Dynamic Implicit-Solvent Coarse-Grained Models of Lipid Bilayer Membranes : Fluctuating Hydrodynamics Thermostat

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Abstract: We introduce a thermostat based on fluctuating hydrodynamics for dynamic simulations of implicit-solvent coarse-grained models of lipid bilayer membranes. We show our fluctuating hydrodynamics approach captures interesting correlations in the dynamics of lipid bilayer membranes that are missing in simulations performed using standard Langevin dynamics. Our momentum conserving thermostat accounts for solvent mediated momentum transfer by coupling coarse-grained degrees of freedom to stochastic continuum fields that account for both the solvent hydrodynamics and thermal fluctuations. We present both a general framework and specific methods for how to couple the particle and continuum degrees of freedom in a manner both consistent with statistical mechanics and amenable to efficient computational simulation. For self-assembled vesicles, we present results for the diffusivity of lipids and their spatial correlations and make comparisons with the standard Langevin thermostat. We find the fluctuating hydrodynamics yields within the bilayer interesting lipid flow correlations that exhibit vortex-like structures that are similar to those observed in explicit-solvent bilayer simulations. The introduced fluctuating hydrodynamics approach provides powerful new methods for performing dynamical studies using implicit-solvent models.

Many coarse-grained models have been developed for equilibrium studies of lipid bilayer membranes [12–17, 19–21, 23–26]. To achieve in simulations access to length-scales and time-scales difficult to attain in fully atomistic molecular dynamics, these coarse-grained lipid models have been developed to provide a reduced description of the molecular degrees of freedom and often remove entirely representation of the solvent degrees of freedom [14–16, 19, 21, 23, 25]. In such implicit-solvent models, the solvent contributions are treated through effective interaction terms within an effective potential for the free energy. Dynamical processes are then often investigated using Langevin dynamics [15, 16, 21, 23]. However, for many problems this approach is insufficient since it neglects important correlations and dynamic contributions from the momentum transfer that would have occurred through the solvent. To incorporate these effects, we introduce a thermostat based on fluctuating hydrodynamics for dynamic simulations of implicit-solvent coarse-grained models [10]. Our approach couples the coarse-grained degrees of freedom to a stochastic continuum field that accounts for both the solvent hydrodynamics and thermal fluctuations. We present both a general mathematical framework and specific methods for how to couple these different mechanical descriptions in a manner consistent with statistical mechanics and amenable to efficient computational simulation [8, 9, 28]. We remark that in related work further studies using the method in the overdamped regime incorporating shear [28] is being investigated in [27]. For self-assembled vesicles, we present results for dynamical properties of our fluctuating hydrodynamics bilayer model making a particular comparison with the widely used Langevin thermostat. We investigate the diffusivity of lipids within the bilayer and the spatial correlations between the motions of an individual lipid and those of its surrounding neighbors. We then study the pair correlation tensor for the motions of lipids within the bilayer. We find the lipid motions exhibit interesting collective flows with vortex-like structures that appear to be similar to those observed in explicit solvent bilayer simulations [3]. These results demonstrate that our momentum conserving fluctuating hydrodynamics thermostat captures important solvent mediated effects not accounted for in conventional Langevin dynamics. These results further suggest that the introduced fluctuating hydrodynamics methods provide a powerful new approach to extend implicit-solvent coarse-grained models for use in performing studies of dynamical phenomena.

Many implicit-solvent coarse-grained models have been developed for equilibrium studies of lipid bilayer membranes [15–17, 19, 20, 23, 25, 26]. These models capture at different levels of resolution molecular features of lipids. To demonstrate our approach, we shall focus on the specific coarse-grained lipid model developed by Cooke. Kremer, and Deserno [15, 16]. In this model each lipid is represented by three coarse-grained units.

