Randomly Triangulated Surfaces as Models for Fluid and Crystalline Membranes

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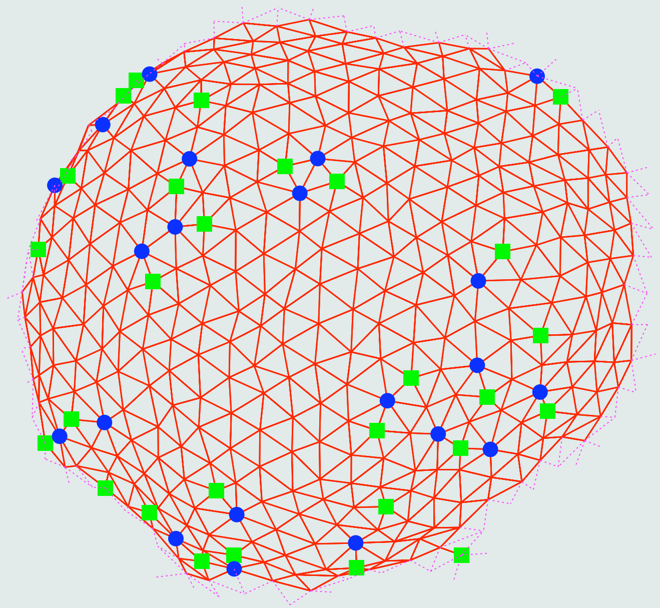


