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Dissipative Particle Dynamics, Overview

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Synonyms

Coarse-grained molecular dynamics; Fluctuating
hydrodynamics; Mesoscopic simulation; Rheol-
ogy; Soft matter

Definition

Dissipative particle dynamics (DPD) is a stochas-
tic mesoscopic simulation technique that
describes *clusters* of molecules moving together
in a Lagrangian fashion subject to simplified
pairwise conservative, dissipative and random
forces.

Introduction

Natural systems can be described at different
scales based on both spatial and temporal size.
In general, there are three different scales, i.e.,
micro-, meso-, and macroscales. A microscopic

event occurs at nanometers in length and nano-
seconds in time or, even less, governed by quan-
tum mechanics or classical laws. Macroscale
describes physical objects or phenomena that
are measurable and visible directly with the
naked eye, and thus, the mean free path of mole-
cules is far smaller than the characteristic length
of the geometry. A macroscopic event is usually
described by continuum partial differential equa-
tions (PDEs), such as Navier-Stokes equations
for fluid dynamics. Mesoscale is somewhat in
between, which is typically in order of microme-
ters and microseconds. Examples of such
mesoscopic systems include colloidal suspen-
sion, polymer solution, and biological mem-
branes. Since the behaviors of such systems can
be much more complex than that of a simple
fluid, they are usually called complex fluids.
There exist broad applications of complex fluid
systems in industrial technologies, especially in
the field of biological and biomedical sciences
such as biochemical lab-on-a-chip systems, sep-
aration devices, and drug delivery systems.

Computer simulations have become an essen-
tial part of mathematical modeling of many nat-
ural systems in modern science and technology,
serving as a bridge between theories and experi-
ments (see Fig. 1). Molecular dynamics (MD) has
emerged as one of the first and yet widely used
simulation methods in many areas of physics and
chemistry starting from the 1950s. However, the
classical MD is practical only for simulations up
to microscales. It is difficult to simulate larger
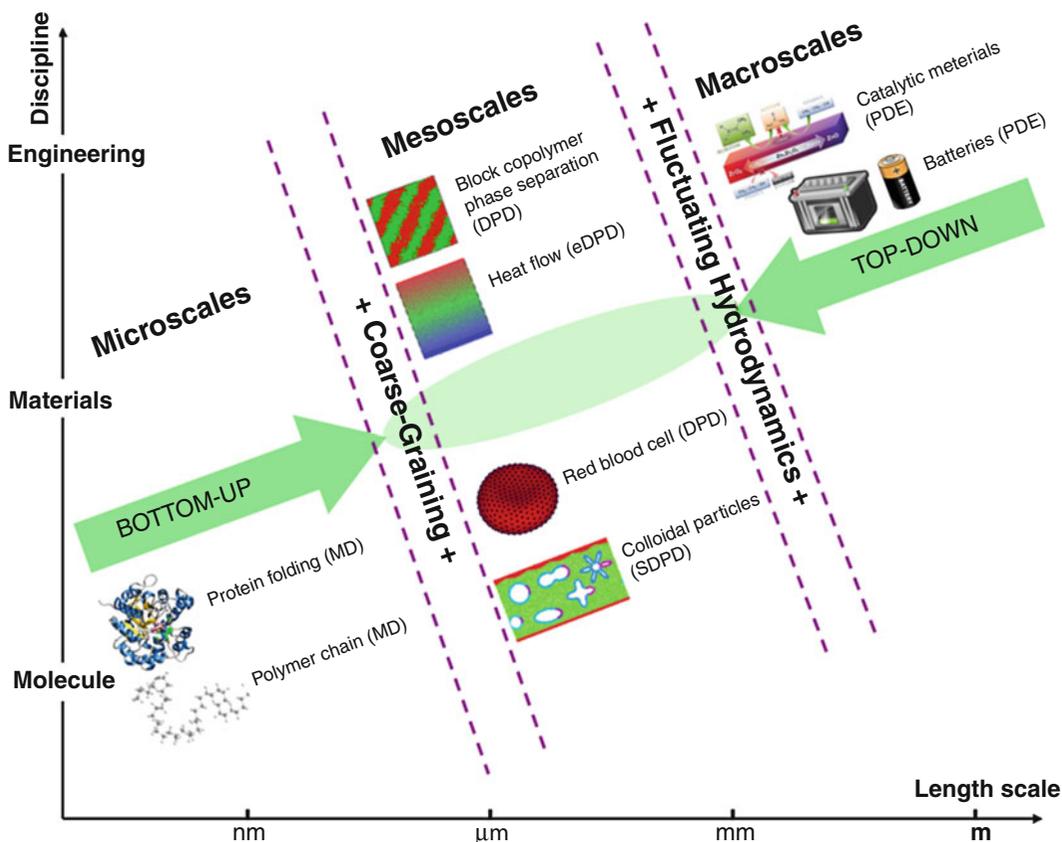
Dissipative Particle Dynamics, Overview, Fig. 1 Illustration of the length scales in "soft" materials. MD, DPD, and PDE stand for molecular dynamics, dissipative particle dynamics, and partial differential equations, respectively, and eDPD and SDPD indicate energy-conserving DPD and smoothed DPD, respectively

