Self-Assembled Lipid Bilayer Membranes: Exploring a Single-Bead Model

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Motivations

- **Kinetics** of lipid bilayer membranes are important in many biological processes.
  - raft formation
  - budding
  - endocytosis
- **Coarse-grained models** allow for computational efficiency for practical investigations.
- **Highly tunable models** allow for the exploration of different phases and kinetic regimes.
- **Many types** of coarse-grained models
  - represent atomic groups as CG units.
  - represent several lipid molecules as one bead.
  - implicitly handle solvent degrees of freedom.

Pairwise Potential Function

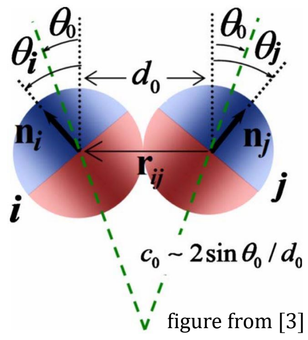


figure from [3]

Overview

- Particle separation and relative orientation dictate interaction.
- Soft-Sphere potential used for translational separation.

Interaction Potentials

$$U(\mathbf{r}_{ij},\mathbf{n}_i,\mathbf{n}_j) = \begin{cases} u_R(r) + [1-\phi(\hat{\mathbf{r}}_{ij},\mathbf{n}_i,\mathbf{n}_j)]\epsilon, & r < r_{\min} \\ u_A(r)\phi(\hat{\mathbf{r}}_{ij},\mathbf{n}_i,\mathbf{n}_j), & r_{\min} < r < r_c \end{cases}$$

$$u(r) = \begin{cases} u_R(r) = \epsilon\left[\left(\frac{r_{\min}}{r}\right)^4 - 2\left(\frac{r_{\min}}{r}\right)^2\right], & r < r_{\min} \\ u_A(r) = -\epsilon\cos^{2\zeta}\left[\frac{\pi}{2}\frac{(r-r_{\min})}{(r_c-r_{\min})}\right], & r_{\min} < r < r_c \end{cases}$$

$$a = (\mathbf{n}_i \times \hat{\mathbf{r}}_{ij}) \cdot (\mathbf{n}_j \times \hat{\mathbf{r}}_{ij}) + \sin\theta_0(\mathbf{n}_j - \mathbf{n}_i)\cdot\hat{\mathbf{r}}_{ij} - \sin^2\theta_0$$

$$\phi = 1 + \mu[a(\hat{\mathbf{r}}_{ij},\mathbf{n}_i,\mathbf{n}_j) - 1]$$

More details in [1,2].

Langevin Dynamics

In order to run simulations in the canonical ensemble (NVT), modified equations of motion are used.

Langevin Equations

$$m\ddot{\mathbf{r}} = -\nabla_r U - \zeta_r\dot{\mathbf{r}} + \mathbf{F}_r(t)$$
$$I\ddot{\mathbf{n}} = -\nabla_n U - \zeta_n\dot{\mathbf{n}} + \mathbf{F}_n(t)$$

$$< \mathbf{F}_r(t)\mathbf{F}_r(t') > = 2k_BT\zeta_r\delta(t-t')$$
$$< \mathbf{F}_n(t)\mathbf{F}_n(t') > = 2k_BT\zeta_n\delta(t-t')$$

- Each particle experiences a stochastic force.
  - Random noise from the implicit solvent.
- The stochastic force is proportional to temperature and drag coefficient.

Velocity Verlet Integration Scheme

Translation:
$$\begin{cases} \mathbf{v}^{n+\frac{1}{2}} = \mathbf{v}^n + \frac{\Delta t}{2}\mathbf{a}^n \\ \mathbf{r}^{n+1} = \mathbf{r}^n + \Delta t\mathbf{v}^{n+\frac{1}{2}} \end{cases}$$

Rotation:
$$\begin{cases} \mathbf{l}^{n+\frac{1}{2}} = \mathbf{l}^n + \frac{\Delta t}{2}\boldsymbol{\tau}^n \\ \mathbf{l}^{n+\frac{1}{2}} \to \boldsymbol{\omega}^{n+\frac{1}{2}}, \quad \mathbf{q}^n \to \hat{\mathbf{n}}^n \\ \hat{\mathbf{n}}^{*,n+1} = \hat{\mathbf{n}}^n + \Delta t\boldsymbol{\omega}^{n+\frac{1}{2}}, \quad \hat{\mathbf{n}}^{n+1} = \frac{\hat{\mathbf{n}}^{*,n+1}}{|\hat{\mathbf{n}}^{*,n+1}|} \\ \hat{\mathbf{n}}^{n+1} \to \mathbf{q}^{n+1} \end{cases}$$