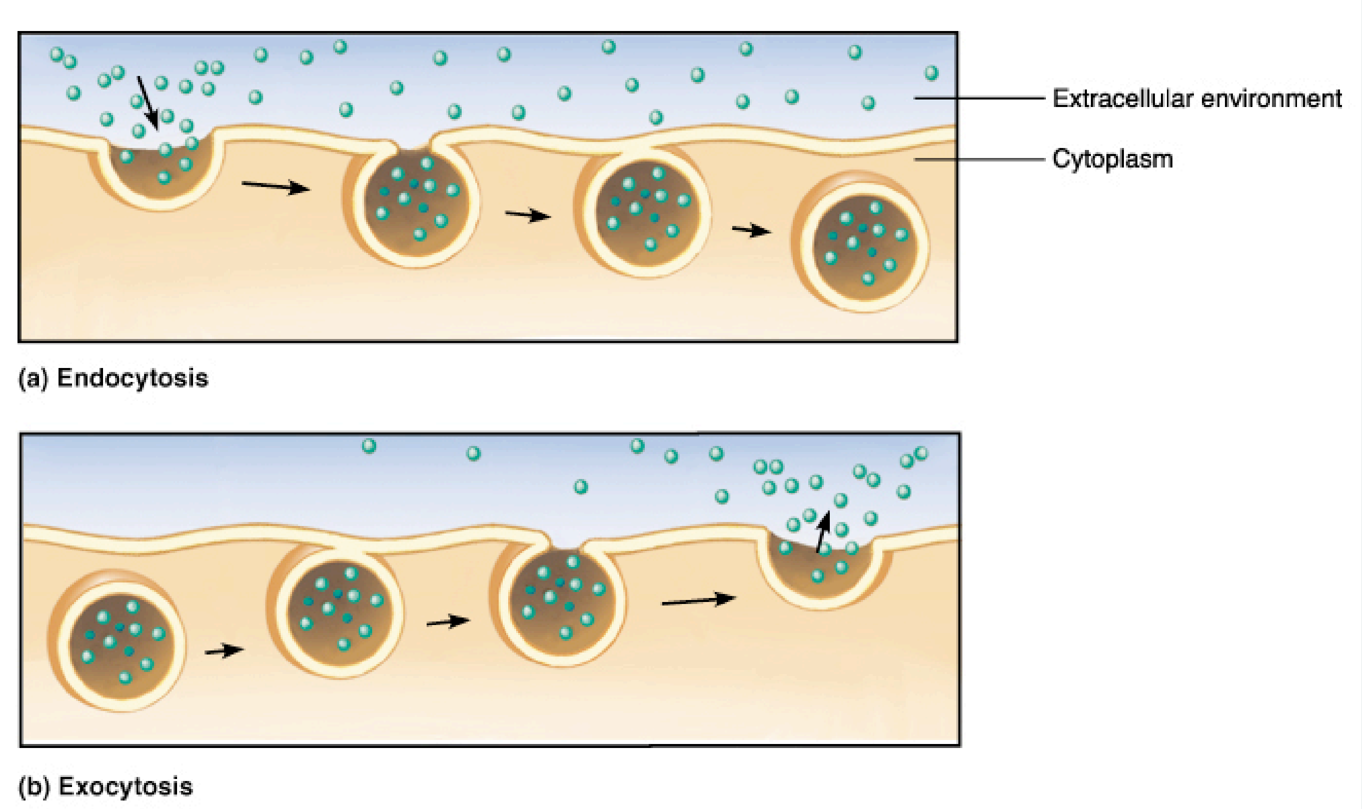
Motivation: Endo- and Exocytosis

Membrane transport of macromolecules and particles:

endocytosis

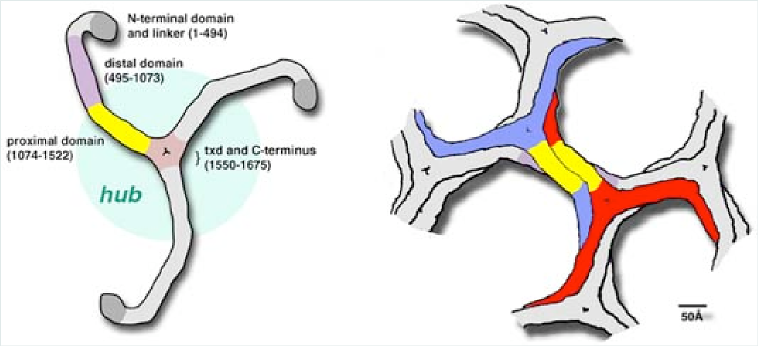
and

exocytosis

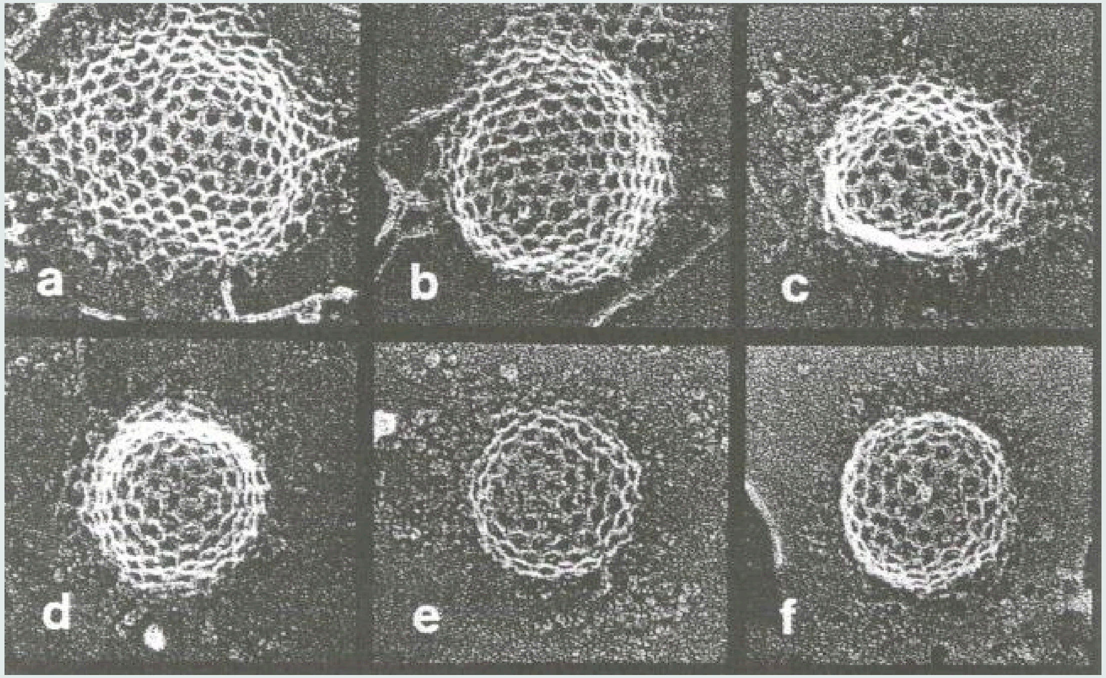


Clathrin-Mediated Endocytosis

Endocytosis in cells is controlled adsorption of clathrin proteins:



Clathrin triskelions form hexagonal networks:



Heuser, J. Cell Biol. (1989)

ph-Induced Budding: Microcages

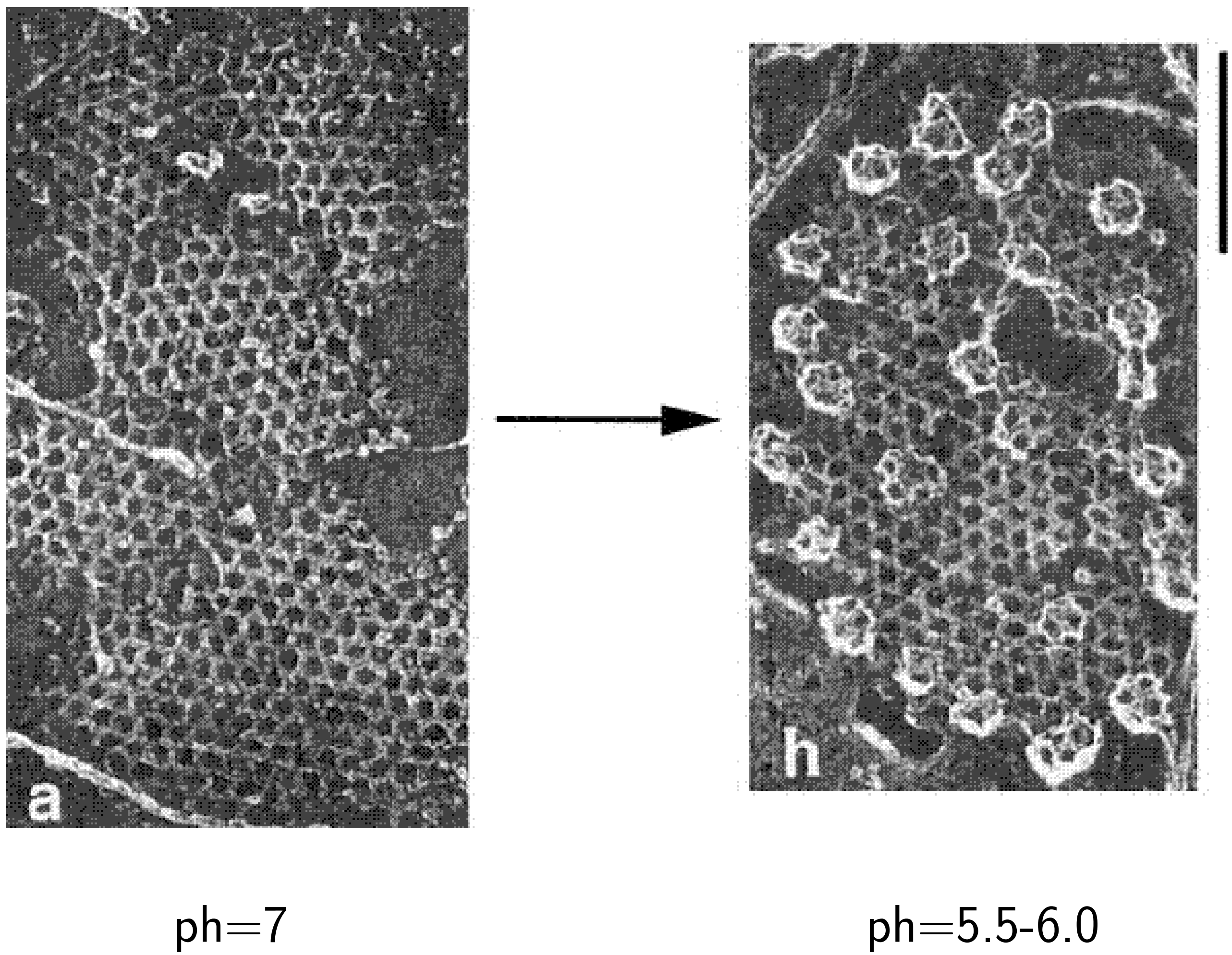
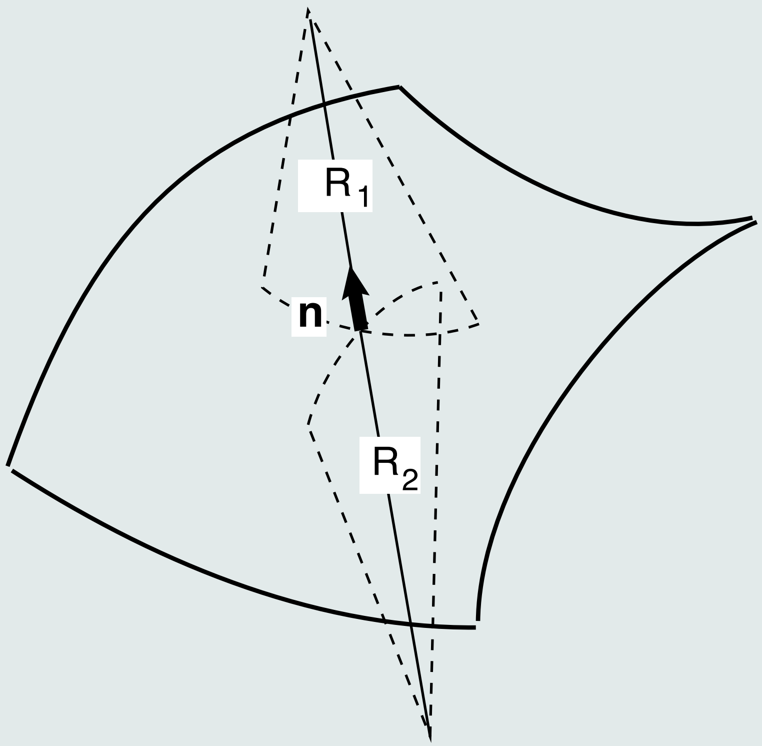