and more complex systems because of prohibitively expensive computations. Meanwhile, sophisticated computational and numerical discretization techniques have been developed over the past decades for the solution of PDEs at macroscale, such as various computational fluid dynamics (CFD) methods. However, these PDEs are inadequate to capture mesoscopic events in complex fluids, since these PDEs are based on simple constitutive equations, while the dynamics of a complex fluid is fundamentally affected by its microscopic structure. Furthermore, the standard PDE formulations often ignore the stochastic nature of a system observed at mesoscale, which is a characteristic feature for many physical phenomena.

Mesoscopic simulation methods have been developed to overcome the aforementioned

problems, aiming at modeling complex fluids with efficient computational costs. Dissipative particle dynamics (DPD), which describes *clusters* of molecules moving together in a Lagrangian fashion, is a typical mesoscopic simulation method for the dynamic and rheological properties of simple and complex fluids [1]. DPD combines Lagrangian features from MD and coarser spatial-temporal scales from lattice-gas automata (LGA), and, therefore, it is faster than MD and more flexible than LGA. The first form of DPD was reformulated by Espanöl and Warren such that it produces a correct thermal equilibrium state [2]. This is considered as the standard form of DPD. Several improved DPD models [3–6], which are capable of representing complicated fluid properties more accurately, as well as efficient algorithms have also been developed.

Rigorous foundations of DPD methodology have also been investigated by both top-down (from macroscopic description to mesoscopic description) and bottom-up (from microscopic to mesoscopic) approaches.

Theoretical Formulation

In a DPD simulation, a particle represents a cluster of molecules, and the position and momentum of the particle are updated in a continuous phase space at discrete time steps. The equation of motion and pairwise interacting forces of particles read

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

where $\mathbf{r}_i$, $\mathbf{v}_i$, and m_i are position, velocity, and mass of particle i, respectively. $\mathbf{F}_{ij}^C$ is referred to as conservative force obtained from a prescribed potential between particles i and j. It is repulsive and leads particles to be evenly distributed in space. Roughly speaking, it can be understood as a pressure force; $\mathbf{F}_{ij}^D$ has a negative sign and is proportional to the velocity difference of two particles. Therefore, it is dissipative and resists velocity difference of any interacting pair of particles. Hence, $\mathbf{F}_{ij}^D$ dissipates the kinetic energy of the system. This amount of energy must be put back into the system, to keep the system at a constant temperature. $\mathbf{F}_{ij}^R$ is exactly for this purpose. It is a random force and injects kinetic energy back into the system. Effectively, $\mathbf{F}_{ij}^D$ and $\mathbf{F}_{ij}^R$ implement a thermostat so that thermal equilibrium is achieved. The magnitudes and functional forms of the two forces are related by the so-called *fluctuation-dissipation theorem*. The typical forms of the three forces are as follows [2, 7]:

$$\mathbf{F}_{ij}^C = a_{ij}\omega^C(r_{ij})\mathbf{e}_{ij}, \quad (2a)$$

$$\mathbf{F}_{ij}^D = -\gamma\omega^D(r_{ij})(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\mathbf{e}_{ij}, \quad (2b)$$

$$\mathbf{F}_{ij}^R = \sigma\omega^R(r_{ij})\theta_{ij}\delta t^{-1/2}\mathbf{e}_{ij}, \quad (2c)$$

where a_{ij}, γ, and σ reflect, respectively, the strength of conservative, dissipative, and random forces. Here, θ is a *Gaussian white noise* ($\theta_{ij} = \theta_{ji}$), and $\mathbf{e}_{ij}$ is the unit vector pointing from particle j to i; also, ω^C, ω^D, and ω^R are unspecific weighting functions of relative distance r_{ij}. A common choice of the weighting functions is

$$\omega^C(r_{ij}) = \begin{cases} (1 - r_{ij}/r_c)^s, & r_{ij} < r_c, \\ 0, & r_{ij} \geq r_c, \end{cases} \quad (3)$$

$$\omega^R(r_{ij}) = \begin{cases} 1 - r_{ij}/r_c, & r_{ij} < r_c, \\ 0, & r_{ij} \geq r_c, \end{cases} \quad (4)$$

where $s = 1$ is the most widely adopted for the classical DPD method. However, other choices (e.g., $s = 0.25$) for the envelopes have also been used. Also, r_c is the cutoff radius, which defines the extent of the interaction range.

To satisfy the fluctuation-dissipation theorem, two conditions must be further enforced [2]:

$$\omega^D(r_{ij}) = \left[\omega^R(r_{ij})\right]^2, \quad \sigma^2 = 2\gamma k_B T, \quad (5)$$

where k_B is the Boltzmann's constant and T is the absolute temperature.

Two important implications of the DPD forces in Eq. 2 must be explicitly noted: firstly, DPD is considered as a reduction model of the underlying microscopic dynamics. By construction, it focuses on the coarse-grained properties and intentionally ignores irrelevant degrees of freedom on the microscopic level. As a result, interparticle potential (the derivative of which is $-\mathbf{F}_{ij}^C$) is much softer than that of MD method; hence, it can potentially access longer time and length scales than are possible using conventional MD simulations. Furthermore, $\mathbf{F}_{ij}^D$ and $\mathbf{F}_{ij}^R$ together account for the lost microscopic information. Secondly, by design, all three forces act along the line of particle centers $\mathbf{e}_{ij}$ and are symmetric by interchanging particle indices. Therefore, the momentum is locally conserved. The fulfillment of the conservation laws guarantees

that a DPD system approaches the PDEs of fluid dynamics, such as Navier-Stokes equations, at the macroscopic scale.

For the purpose of modeling simple and complex fluids, α, γ (or σ), and s are free parameters to calibrate so that the desired properties of a target system can be achieved. The time evolution of velocities and positions of particles is determined by Newton's second law of motion similar to the MD method, which is usually integrated using a modified velocity-Verlet algorithm [7].

Extensions of DPD

The classic DPD method is a minimal working version for mesoscopic simulations of fluids. Due to the lack of necessary degrees of freedom, it cannot model some specific problems, e.g., heat flow in non-isothermal systems and liquid-vapor interface in two-phase fluid systems. To this end, extra degrees of freedom, such as an internal energy variable and freedom to alter the equation of state, have been introduced to DPD system for particular applications [8]. In this section, several extensions of the DPD method will be described briefly.

