values obtained from MD simulations. Figure 2
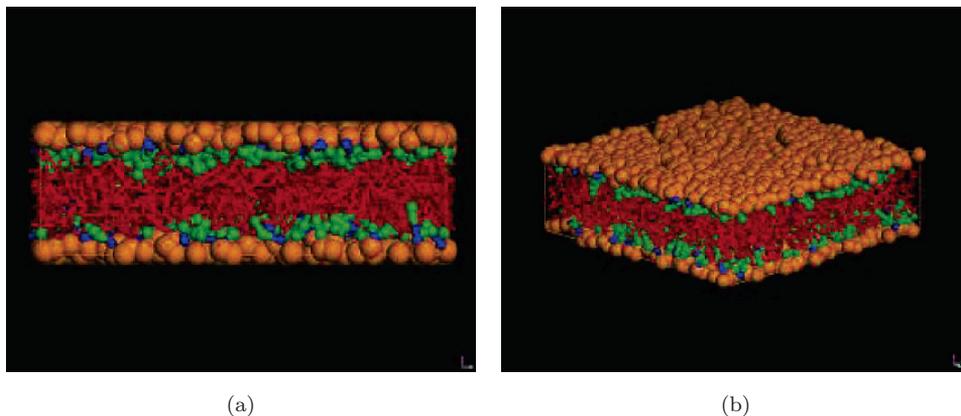
Fig. 2.   Morphology of the clay-nylon 6 nanocomposite system obtained via DPD simulation: (a) perspective view and (b) frontal view. Orange-clay; blue-surfactant head; green-surfactant tails; red-polymer. Reprinted with permission from Scocchi *et al.* [2007b]. Copyright 2006 American Chemical Society.

shows the morphology of clay–nylon 6 nanocomposites obtained from DPD simulation, which is in good agreement with earlier experimental and atomistic simulation results.

Recent studies have claimed that the motor proteins can be a potential tool for powering future nano-bio-mechanical systems. With an aim to study the interaction between the protein motors and bio-filaments, and to investigate the effects of motor density and the length of microtubule on the microtubule motion, Chen *et al.* [2007] conducted DPD simulations of molecular motors attached to a microtubule. In Bedau *et al.* [2006] a simple form of ligation was investigated by a DPD model extended to include the dynamic making and breaking of strong bonds. In Gazzola *et al.* [2007] and Buchanan *et al.* [2008], it was shown that the incorporation of the chemical reactions into the DPD model enables the additional study of the interplay between chemical reactions and self-assembly processes. More interestingly, the coupled diffusion, self-assembly, and chemical reaction processes required to model a full life cycle of a protocell were reported by Fellermann *et al.* [2007] and Fellermann and Solé [2007], using a DPD framework.

In addition to successful application of DPD in the areas discussed in the earlier sections on polymeric related fields, there are some other publications connected to DPD simulations, which are more general and related to various fluidic systems. Thus, in the following sub-sections, we shall classify and discuss these specific categories, and review some of the most representative works in these categories.

3.1. *Suspension flow and colloidal system*

Understanding the rheological properties of colloidal suspensions with particles of different sizes, shapes and compositions which are suspended in different mediums

of various conditions, is one of the key issues in its modelling and simulation. The industrial applications of these suspensions range from paints, coating fluidized beds to oil recovery. In addition to continuum based approaches like Brownian dynamics (see Ball and Melrose [1997] for more details) or Stokesian dynamics, which are computationally expensive for high shear rates Boek *et al.* [1997], there are alternative mesoscopic techniques such as the Lattice Boltzmann method (LBM) and DPD. The DPD simulation of suspensions is a possible way to accommodate continuum hydrodynamics at large length scales, while it is also capable of capturing some degree of molecular details. In the following discussion, we review the most representative works which used DPD to simulate colloidal suspensions.