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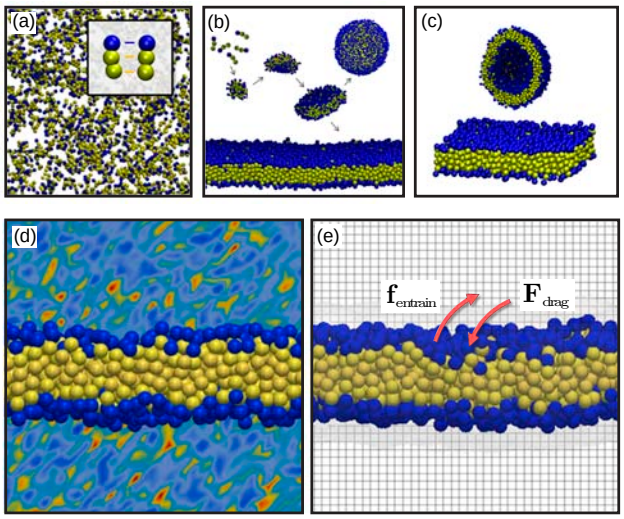

FIG. 1. Implicit-Solvent Coarse-Grained Lipid Model : (a) Individual lipids are modeled by three coarse-grained units that interact to mimic amphiphilic molecules [15]. Starting from a concentrated solution of model lipids, structures are self-assembled. (b) The self-assembly proceeds initially through the formation of aggregates that resemble micelles which subsequently merge into larger disk-like structures. (c) These structures merge further and after reaching a critical size they either orient to span the entire periodic domain as a planar bilayer or wrap spontaneously to form a vesicle. (d) Solvent degrees of freedom are represented by a stochastic velocity field to capture both hydrodynamic momentum transfer and thermal fluctuations. (e) The fluctuating hydrodynamic fields of the solvent are represented on an Eulerian lattice and coupled bidirectionally to the Lagrangian degrees of freedom of the lipids through two interrelated force terms.

The first unit accounts for the polar hydrophilic head group of the lipid and the remaining two units account for the hydrophobic groups along the hydrocarbon tail of the lipid, see Figure 1. An effective interaction potential is developed that takes into account the hydrophobic-hydrophilic effect, excluded volume interactions, and van der Waal's attraction. An important feature is the introduction in the coarse-grained model between the tail units a long-range attractive interaction that also has a broad energy well. This was found to be important to capture the solvent mediated effects that robustly drive bilayer formation while also yielding a fluid phase [15].

Extensive studies have been performed to parameterize this lipid model to obtain reasonable equilibrium properties, such as the bilayer bending elasticity, compression modulus, average area per lipid, and tension [15]. Throughout, we shall use the specific parameterization given in Table I. An important feature of the lipid model is the self-assembly of stable bilayer structures from a solution of lipids. For our studies, we have performed simulations over long trajectories to self-assemble both planar bilayer sheets and vesicles, see Figure 1. In the interest of conciseness in the current presentation of our

Parameter	Description	Value
σ	lipid radius	1.0 nm
ϵ	energy scale	2.5 kJ·M^{-1}
m_0	reference mass	1 amu
w_c	energy potential width	1.2σ
m	lipid mass	720 m_0
τ	time-scale	$\sigma\sqrt{m_0/\epsilon} = 0.6$ ps
k_BT	thermal energy	1.0 ϵ
ρ	solvent mass density	602 m_0/σ^3
μ	solvent viscosity	383 $m_0/\tau\sigma$
Υ	drag coefficient	7210 m_0/τ

TABLE I. Parameterization of the Fluctuating Hydrodynamics Lipid Model

work, we shall focus on the case of vesicle bilayers.

To account for the missing solvent degrees of freedom, we introduce a thermostat based on continuum stochastic fields that incorporate into the dynamics both hydrodynamic momentum transfer and thermal fluctuations. We do this by introducing the fluctuating hydrodynamic equations

$$\rho\frac{d\mathbf{u}}{dt} = \mu\Delta\mathbf{u} - \nabla p + \mathbf{f}_{\text{entrain}} + \mathbf{f}_{\text{thm}} \tag{1}$$

$$\nabla\cdot\mathbf{u} = 0 \tag{2}$$

which are bidirectionally coupled to the coarse-grained particle equations

$$m\frac{d\mathbf{V}}{dt} = \mathbf{F}_{\text{drag}} + \mathbf{F}_{\text{body}} + \mathbf{F}_{\text{thm}} \tag{3}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{V}. \tag{4}$$