Energy-Conserving DPD

The classic DPD method is limited to isothermal systems and is not valid for modeling non-isothermal processes because the energy is not conserved in particle interactions. To extend the standard formulation of DPD with application to heat flow in non-isothermal fluid systems, the conservation of energy was applied to DPD by introducing the particle internal energy ε_i as an additional variable [3]. Along this new variable, a local entropy function $s(\varepsilon_i)$ and the temperature $T_i = (\partial s_i / \partial \varepsilon_i)^{-1}$ are defined for each particle. The energy-conserving DPD model is known in the literature as eDPD or DPDE, where for interacting particles, the dissipation induced by the dissipative forces is utilized in raising the internal energy of the particles through viscous heating. Moreover, the temperature differences between particles produce variations in the internal energies through heat conduction.

The key aspect of eDPD is that the temperature T_i is defined on each particle, and the fluctuation-dissipation theorem is applied locally based on the particle temperature T_i rather than the thermodynamic temperature of the system. As a result, eDPD allows temperature gradients and can be used in non-isothermal problems, where thermal transport plays a critical role.

Many-Body DPD

The conservative force $\mathbf{F}_{ij}^C$ is responsible for the thermodynamic behavior of the DPD system and has the form shown in Eq. 2. For a single-component DPD fluid, the equation of state (EOS) of the system can be approximated as $p = \rho k_B T + \alpha a_{ij} \rho^2$, which is a quadratic function of the particle density ρ. This monotonic function of EOS does not contain a van der Waals loop and excludes the possibility of simulating phenomena involving vapor-liquid coexistence or free surface.

To model vapor-liquid coexistence, the many-body DPD (MDPD) was developed by modifying the expression of the conservative force [5]. A direct way to produce higher order terms in EOS is making the conservative force in MDPD dependent not only on the interparticle distance but also on the instantaneous local particle density. Therefore, the conservative force in MDPD is effectively a many-body force and it generally includes both attractive and repulsive components. With higher order terms in EOS, MDPD has been successfully applied to simulations of droplet- and wetting-related phenomena.

Fluid Particle Model

The fluid particle model (FPM) is a generalization of the classic DPD method [4]. FPM considers both linear and angular momenta of the particles and includes both central and noncentral forces between particles, while the classic DPD method considers only linear momentum and includes only central forces. By introducing torques and angular velocities of the particles, both linear and angular momenta of FPM are

conserved. Also, the dissipative and random forces in FPM satisfy the fluctuation-dissipation theorem, and they together act as a thermostat to maintain the temperature of the FPM system at a constant.

Since the rotational motion of individual particle is included, FPM shows high computational efficiency in studying the dynamical and rheological properties of colloidal suspensions in simple fluid solvents. The reason is that each colloidal particle can be represented by a single FPM particle rather than a cluster of particles. FPM has been used to investigate a range of rheological behaviors and volume fractions of the colloidal suspensions and shows good agreement with experimental and theoretical results.

Smoothed DPD

The classic DPD model is a bottom-up approach and it is usually considered as a coarse-grained MD model, in which particles are governed by a coarse-grained force field. Similarly to the MD method, the inputs of DPD are the particle interactions, while the macroscale quantities, such as viscosity, diffusivity, compressibility, and EOS, are output properties. As a result, DPD has no restrictions on constitutive equations, which provides flexibility in modeling complex materials and multicomponent systems. However, a shortcoming of DPD is that it employs empirical expressions for the particle interactions, and its parameters are not related in a straightforward way to usual macroscale quantities. Therefore, in practice, the DPD units have to be mapped to physical units based on output properties.

Alternatively, *smoothed* DPD (SDPD) is a top-down approach [6]. It was developed from smoothed particle hydrodynamics (SPH). In fact, SDPD is a Lagrangian discrete model for simulating Navier-Stokes hydrodynamics that includes thermal fluctuations consistently. Unlike the classic DPD method, the parameters in the governing equations of SDPD have clear physical meaning. The inputs are the viscosity, equation of state, temperature, and other parameters required by the fluctuating Navier-Stokes equations. However, since the constitutive equations and macroscale properties of the system must be given as inputs, SDPD works well with simple fluids but loses its effectiveness in modeling complex materials.