Boek *et al.* [1997] investigated the rheological properties of suspension of large colloidal particles such as spheres, rods and disks in a liquid of interacting point particles. They found the DPD method highly efficient for the calculation of hydrodynamic interactions compared to methods which use continuum models for the solvent. In Boek *et al.* [1996, 1997], the viscosity as a function of shear rate and volume fraction of the suspended particles was calculated using DPD, and the results for dilute suspensions of rods and disks were in excellent agreement with theoretical predictions. In addition, for the semidilute regime, they found similar "Doi-Edwards" scaling behaviour for the concentrated rod suspensions. In an exposition on the issues and complications of using DPD to simulate colloids, Whittle and Dickinson [2001] noted that an increase in the size of the colloidal particles compared with the fluid particles is expected to improve the quality of the hydrodynamic interactions, but this also increases the total number of particles in the simulation and is thus computationally costly. An additional complication arises from the depletion effects caused by structuring of the small particles between adjacent larger particles. With regard to these finite size and resolution effects in the DPD simulation of colloidal systems, Boek and Van Der Schoot [1998] examined the fluid flow through a periodic array of spheres, rheology of suspended spheres and aggregation of solid spheres caused by depletion flocculation. They found that for the case of fluid flow through arrays, the size of system does not affect dimensionless drag, while for higher solid volume fractions, it was necessary to increase the system size to avoid the finite size and resolution effects.

Gibson *et al.* [1998, 1999b] used DPD to effectively simulate adsorption of colloidal particles onto a polymer-coated surface and their results achieved good agreement with the theoretical predictions, in that as the size of the polymers relative to the colloidal particle increases or similarly as density of the polymers increases, the adsorption of particles onto the surface would be less likely. Van Der Kooij *et al.* [2001] obtained good results for the intrinsic viscosity of hard plate suspension by studying the rheology of dilute suspensions of these hard plate-like colloids through combining rheological measurements on suspensions of sterically stabilized plate-like colloids with DPD modelling for disks.

Kim and Phillips [2004] studied flows around spheres and cylinders at finite Reynolds numbers with a finite fluid inertia in DPD simulations. Flow around immobile objects and translation and rotation of mobile objects were investigated and it was shown that under computationally feasible conditions, DPD simulations are quantitatively accurate up to Reynolds numbers of 50∼100, and the inaccuracies at higher Reynolds numbers can be attributed to compressibility effects. Later, Chen *et al.* [2006] estimated the drag force and torque of uniform and shear flow around a stationary sphere by employing DPD simulation, and they observed the importance of the dissipative coefficient on the resulting values of the drag force and torque.

In Darias *et al.* [2003], suspensions constricted in cylindrical geometries were investigated using DPD. In this DPD model, the suspended soft spheres interact via a conservative force while the continuum phases interact through DPD forces. Pryamitsyn and Ganesan [2005] devised a simple extension of the DPD approach to model the rheology of macroparticles in complex fluid solvents, and in addition, they were also able to track the glass transition and related dynamical phenomena of their suspension model. Later, De Palma *et al.* [2006] applied the DPD method to simulate the flow driven by a peristaltic micropump which consists of several colloidal spheres, and they obtained a detailed description of local flow properties which were reasonably accurate when compared with corresponding experimental data.

Martys [2005] performed a series of simulation tests in order to compare the DPD results of various suspension models with other theoretical predictions, and he found that the original DPD method recovers the flow of a suspension for volume fractions in the dilute to semidilute systems regime well. However, at higher volume fractions and Peclet numbers Pe, he found that it was necessary to adjust the time step and explicitly include lubrication forces into the DPD algorithm in order to consider important phenomena that must be resolved at small time and length scales. Satoh and Chantrell [2006] first modelled the interactions between dissipative and magnetic particles of two magnetic particle system using an idealised model potential, and then moved on to study ferromagnetic colloidal dispersion in a multi-magnetic particle system. The DPD simulations were carried out to investigate particle aggregates and the pair correlation function along an applied magnetic field direction, and the results were found to be in good agreement with those of Monte Carlo and Brownian dynamics simulations.