FIGURE 4 A clathrin network initially at neutral pH is acidified to pH 5.5–6.0, resulting in the formation of “microcages,” which are devoid of cell membrane and inhibit endocytosis. Bar, 0.2 μm. Reproduced from Heuser (1989) by permission of The Rockefeller University Press.

Fluid Membranes: Curvature Elasticity

Shape of fluid membranes is controlled by curvature energy:

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



κ: bending rigidity

$\bar{\kappa}$: saddle-splay modulus

C_0: spontaneous curvature

Canham, J. Theor. Biol. (1970); Helfrich, Z. Naturforsch. (1973)

Domain-Induced Budding in Fluid Membranes

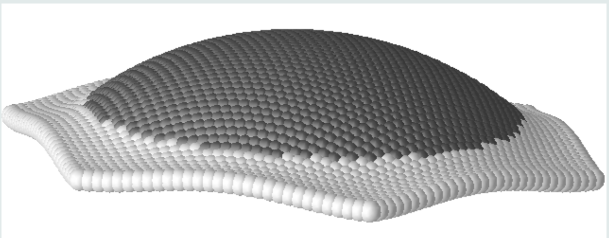
Consider a domain of component A with radius R in a membrane of component B.

Two components are characterized by spontaneous (or preferred) curvatures C_A and C_B.