Applications in Different Fields

In the past decade, the DPD method has been successfully extended to many applications including simple fluid hydrodynamics, polymer solutions and melts, biological membranes, colloidal suspensions, and blood flow [9, 10]. A few examples are presented in the following:

Polymer Solution

A polymer is a large molecule composed of many repeated subunits bonded together. In DPD, a polymer can be represented by linking collections of particles into chains with appropriate spring forces expressed as $\mathbf{F}_{ij}^S = k_{\text{bond}}(1 - r_{ij}/r_0)\mathbf{e}_{ij}$ [9]. Numerous simulations have testified that the DPD model is capable of capturing many essential physical phenomena of the polymer systems. For example, the DPD model has been applied to polymers in solution to study effects of solvent quality on the conformation and relaxation of polymer chains [11]. The dynamics of polymer chains in simple shear flow such as Couette and Poiseuille flow have also been simulated. Simple shear flows are commonly generated by imposing a constant driving body force (Poiseuille flow), or a driving velocity on the boundary shear planes (Couette flow). The static and dynamic properties of polymer chain under shear, such as radius of gyration, diffusivity, and viscosity, were computed and compared to experimental results [12]. The conformational changes and translocation dynamics of polymer and DNA molecules through microfluidic channels have also been investigated by DPD [13].

Amphiphilic Systems

Amphiphilic molecules, which contain hydrophilic head and hydrophobic tails, can be synthesized with various structures of the block type. In a selective solvent of one of the blocks, they can self-assemble into a wide variety of morphologies. A typical model of amphiphilic molecules
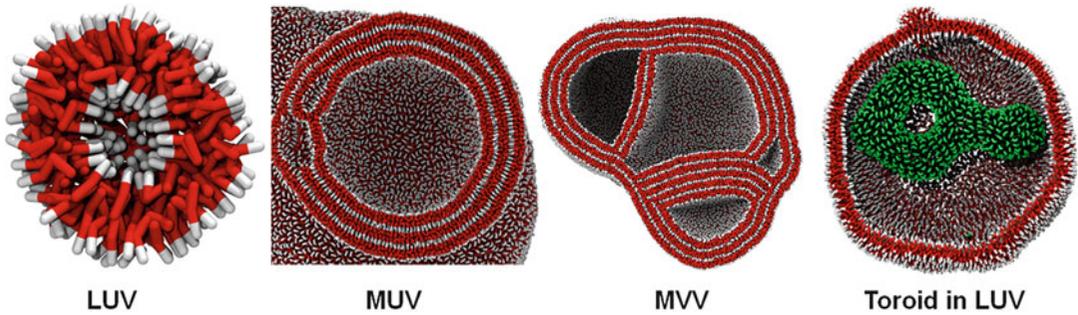
Dissipative Particle Dynamics, Overview, Fig. 2 Self-assembled complex microstructures of amphiphilic molecules. These microstructures included: large unilamellar vesicle (*LUV*), multilamellar vesicle (*MLV*), multivesicular vesicle (*MVV*), and a toroid in LUV. The hydrophilic and hydrophobic particles are rendered in *white* and *red*/*green*, respectively. Slices of these shapes are shown for clarity

is the two-letter ("black-and-white") H-T model, composed of a single head particle (denoted by H) and a linear chain of tail particles (denoted by T). The amphiphilic molecules are then immersed in solvent bath (denoted by W).

To model the amphiphilic nature of amphiphilic molecules, the hydrophobic and hydrophilic interactions emerge from the relative interaction strengths. In theory, the functional dependence of the Flory-Huggins parameter χ [14] on DPD repulsion parameter a_{ij} places the simulation results in the proper context. The relationship between a_{ij} and χ has been established by Groot and Warren [15]: $a_{ij} = a_{ii} + 3.27\chi_{ij}$ at particle density $\rho = 3$ and $a_{ij} = a_{ii} + 1.45\chi_{ij}$ at $\rho = 5$. Typically, for simplicity, the repulsive parameter related to the interaction between two alike DPD particles (H-H, T-T, W-W, and H-W) is treated the same, while the parameter related to the interaction between the hydrophilic and hydrophobic particles (H-T and T-W) is made larger than the repulsion parameter between two similar particles, which ensures that the hydrophobic tails of amphiphilic molecules are sufficiently shielded from the hydrophilic head and solvent. Various morphologies, such as spherical and cylindrical micelles, toroids, bilayers, and vesicles, have been observed depending on the selectivity of solvents, amphiphilic concentration, and the structure of the amphiphilic molecules [16]. A selection of vesicle shapes obtained from the DPD simulations is displayed in Fig. 2.