The $\mathbf{u}$ denotes the velocity of the solvent fluid and $\mathbf{X}, \mathbf{V}$ denotes the collective positions and velocities of the coarse-grained particles. The p denotes the pressure that imposes the incompressibility of the solvent fluid, $\nabla\cdot\mathbf{u} = 0$. The ρ is the mass density of the solvent, μ is the shear viscosity, and m is the excess mass matrix for the coarse-grained particles. The forces acting on the coarse-grained particles is denoted by $\mathbf{F}_{\text{body}} = -\nabla\Phi$, where $\Phi[\mathbf{X}]$ is the potential energy.

The momentum is transferred from the solvent fluid to the coarse-grained particles through the drag term $\mathbf{F}_{\text{drag}} = -\boldsymbol{\Upsilon}(\mathbf{V} - \Gamma\mathbf{u})$. The momentum is transferred from the coarse-grained particles to the solvent through the fluid entrainment term $\mathbf{f}_{\text{entrain}} = \Lambda[-\mathbf{F}_{\text{drag}}]$. We remark that in principle more detailed descriptions of the momentum transfer between fluids and solid bodies could be used. However, in practice an important consideration motivating our specific choice is that the transfer terms must (i) be amenable to the development of efficient computational methods, and (ii) be amenable to analysis to provide readily a way of introducing thermal fluctuations that yield a well-founded model with respect to statistical mechanics. With this in mind, a number of

additional conditions arise naturally for the operators. First, we require the $\boldsymbol{\Upsilon}$ operator to be positive definite. We take it here simply to be $\boldsymbol{\Upsilon} = \Upsilon\mathcal{I}$, where Υ is a scalar drag coefficient and $\mathcal{I}$ is the identity tensor. We introduce the operator Γ to obtain locally from the solvent momentum field a reference velocity useful in determining the local drag force. We introduce the operator Λ for the drag interaction to model how the equal-and-opposite forces exerted on the solvent molecules are spatially distributed within the solvent-fluid body. Interestingly, an important constraint is that these operators be adjoints $\Gamma = \Lambda^*$. This is required to ensure the dissipation only occurs through the Υ-drag term, and not merely as a consequence of the interconversion of quantities by the operators Γ, Λ, see [8, 22]. For related reasons, these adjoint conditions also prove essential when introducing the thermal fluctuations to greatly simplify the form of the correlations of the stochastic driving fields and the algorithms needed for their computational generation [8].

We account for thermal fluctuations through the stochastic driving fields $\mathbf{f}_{\text{thm}}$ and $\mathbf{F}_{\text{thm}}$. These are taken to be δ-correlated Gaussian random fields with the covariances

$$\left\langle \mathbf{f}_{\text{thm}}(s)\mathbf{f}_{\text{thm}}(t)^T \right\rangle = -2k_BT\left(\mu\Delta - \Lambda\Upsilon\Gamma\right)\delta(t-s) \quad (5)$$

$$\left\langle \mathbf{F}_{\text{thm}}(s)\mathbf{F}_{\text{thm}}(t)^T \right\rangle = 2k_BT\Upsilon\,\delta(t-s) \quad (6)$$

$$\left\langle \mathbf{f}_{\text{thm}}(s)\mathbf{F}_{\text{thm}}(t)^T \right\rangle = -2k_BT\Lambda\Upsilon\,\delta(t-s). \quad (7)$$

Under the rather general conditions we have outlined, the equations 1– 7 can be shown to manifest stochastic dynamics that yield results consistent with equilibrium statistical mechanics [8]. We refer to this general coarse-grained fluctuating hydrodynamics approach and related computational methods as the Stochastic Eulerian Lagrangian Method (SELM).

