Randomly Triangulated Surfaces as Models for Fluid and Crystalline Membranes

G. Gompper

Institut für Festkörperforschung, Forschungszentrum Jülich
Motivation: Endo- and Exocytosis

Membrane transport of macromolecules and particles:

- endocytosis
- and
- exocytosis
Clathrin-Mediated Endocytosis

Endocytosis in cells is controlled adsorption of clathrin proteins:

Clathrin triskelions form hexagonal networks:

ph-Induced Budding: Microcages

Figure 4: A clathrin network initially at neutral pH is acidified to pH 5.5-6.0, resulting in the formation of "microcages," which are devoid of cell membrane and inhibit endocytosis. Bar, 0.2 μm. Reproduced from Heuser (1989) by permission of The Rockefeller University Press.
Shape of fluid membranes is controlled by curvature energy:

$$\mathcal{H}_l = \int dS \left\{ \frac{\kappa}{2} \left( \frac{1}{R_1} + \frac{1}{R_2} - C_0 \right)^2 + \bar{\kappa} \frac{1}{R_1 R_2} \right\}$$

- $\kappa$: bending rigidity
- $\bar{\kappa}$: saddle-splay modulus
- $C_0$: spontaneous curvature

**Domain-Induced Budding in Fluid Membranes**

Consider a domain of component $A$ with radius $R$ in a membrane of component $B$. Two components are characterized by spontaneous (or preferred) curvatures $C_A$ and $C_B$.

The domain boundary has line tension $\lambda$.

\[
\mathcal{H} = \frac{\kappa_A}{2} \int_A dS (H - C_A)^2 + \frac{\kappa_B}{2} \int_B dS (H - C_B)^2 + \lambda \oint ds
\]

Budding:

\[
\frac{\lambda R}{\kappa} + 2C_AR = 4
\]

Budding of Crystalline Domains

Main new feature compared to fluid domains: in-plane shear elasticity
long-range crystalline order

Formation of bud requires crystal defects: five-fold disclinations
Questions

• How are topological defects (disclinations) generated?
  – interior acquisition: dislocation unbinding inside domain
  – exterior acquisition: disclinations enter from boundary

• Location of budding transition $C_0(R), \lambda(R)$?
Simulations of Membranes

Modelling of membranes on different length scales:

- (a) Atomistic
- (b) Coarse-grained
- (c) Solvent-free
- (d) Triangulated
Simulations of Membranes

Dynamically triangulated surfaces

Hard-core diameter $\sigma$
Tether length $L: \sigma < L < \sqrt{3}\sigma$

$\rightarrow$ self-avoidance

Dynamic triangulation:

Phase Behavior of Planar Network Models

Only parameter: Tether length $\ell_0$ controls in-plane density

$\ell_0/\sigma = 1.53$

$\ell_0/\sigma = 1.55$

Budding of Crystalline Domains: Vesicles Shapes

Shapes for fixed spontaneous curvature and increasing line tension $\lambda$:

$\lambda/k_B T = 1.5$  $\lambda/k_B T = 3.0$  $\lambda/k_B T = 5.0$

Phase Behavior for Crystalline Domains

Length of domain boundary:

\[ N_A = 92 \]

\[ N_A = 184 \]

Phase Behavior for Crystalline Domains

Construct phase diagram:

\[ \frac{\lambda}{\kappa} R + \gamma_0 C_0 R = \Gamma(R) \]

with \( \gamma_0 = 0.84 \) and

<table>
<thead>
<tr>
<th>( \Gamma(R) )</th>
<th>( N )</th>
<th>( R/\sigma )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.39 ± 0.02</td>
<td>92</td>
<td>6.18</td>
</tr>
<tr>
<td>3.45 ± 0.03</td>
<td>184</td>
<td>8.74</td>
</tr>
<tr>
<td>3.68 ± 0.05</td>
<td>368</td>
<td>12.4</td>
</tr>
</tbody>
</table>
Defects in Flexible Membranes: Buckling

For flexible membranes, buckling reduces elastic energy.

Fivefold disclinations: \((s = 2\pi/6)\)

Stretching

\[ E_s = \frac{1}{32\pi} K_0 s^2 R^2 \]

Buckling

\[ E_b = s\kappa \ln(R/a) \]

Buckling favorable for \(R\) larger than bucking radius

\[ R_b = 10 \left( \frac{\kappa}{K_0 s} \right)^{1/2} \]

Scaling Arguments

Four regimes can be distinguished for increasing $R$:

- Spherical: \( \Gamma(R) = 4 + K_0 R^2 / \kappa \ < 8 \)
- Cone-like corners: \( \Gamma(R) \sim \ln(R/a) \)
- Deformed icosahedron: \( \Gamma(R) \sim R^{1/3} \)
- Hexatic phase: \( \Gamma(R) \sim \ln(R/a) \)

Conclusion:

- Budding of crystalline domains qualitatively different than for fluid domains!

Bud Formation Dynamics

(Top view — embedding fluid membrane not shown)

0.1 million MCS  
0.5 million MCS  
2.0 million MCS

- Defects are generated at boundary, diffuse into interior
Formation of Microcages

Quench to state of high spontaneous curvature with high Young modulus:

Budding of crystalline domains in fluid membranes:

- Defects generated at domain boundary, diffuse into interior.
- Line tension $\lambda$, spontaneous curvature $C_0$ monotonically decreasing with domain size $R$.