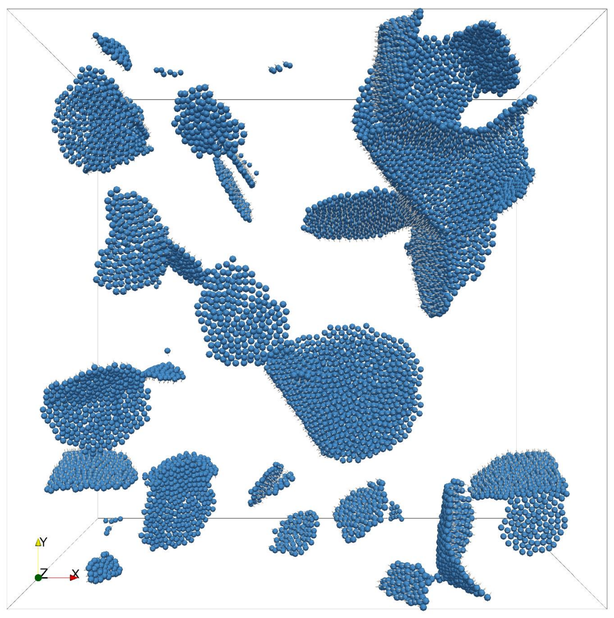
Forces are then recalculated on each particle, and the final velocity and angular velocity vectors are calculated with

$$\begin{cases} \mathbf{v}^{n+1} = \mathbf{v}^{n+\frac{1}{2}} + \frac{\Delta t}{2}\mathbf{a}^{n+1} \\ \mathbf{l}^{n+1} = \mathbf{l}^{n+\frac{1}{2}} + \frac{\Delta t}{2}\boldsymbol{\tau}^{n+1} \end{cases}$$

Global error for position and velocity is $O(\Delta t^2)$.

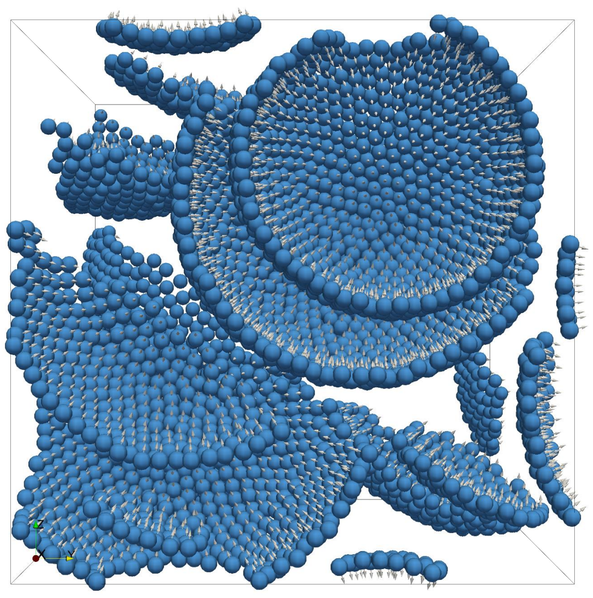
Self-Assembling Sheets and Vesicles

Sheets



- Sheets bend due to thermal forces and the edge effect
- Over time, sheets coalesce to form larger sheets

Spherical Vesicles (imposed curvature)



Parametrization

Potential Parameters

r_c: interaction cutoff distance
μ: penalty for non-preferred orientation
ζ: steepness of repulsive branch
θ_0: preferred relative orientation

Simulation Parameters

$\zeta_{r,n}$: dampening coefficients for Langevin Equation
Δt: timestep for simulation
k_BT: temperature of system

Reduced Units

To keep all quantities in a reasonable numerical range, all values computed are unitless, and are given in terms of combinations of three physical scales. Units can be found by picking values for these characteristic scales.

ϵ: energy
σ: length
m: mass of a bead

Summary and References

Summary

- Implemented model and Velocity Verlet integrator for orientations in LAMMPS.
- Self-assembling sheets in large parameter ranges.
- Forced spherical vesicle formation.
- Checking consistency between Nose-Hoover thermostat and Langevin equation for canonical ensemble simulations.
- Exploring properties of spherical vesicles.

References

1. **Computer Simulations of Self-Assembled Membranes**, J.-M. Drouffe, A. C. Maggs and S. Leibler, Science, (1991).
2. **Fluid Membranes Can Drive Linear Aggregation of Adsorbed Spherical Nanoparticles,** An'ela S˘aric´ and Angelo Cacciuto, Phys. Rev. E., (2012).
3. **One-particle-thick, Solvent-free, Course-grained Model for Biological and Biomimetic Fluid Membranes,** Hongyan Yuan, Changjin Huang, Ju Li, George Lykotrafitis, and Sulin Zhang, Phys. Rev. E, (2010).

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