In the present work, we shall use throughout the following specific coupling operators

$$\Gamma\mathbf{u} = \int_\Omega \eta\left(\mathbf{y} - \mathbf{X}(t)\right)\mathbf{u}(\mathbf{y},t)d\mathbf{y} \quad (8)$$

$$\Lambda\mathbf{F} = \eta\left(\mathbf{x} - \mathbf{X}(t)\right)\mathbf{F}. \quad (9)$$

While other choices are possible, and may be desirable, this approach is based on the Stochastic Immersed Boundary Method [9]. The kernel functions $\eta(\mathbf{z})$ are chosen to be the Peskin δ-Function developed in [22]. This choice is made instead of a Dirac δ-Function to ensure a model in which the mobility of individual particles have a finite effective hydrodynamic radius within the fluid [9]. This choice also has important numerical properties that ensure to a good approximation that there is translational invariance of the coupling despite the breaking of this symmetry by the discretization lattice of the fluid [9, 22]. This specific coupling scheme has been shown to provide a computationally efficient method for obtaining far-field hydrodynamic correlations and has a well-characterized near-field interaction [5–7, 9].

To compare the introduced SELM fluctuating hydrodynamics thermostat with more conventional approaches, we consider the Langevin dynamics in two particular cases. We first consider Langevin dynamics where the drag coefficient Υ is comparable to the Stokes drag of a particle of size σ immersed in water, $\Upsilon = 7210\ m_0/\tau$. We then consider the case corresponding to Langevin simulations often reported in the literature where the drag coefficient is taken artificially small to achieve efficient equilibration and sampling, $\Upsilon = 0.06\ m_0/\tau$ [15, 16]. These two cases provide a useful baseline for comparisons. For the SELM fluctuating hydrodynamics, we shall use throughout the Stokes drag in water for the solvent-lipid coupling strength $\Upsilon = 7210\ m_0/\tau$. For the reference Lennard-Jones units σ, ϵ, m_0, see Table I.

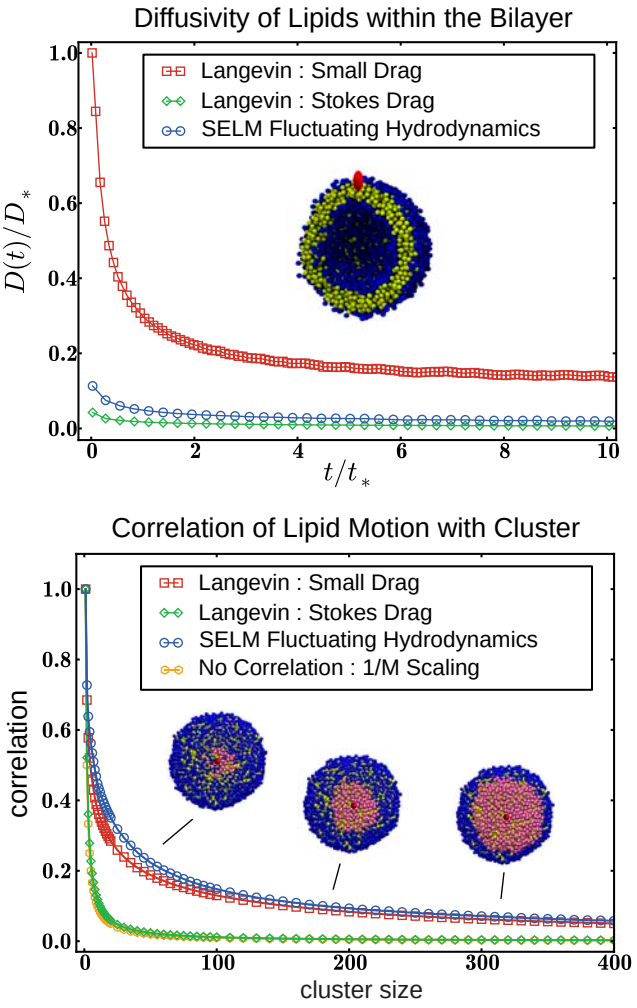

FIG. 2. The diffusivity and correlations of lipids within the vesicle bilayer. While Langevin dynamics with Stokes drag and the SELM fluctuating hydrodynamics exhibit similar lipid diffusivities, the Langevin dynamics with Stokes drag exhibits almost no lateral correlations between lipid motions. Retaining such spatial correlations, even for small lipid diffusivities, is an important consequence of the momentum conservation of the SELM fluctuating hydrodynamics thermostat.

