

A simulation model for amphiphilic molecules in a mesoscale solvent

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Abstract

We present a stochastic rotation dynamics model of amphiphilic molecules. Vesicle formation of amphiphilic molecules in a thermal fluctuating fluid is demonstrated in this paper. In the model, the interaction of amphiphilic molecules is represented by Lennard–Jones potentials, and stochastic rotation dynamics [T. Ihle, D.M. Kroll, Stochastic rotation dynamics: A Galilean-invariant mesoscopic model for fluid flow, *Phys. Rev. E* 63 (2001) 020201(R)] of mesoscopic particles has been adopted to reproduce the correct hydrodynamics of solvent fluids at the macroscopic scale. The amphiphilic molecules and the solvent particles interact via Boltzmann sampling of a color potential as suggested in a previous paper [Y. Inoue, Y. Chen, H. Ohashi, A mesoscopic simulation model for immiscible multiphase fluids, *J. Comput. Phys.* 201 (2004) 191] to reproduce a phase separation between hydrophobic atoms and solvent fluids.

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1. Introduction

A vesicle is a spherical closed bilayer formed by amphiphilic molecules. Investigations of both vesicles and their dynamics are important for our understanding of biology because vesicles can be regarded as a simple cellular model in biological systems.

A large variety of simulation models which reproduce the self-assembly of vesicles has been developed. Noguchi and Takasu [3] have shown Brownian dynamics (BD) simulations of amphiphilic particles self-assembling into a vesicle without solvent particles, where the amphiphilic particle consists of one hydrophilic particle and two hydrophobic particles. They defined a multi-body potential energy between hydrophobic parts to mimic the so-called hydrophobic effect. However, because of the lack of the explicit solvent, the BD model may not capture how hydrodynamics affects the macroscopic dynamics of amphiphilic molecules. Yamamoto et al. [4] have developed a dissipative particle dynamics (DPD) model of amphiphilic molecules, in which the DPD amphiphilic molecules can spontaneously assemble into a vesicle when suspended amongst explicit solvent particles. Since DPD features

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a soft repulsive force between particles, one can use a relatively large time step compared to that used in molecular dynamics simulations. Thus, DPD can access the hydrodynamic regime but is restricted to small simulation boxes due to the high computational cost. A more realistic molecular model, but still at the mesoscale, has been suggested by Marrink and Mark [5], in which DPPC lipids are represented by twelve coarse-grained atoms and the water molecules are represented by single coarse-grained atoms. Their result of the electron density distribution measured along the bilayer normal quantitatively agrees with those obtained by atomistic molecular dynamics simulations; coarse-grained DPPC showed spontaneous aggregation into vesicles.

All the models mentioned above can reproduce spontaneous aggregation into a vesicle. However, simulations of dynamics of vesicles with hydrodynamics at the sub-micrometer scale are impossible for BD [3] due to the lack of hydrodynamics, and impracticable for DPD [4] and MD [5] due to the computational costs of the calculations of many solvent particles. Thus, a novel simulation model, which would be capable of simulations of vesicles on long time scales and over long distances, is required.

2. A novel simulation model for amphiphilic molecules in a fluid

2.1. A fluid model

We focus on the dynamics of amphiphilic molecules and vesicles together with their hydrodynamic interactions, such as how amphiphilic molecules aggregate in a flow field or the dynamics of a vesicle in a flow field. While most of the computational time is occupied by the calculation of the motions of solvent particles, we are interested in some of the degrees of freedom of solutes at the micro scale, at which the solutes interact with the dynamics of the solvents, but yet the microscopic details are of less interest. In this case, we require a mesoscopic simulation model of solvent dynamics which is simple and has a much lower cost compared with that of atomistic models, yet still accounts for the dynamics over long times and large distances. One such candidate is stochastic rotation dynamics (SRD) [1]. SRD is an improved version of the Malevanets–Kapral model [6] which satisfies Galilean invariance of macroscopic equations. In the model, the particle dynamics consists of two processes, namely, streaming and collision. In the streaming, the position vector of each particle is shifted through a unit time interval as follows:

$$\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\Delta t. \quad (1)$$

Here $\mathbf{r}_i(t)$ and $\mathbf{v}_i(t)$ are the position and the velocity vectors of particle i at time t . In the collision, the space is divided into a square lattice with links of unit length, and particles exchange their momentum and kinetic energy if they happen to reside in the same lattice cell. The process is formulated as follows:

$$\mathbf{v}_i(t + \Delta t) = \mathbf{V}([\mathbf{r}_i(t)]) + \mathbf{\Omega}(\mathbf{v}_i(t) - \mathbf{V}([\mathbf{r}_i(t)])). \quad (2)$$

Here, $\mathbf{\Omega}$ indicates a rotation matrix for the particle collision and $\mathbf{V}([\mathbf{r}_i(t)])$ is the velocity of the center of mass for those “colliding particles” in the following way. The bracketed vector $[\mathbf{r}_i]$ stands for the integer part of \mathbf{r}_i . Taking the mass of particle i as m_i , $\mathbf{V}([\mathbf{r}_i(t)])$ can be calculated as

$$\mathbf{V}(\mathbf{X}, t) = \frac{1}{M(\mathbf{X}, t)} \sum_i m_i \mathbf{v}_i(t) \delta_{\mathbf{X}[\mathbf{r}_i(t)]}. \quad (3)$$

Here, \mathbf{X} is an arbitrary lattice point vector which only has integer components and we define $\delta_{\mathbf{X}[\mathbf{r}_i(t)]}$ as

$$\delta_{\mathbf{X}[\mathbf{r}_i(t)]} = \prod_{\alpha} \delta_{X_{\alpha}[\mathbf{r}_i(t)]_{\alpha}}. \quad (4)$$

Here, α takes the x -, y -, z -component of the vector, and δ_{ab} indicates the Kronecker delta function, $\delta_{ab} = 1$ ($a = b$); $\delta_{ab} = 0$ ($a \neq b$). The total mass in a lattice cell is

$$M(\mathbf{X}, t) = \sum_i m_i \delta_{\mathbf{X}[\mathbf{r}_i(t)]}. \quad (5)$$

Before the collision step, a random shift of the lattice is implemented. The random shifts reduce multiple correlations between SRD particles and more importantly it makes them independent of an imposed homogenous flow. In this

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