For simulation of ordered colloidal structures, Dzwinel and Yuen [2000] and Dzwinel *et al.* [2002] used a Lennard-Jones-type potential to define the colloidal particle system and DPD particles to mimic the solvent. The phase transition of particles and spontaneous creation of spherical or worm-like micelles and their crystallization in stable hexagonal or wormlike structures were observed. In addition, the strongly variable properties such as the viscosity and partial pressure of the DPD solvent were found to be crucial in determining the speed of crystallization.

3.2. *Phase separation of immiscible fluids and mixtures*

The growth kinetics of immiscible fluids and simulating the phase separation of these mixtures is another interesting issue in soft matter modelling. A variety of techniques such as cell dynamical systems with/without Oseen tensor hydrodynamics, time dependent Ginzburg-Landau models, lattice-gas automata (LGA) and LBM have been used to simulate these systems Coveney and Novik [1996]. However, DPD is proving to be an alternative technique which combines the best aspects of LGA and MD to investigate these systems Arce et al. [2006].

Employing DPD, Coveney and Novik [1996] and Novik and Coveney [1997] investigated the domain growth and phase separation in two-dimensional binary immiscible fluids. They studied the scaling laws for the domain size growth $R(t) \sim t^n$ for both symmetric and asymmetric quenches and found the two-dimensional growth exponents being $n = 1/2$ and $n = 2/3$ at early and late times, respectively, for symmetric quenches, while $n =1/3$ throughout for asymmetric quenches. Furthermore, Laplace's law was validated by a series of simple bubble experiments and the existence of surface tension between the two phases was confirmed. Subsequently, Novik and Coveney [2000] studied the domain growth and phase separation of hydrodynamically correct binary immiscible fluids of differing and equal viscosity, as a function of minority phase concentration, in both two and three spatial dimensions. For the latter three-dimensional case, it was observed that the characteristic domain size scales as $n =1/3$ for simulations of differing and equal viscosity fluids developing from symmetric and slightly off-critical quenches, see Fig. 3. Later, based on difference in dynamic properties and particularly by adjustment of friction coefficients of DPD model, Yaneva *et al.* [2005] proposed a model of a binary mixture.

The effect of volume fraction, radius, and mass of nanoparticles on the dynamics and morphologies of phase separation in three-dimensional fluids containing nanospheres was investigated by authors Laradji and Hore [2004] using DPD. At low to moderate volume fractions of nanoparticles, the growth law was found to be similar to pure binary mixtures. However, slower growth regimes were observed as the volume fraction of the nanospheres is increased or their radius decreased, which is associated with crystallization of the nanoparticles within the preferred component. More recently, for moderate volume fraction of nanoparticles, Hore and Laradji [2007] explored the microphase separation induced by interfacial segregation of isotropic nanoparticles interacting symmetrically with the two fluids. Liu *et al.* [2007a] studied the influence of polymerization on the phase separation of binary immiscible mixtures via DPD in two dimensions. They observed that during polymerization the bulk viscosity increased which slows down the spinodal decomposition process and suppressed the speed of phase separation.