We first study the diffusivity of individual lipids within the bilayer. We define the time-dependent diffusivity as $D(t) = \langle(\mathbf{X}(t)-\mathbf{X}(0))^2\rangle/t$ and non-dimensionalize by the small drag Langevin diffusivity $D_*(0) = 5.58\times10^{-3}\sigma^2/\tau$ and time-scale $t_* = \sigma^2/D_*(0) = 179.28\tau$. We find the SELM fluctuating hydrodynamics thermostat exhibits a diffusivity comparable but larger than the Langevin dynamics with Stokes drag, see Figure 2. For the SELM diffusivity we attribute this to two related mechanisms that reduce relative to the Langevin dynamics the dissipation associated with the collective internal rearrangement modes of the lipids within the bilayer. The first is the local conservation of momentum that transmits momentum between lipids inducing local correlations and flows. The second is that the drag force acting on lipids depends only on the relative difference in velocity between the hydrodynamic field and the lipids. This allows for more coordinated motions and rearrangements of the lipids and the fluid body that are ultimately less dissipative. In contrast, for the Langevin dynamics the fluid is treated as a fixed undeformable ambient medium to which momentum is ceded. Interestingly, this result is somewhat in opposition to the alternative intuition that might have predicted the diffusivity under SELM dynamics would be smaller than the Langevin dynamics with Stokes drag as a consequence of the hydrodynamics contributing additional local correlations requiring larger-scale collective motions.

We investigate this effect by considering the spatial correlations between the motions of an individual lipid and those in a surrounding patch of lipids in its neighborhood. We consider the displacements $\Delta_0 X$ of a given reference lipid over a time δt and its correlation with the displacement $\Delta_M X$ of the center-of-mass of a patch consisting of the M nearest neighbors. We define the lipid-patch correlation as $c_M = \langle\Delta_0 X \Delta_M X\rangle / \langle\Delta_0 X^2\rangle$. For lipids that diffuse with only short-ranged correlations, we expect as a base-line for the correlation to decay in M like $c_M \sim 1/M$, see Figure 2. For the Langevin dynamics with Stokes drag we find there are no significant spatial correlations and the predicted scaling $\sim 1/M$. Interestingly, for the Langevin dynamics with small drag we do find significant spatial correlations. In this regime, this is explained by the significant inertial effects that allow for momentum to be transferred through multiple collisions between lipids before being suppressed. This is in stark contrast to the case with Stokes drag where inertial effects are strongly suppressed. Importantly, for the SELM fluctuating hydrodynamics that use the same Stokes drag coefficient, the long-range spatial correlations persist. We attribute this to momentum conservation of the SELM fluctuating hydrodynamics thermostat. For the SELM dynamics, the drag does not result in any net loss of momentum, instead momentum is only transferred between the lipid degrees of freedom to the continuum solvent degrees of freedom. The momentum in the hydrodynamic fields then facilitates lateral transfer between lipids over a long-range.