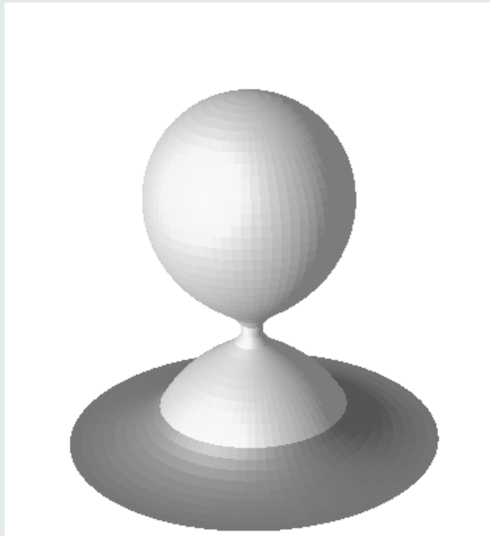
The domain boundary has line tension λ.

$$\mathcal{H} = \frac{\kappa_A}{2}\int_{\mathcal{A}} dS\,(H - C_A)^2 + \frac{\kappa_B}{2}\int_{\mathcal{B}} dS\,(H - C_B)^2 + \lambda\oint ds$$

Budding:



$\longrightarrow$



$$\frac{\lambda R}{\kappa} + 2C_A R = 4$$

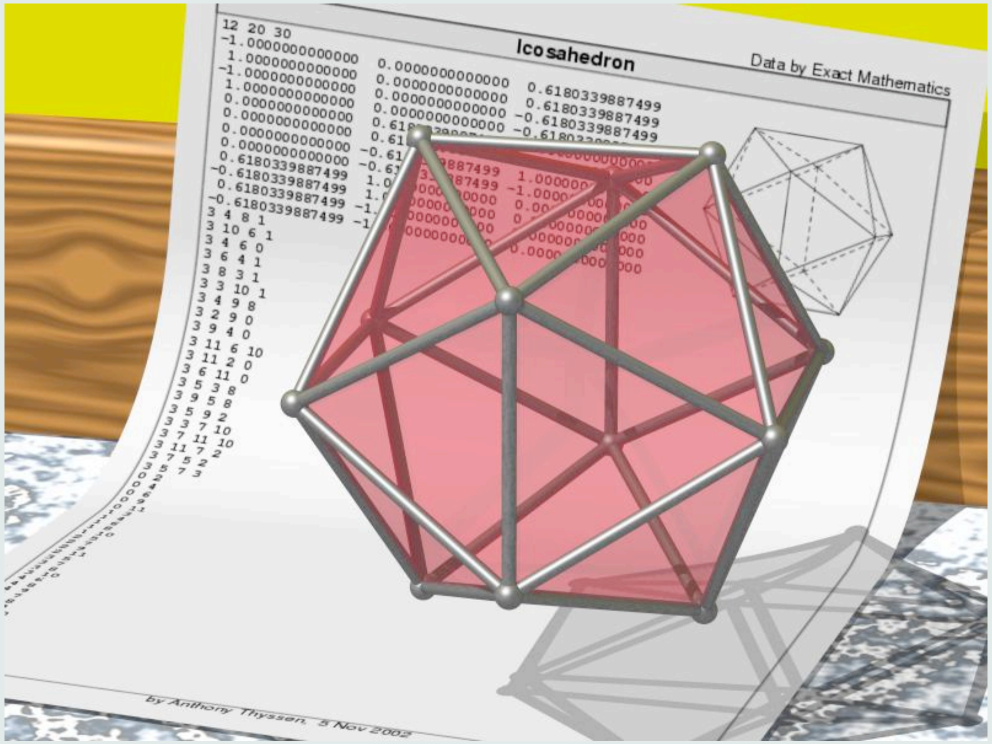
Lipowsky, J. Phys. II France (1992)