3.3. *The thin film evolution and dynamics of drop*

There are various types of industrial and biological systems associated with suspension of droplets, deformation of individual drops in multiphase flow environments,
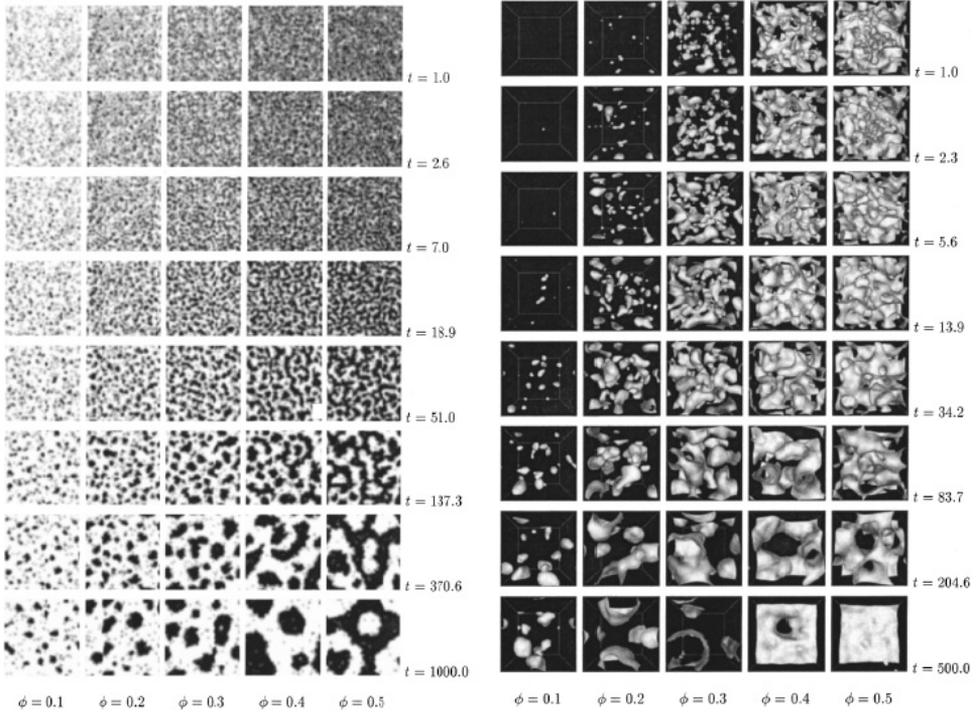
Fig. 3.   Time evolution of five sample simulations of two (left) and three (right) dimensional equal viscosity fluid of different minority phase fractions varying from $\phi = 0.1$ to $\phi = 0.5$. Reprinted with permission from Novik and Coveney [2000]. Copyright 2000 by the American Physical Society.

and wetting processes. Until now and probably due to certain theoretical and experimental inadequacies, the physics of the dynamics of the drop's motion and its shape and stability have not been fully understood. Accurate and robust numerical simulation techniques which can handle mesoscopic time and length scales are key tools which can help us to extract and understand the underlying physics of these complex systems, and DPD seems to be the proper mesoscale method which has recently attracted the attention of many investigators in this area.

Employing MD and/or DPD, Dzwinel and Yuen [1999] and Dzwinel *et al.* [2000] studied the gravitational fall of a fluid film positioned on the underside of a plate (Raleigh-Taylor flow), and they observed the short-time rupture of the thin film, its break up into contracted droplets and spikes, and finally the formation of bubbles. Moreover, formation of fingering instability, rivulets and horseshoe patterns were also observed. Later, Kong and Yang [2006] used DPD to study the effects of substrate topology on contact angle hysteresis. They found that discontinuous solid substrates (DSS) have relatively larger contact angle hysteresis at lower temperature, while from dynamic wettabilty viewpoint, a continuous solid substrate (CSS) is more suitable for building an ultrahydrophobic or ultralyophobic surface. More recently, a method to model adhesive, solid boundaries for the treatment of

solid-liquid interfaces was introduced by Henrich *et al.* [2007], and it was applied in a DPD framework to examine forced wetting and behaviour of dynamic angles.