By adding a bond-bending potential to the hydrophobic tails, a rod-coil amphiphilic molecule can be modeled. Based on the functionality of the rigid-rod blocks, there is growing interest in amphiphilic systems with rod-coil structures, and a number of intriguing phases, including wavy lamellae, zigzags, and hollow spherical micelles, have been observed through self-assembly from DPD simulations [17]. These simulations have shown the applicability of DPD method to study the self-assembly process of amphiphilic systems.

Blood Flow

Blood is primarily composed of microscopic cellular particles such as red blood cells (RBCs), leukocytes, and platelets. The most abundant cells in vertebrate blood are RBCs. A human RBC is a nucleus-free cell with a biconcave shape when not subject to any external stress and is approximately 8.0 μm in diameter and 2.0 μm in thickness. The RBC membrane consists of a lipid bilayer supported by an attached spectrin-based cytoskeleton, and its extreme deformability allows the RBC to squeeze without any damage when passing through narrow capillaries in microcirculation. A multiscale RBC (MS-RBC) model [18], which is based on spectrin-level RBC model [19], has been developed for blood simulations.

In the MS-RBC model, the membrane of RBC is represented by a two-dimensional triangulated network with a collection of DPD particles, while
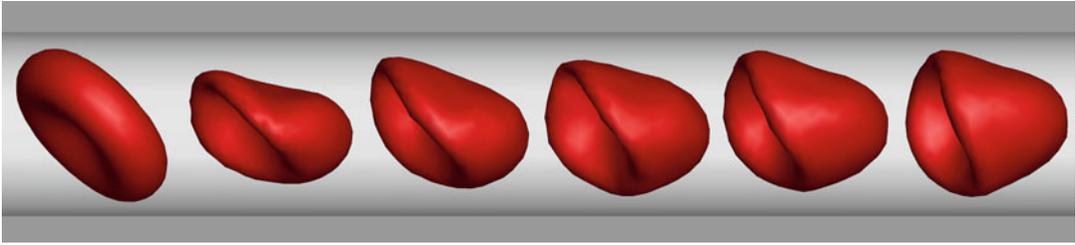
Dissipative Particle Dynamics, Overview, Fig. 3 Sequence of RBC shapes from biconcave to parachute in Poiseuille flow in tube

constraints on the area and volume conservation of RBC are imposed to mimic the area-preserving lipid bilayer and the incompressible interior fluid. The RBC membrane interacts with the fluid particles through DPD forces, and the temperature of the system is controlled through the DPD thermostat. The internal and external fluids are modeled by collections of free DPD particles, and their separation is enforced by bounce-back reflections of these particles at the RBC membrane surface. The MS-RBC has been successfully applied in RBC simulations, such as RBC dynamics in Poiseuille flow (see Fig. 3), RBC thermal fluctuations, and RBCs in diseases like malaria and sickle cell anemia [20].

Outlook

As a coarse-grained molecular dynamics method, dissipative particle dynamics has been demonstrated to be a promising mesoscopic method for simulating the dynamic and rheological properties of simple and complex fluids. The classical DPD method and its extended models have already been applied successfully to a wide variety of phenomena occurring at the mesoscales. However, there remain many open questions both with regard to the foundations of the method and in various applications. For example, the issue of memory effects and the scaling up of DPD in even bigger spatiotemporal scales are two important open questions.

Cross-References

- ▶ Computer Modeling and Simulation of Materials
- ▶ Mesoscopic Modeling
- ▶ Multiscale Modeling

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