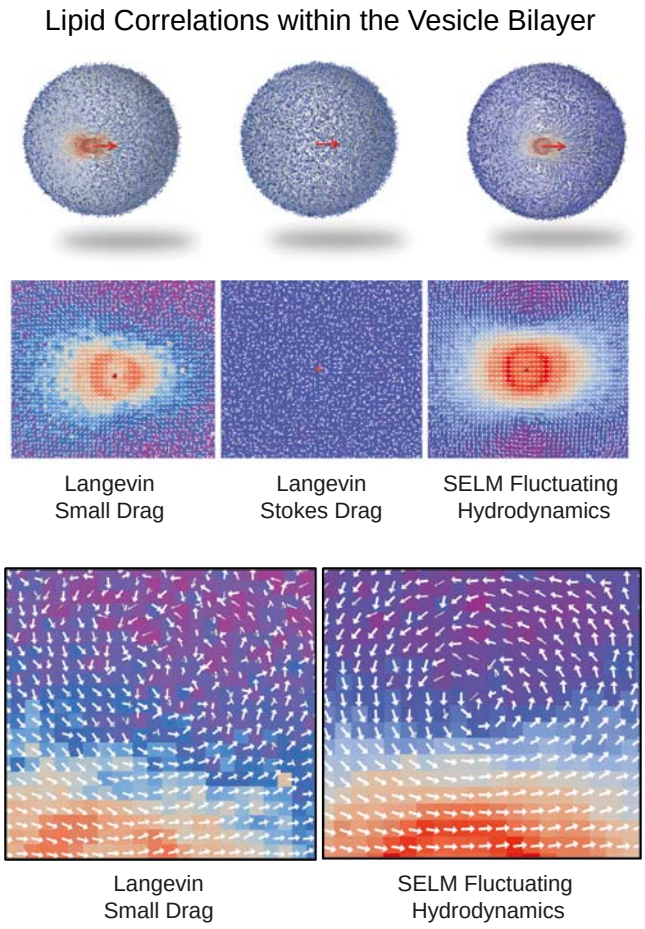

FIG. 3. Lipid flow correlations $\mathbf{w} = \Psi\mathbf{e}_1$ under Langevin dynamics with small drag $\Upsilon = 0.06\ m_0/\tau$, Langevin with Stokes drag $\Upsilon = 7210\ m_0/\tau$, and SELM Fluctuating Hydrodynamics with $\Upsilon = 7210\ m_0/\tau$. The Langevin dynamics with small drag and the SELM Fluctuating Hydrodynamics exhibit vortex-like structures similar to those in explicit-solvent lipid models [3]. In the color map, red indicates flow to the right and purple indicates flow to the left.

To characterize in more detail the lipid spatial correlations, we consider the pair correlation tensor $\Psi(\mathbf{r}) = \langle\Delta_{\mathbf{r}} X \Delta_0 X^T\rangle$. In this notation, the displacements ΔX are taken over the time δt. The subscript $\mathbf{r}$ specifies the displacement vector from the center-of-mass of a reference lipid to the center-of-mass of a second lipid within the bilayer. The vector field $\mathbf{w} = \Psi\mathbf{e}_1$ provides by linear response theory a characterization of the flow of lipids within the bilayer in response to an impulse force in the $\mathbf{e}_1 = (1,0,0)$ direction [11], see Figure 3.

For the Langevin dynamics with Stokes drag the strong suppression of lateral transfer of momentum between lipids yields no discernible lipid flow structures. Interestingly, we find that both the Langevin dynamics with small drag and SELM fluctuating hydrodynamics exhibit significant lipid flow structures. For the SELM fluctuating hydrodynamics, the particular vortex-like flow struc-

ture exhibited is very similar to those that have been observed in explicitly solvated simulations of lipid bilayers, see [3, 18]. Similar lipid flows and spatial correlations have also been offered as an explanation for some results seen in recent neutron scattering experiments [4]. To obtain realistic results for the collective motions of lipids within the bilayer, these results strongly indicate the importance of the thermostat used.

In summary, we have introduced an approach based on fluctuating hydrodynamics to obtain a momentum conserving thermostat for dynamical studies using implicit-solvent coarse-grained models. We have shown that our SELM fluctuating hydrodynamics lipid model yields bilayer dynamics that differ markedly from conventional Langevin dynamics. We have shown that hydrodynamics and momentum conservation play key roles in producing spatial correlations between lipids within the bilayer. In contrast, the non-hydrodynamic Langevin dynamics suppresses these effects. For diffusion within the vesicle bilayer, we have shown the SELM fluctuating hydrodynamics produces interesting vortex-like lipid flows similar to those seen in previous explicit-solvent simulations and in signatures of recent neutron scattering experiments [3, 4, 18]. The results we report indicate that the introduced fluctuating hydrodynamics methods provide a promising set of new approaches for extending implicit-solvent lipid models for studies of dynamical phenomena within lipid bilayer membranes.

Software: For simulations using the SELM fluctuating hydrodynamics thermostat, the software package Mango-Selm is available at `http://mango-selm.org/`.

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