The dynamics of a drop confined through a liquid, and attached on a solid surface under a shear field, was studied by Jones *et al.* [1999]. Through their DPD simulations, they found that the shear field induces contact angle hysteresis in the drop, and this hysteresis increased with the shear rate. Consequently, when the shear rate exceeds a critical value, the drop was inclined to lift off the boundary, and upon elongation of the drop, necks are developed and finally the drop breaks up as the necks rupture upon thinning. Following this, Clark *et al.* [2000] investigated the shape profile and detachment process of pendant drops, and they found that the DPD simulated shape profile was in a complete agreement with the solution of Laplace equation, while the neck formation and detachment of the drop was consistent with the earlier experimental data. In addition, they also investigated the time evolution of the shape of the drop as it underwent the break up process in shear field, and the calculated critical value of the capillary was in reasonable agreement with experimental figures. In Warren [2003b], a many-body DPD model was constructed to cater for vapour-liquid coexistence, and this was used for the simulation of pedant drops. Liew and Mikami [2003] implemented several coarse-graining procedures for soft-matter, which also resulted models able to reproduce liquid-vapour coexistence, and they used this 'soft-attractive-and-repulsive' pair-potential model in combination with DPD to investigate dynamic properties in complex fluids.

DPD simulations of the realignment of a nematic nanodroplet suspended in an isotropic fluid following a switch in the direction of an applied external magnetic field were carried out by Levine and Polimeno [2007], and the results showed significant spatial inhomogeneities in the properties of the nanodroplet, consistent with its fluid structure.

3.4. *Multiphase flows*

There are several applications, such as liquid jet break up, drop collisions, drop break up, mixing and multiphase flows in mircochannels, in which the flow involves different phases. The key issue in these multiphase flow applications is the interfacial physics between different phases of liquid, gas and solid. The DPD method, due to its mesoscopic features, can be a very useful simulation tool in this area. Based on mean field theory, Tiwari and Abraham [2006] proposed a DPD model for two-phase flows involving gas and liquid phases. In the validation of their proposed model, they carried out simulations of problems with interfacial dynamics, such as the small-and large-amplitude oscillations of liquid cylinders and capillary waves. Visser [2006] proposed three methods to handle the friction factor for the interaction between particles of unlike fluids in multi-viscosity systems. The capability of DPD in capturing the qualitative jetting effects which occur during ceramic injection was reported in by Heldele *et al.* [2006].

Liu *et al.* [2006] proposed a combination of short-range repulsive and long-range attractive interactions for the DPD modelling of multiphase systems, and using this model they studied the behaviour of liquid drops in a gas. Later a similar model was used to simulate multiphase fluid flow in microchannel networks Liu *et al.* [2007c], unsaturated fracture junctions Liu *et al.* [2007b] and porous media Liu *et al.* [2007d], which is complex due to interplay of viscous, capillary and gravitational forces, microchannel geometry, and the inflow conditions. Varying injection rates and the fluid-fluid and fluid-wall interaction strengths, and external forces, different modes of flow such as thin film flow, wetting and non-wetting flows, were observed by Liu *et al.* [2007b] and this verifies the viability of the use of DPD methodology in the area of multiphase simulations.

4. Concluding Remarks

The DPD method is a relatively new mesoscopic simulation technique for the simulation of complex systems, and it is capable of addressing certain features where other similar scale methods are unable. However, there are several issues associated with the DPD that may require new development work or future refinements. These include possible new directions in theoretical aspects as well as its applications. In the theoretical development area, some of the interesting challenges can be formulation of more appropriate DPD algorithms and parameters that are capable of handling variety of problems such as multiphase problems, complex heat transfer studies (such as conduction and convection in nano-materials), simulation of biological membranes or macromolecules subject to different flows and geometries, morphology investigation of self-assemblies, etc. Depending on the application; huge computational cost may be required, while fast time-evolution algorithms necessary for the speed up of the simulations are always essential. There are vast opportunities for particle methods to decrease computational cost by improving cell algorithms (such as the Neighbor List method), as well as efficient parallel implementations, [Dzwinel *et al.*, 1999; Boryczko *et al.*, 2002, 2003; Sims and Martys, 2004; Oh and Klein, 2006]. Finally, it would be a major milestone, and just a matter of time when innovative researchers concurrently couple DPD with other particle based methods like MD in order to handle multiscale problems. In the nano-scale regions or close to boundaries where DPD is unable to capture the details of microscale or even nanoscale interactions, more refined techniques can be used while DPD is being used to simulate the bulk region.

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