In the clathrin-controlled budding in cells, many other proteins are involved. What are their roles in the physical mechanism described above?
Flexible Crystalline Vesicles

Defect Scars on Flexible Crystalline Vesicles
Defects on Crystalline Vesicles

**Spherical surfaces:**
Grain boundaries of finite length form to screen long-range deformation field of disclinations

Scar length increases *linearly* with sphere radius $R$

---

Bowick, Nelson, Travesset, Phys. Rev. B (2000);


What happens on *flexible* surfaces ??
Defects on Crystalline Vesicles

Flexible surfaces *without* defects:
Faceting with increasing Föppl-von Kármán number $\gamma = K_0 R^2 / \kappa$

Lobkovsky et al., Science 270 (1995);

Flexible surfaces *with* defects:

- Faceting still exists
- Defect scars get localized for “large” $\gamma$
- Scars get fuzzy at finite temperatures

Defects on Crystalline Vesicles

- Defect scars screen deformation field on surfaces of non-zero Gaussian curvature
- Gaussian curvature localized near corners, with curvature radius $R_b$
- Implies scaling of scar length $L/R$ with $R/R_b$

Hydrodynamics of Membranes and Vesicles
Soft Matter Hydrodynamics

- Vesicles and red blood cells in capillaries and microvessels:

Diseases such as diabetes reduce deformability of red blood cells!
Mesoscale Flow Simulations

Complex fluids: length- and time-scale gap between

- atomistic scale of solvent
- mesoscopic scale of dispersed particles (colloids, polymers, membranes)

→ Mesoscale Simulation Techniques

Basic idea:

- drastically simplify dynamics on molecular scale
- respect conservation laws for mass, momentum, energy

Examples:

- Lattice Boltzmann Method (LBM)
- Dissipative Particle Dynamics (DPD)
- Multi-Particle-Collision Dynamics (MPCD)

Alternative approach: Hydrodynamic interactions via Oseen tensor
Multi-Particle-Collision Dynamics (MPCD)

- coarse grained fluid
- point particles
- off-lattice method
- collisions inside “cells”
- thermal fluctuations

Mesoscale Flow Simulations: MPCD

Flow dynamics: Two step process

Streaming

- ballistic motion
  \[ \mathbf{r}_i(t + h) = \mathbf{r}_i(t) + \mathbf{v}_i(t)h \]

Collision

- mean velocity per cell
  \[ \bar{\mathbf{v}}_i(t) = \frac{1}{n_i} \sum_{j \in C_i} n_j \mathbf{v}_j(t) \]

- rotation of relative velocity by angle \( \alpha \)
  \[ \mathbf{v'}_i = \bar{\mathbf{v}}_i + D(\alpha)(\mathbf{v}_i - \bar{\mathbf{v}}_i) \]
Mesoscale Flow Simulations: MPCD

- Lattice of collision cells: breakdown of Galilean invariance
- Restore Galilean invariance exactly: random shifts of cell lattice

Kinematic viscosity $\nu = \eta/\rho$:

$$\nu_{\text{kin}} = \frac{k_B T h}{a^3} \left[ \frac{5\rho}{\rho - 1} f(\alpha) - \frac{1}{2} \right]$$

$$\nu_{\text{coll}} = \frac{1 - \cos(\alpha)}{18ha} \left( 1 - \frac{1}{\rho} \right)$$


Membrane Hydrodynamics

Interaction between membrane and fluid:

- **Streaming step:**
  bounce-back scattering of solvent particles on triangles

- **Collision step:**
  membrane vertices are included in MPCD collisions

implies *no-slip boundary conditions*.

Membrane Hydrodynamics

Vesicle and Cells in Capillary Flow
Capillary Flow: Fluid Vesicles

- small flow velocities: vesicle axis perpendicular to capillary axis → no axial symmetry!
- discocyte-to-prolate transition with increasing flow

Capillary Flow: Red Blood Cells

- Spectrin network induces shear elasticity $\mu$ of composite membrane
- Elastic parameters: $\kappa/k_B T = 50$, $\mu R_0^2/k_B T = 5000$
Capillary Flow: Elastic Vesicles

Elastic vesicle:
- curvature and shear elasticity
- model for red blood cells

Tsukada et al., Microvasc. Res. 61 (2001)
Capillary Flow: Elastic Vesicles

Shear elasticity suppresses prolate shapes (large deformations)

Flow velocity at discocyte-to-parachute transition

Implies for RBCs: $v_{trans} \simeq 0.2 \, \text{mm/s}$ for $R_{cap} = 4.6 \, \mu\text{m}$
Physiological conditions:
Hematocrit $H_T = 0.45$ — volume fraction of RBCs

Therefore: Hydrodynamic interaction between RBCs very important

First step: Investigate 3 RBCs at low $H_T$. 

Outlook
Summary

- **Mesoscale simulation techniques** are powerful tool to bridge the length- and time-scale gap in complex fluids

- Multi-particle-collision dynamics well suited for hydrodynamics of **embedded particles**: membranes, colloids, polymers

- **Vesicles in flow**: parachute shapes, hydrodynamic interactions