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



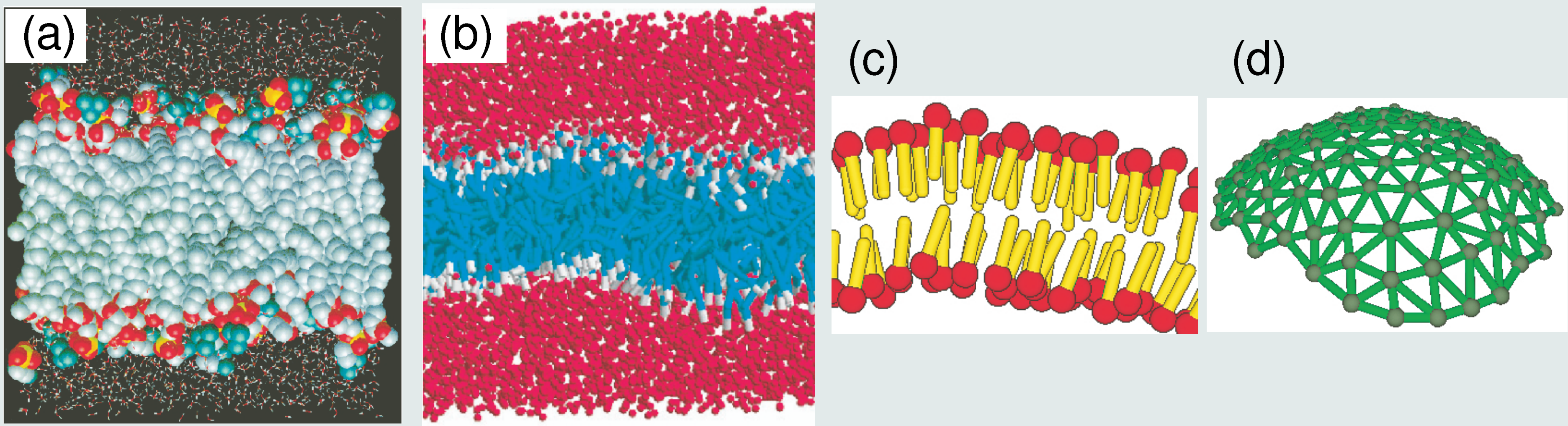
Questions

- 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

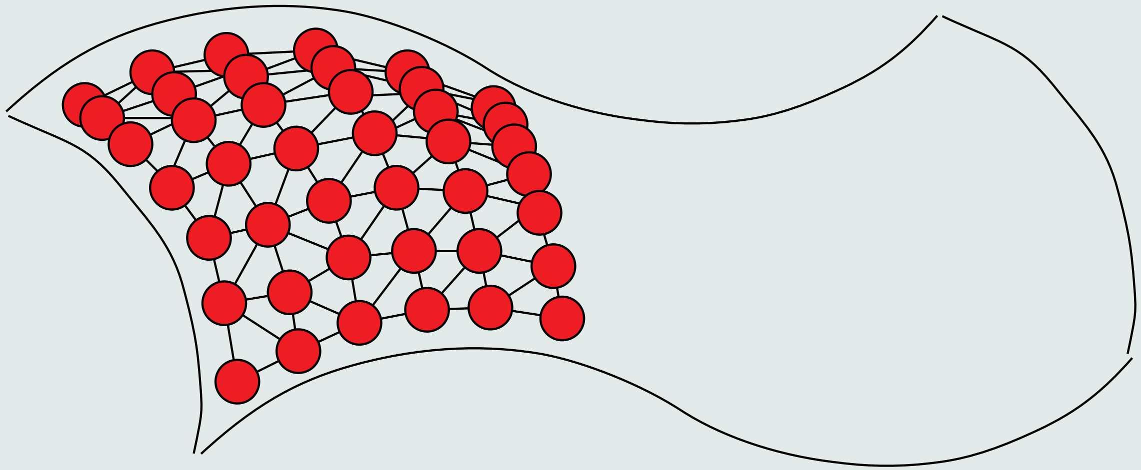
Modelling of membranes on different length scales:



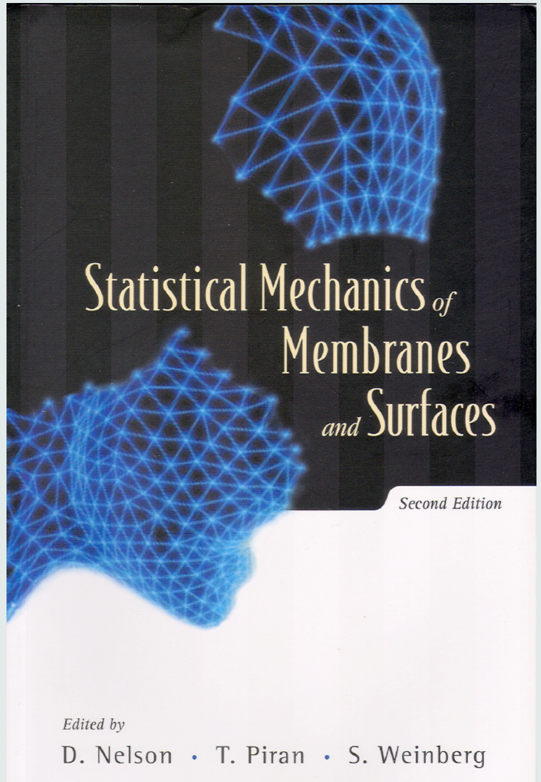
atomistic coarse-grained solvent-free triangulated

Simulations of Membranes

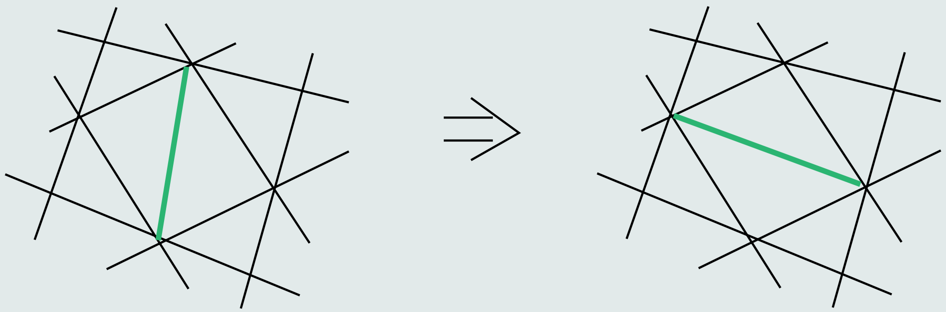
Dynamically triangulated surfaces



Hard-core diameter σ
Tether length L: $\sigma < L < \sqrt{3}\,\sigma$
--> self-avoidance



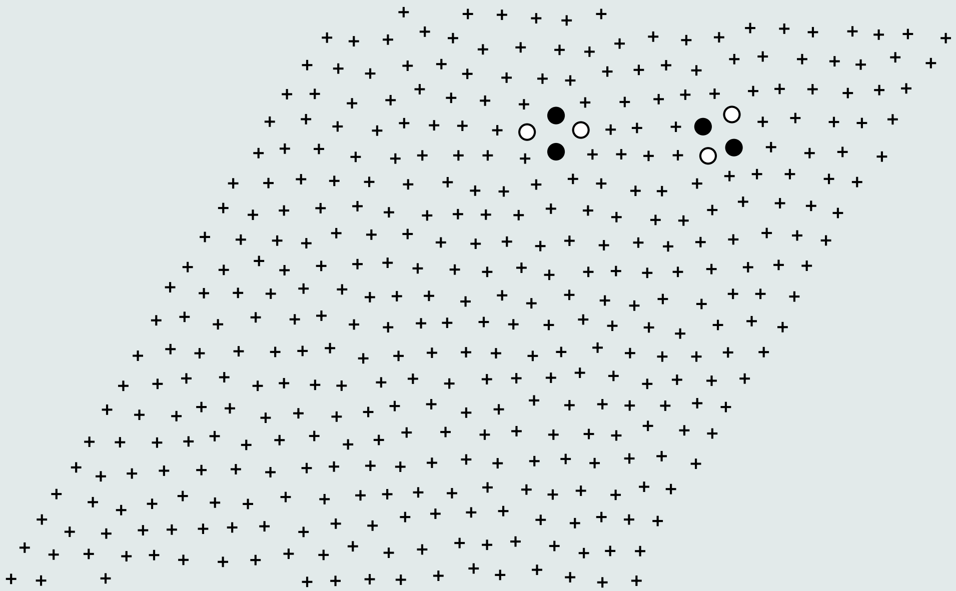
Dynamic triangulation:



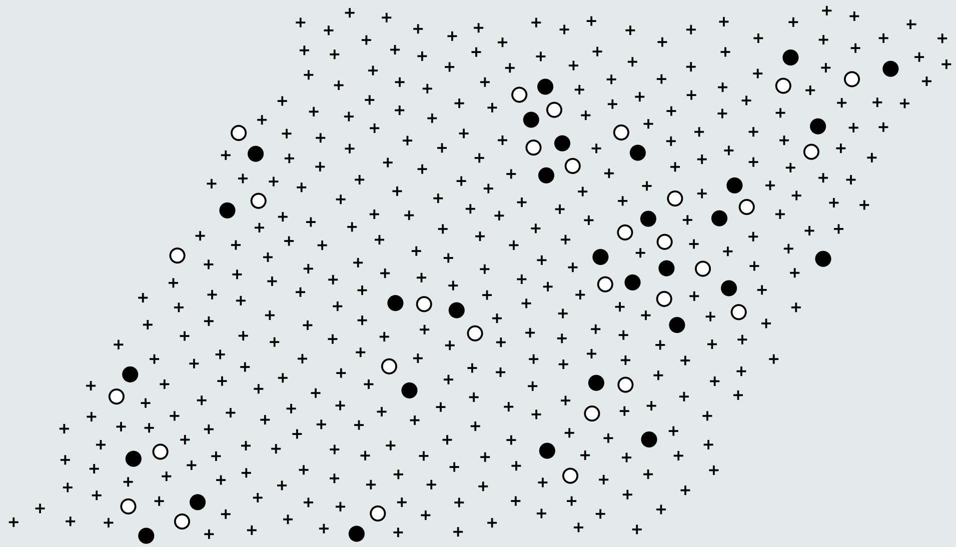
G. Gompper & D.M. Kroll (2004)

Phase Behavior of Planar Network Models

Only parameter: Tether length ℓ_0 controls in-plane density



$\ell_0/\sigma = 1.53$

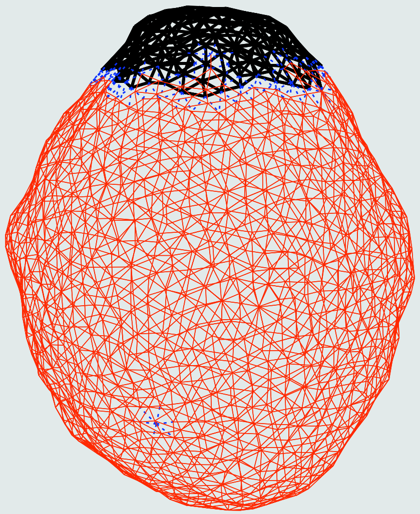


$\ell_0/\sigma = 1.55$

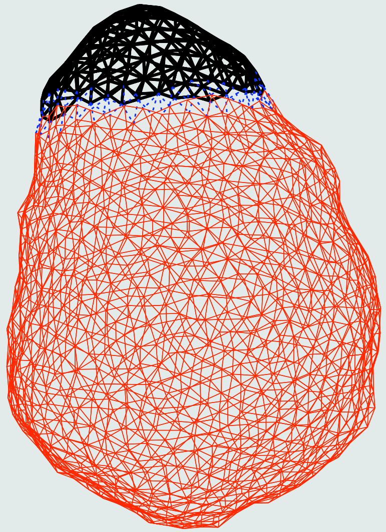
Gompper & Kroll, J. Phys. I France (1997)

Budding of Crystalline Domains: Vesicles Shapes

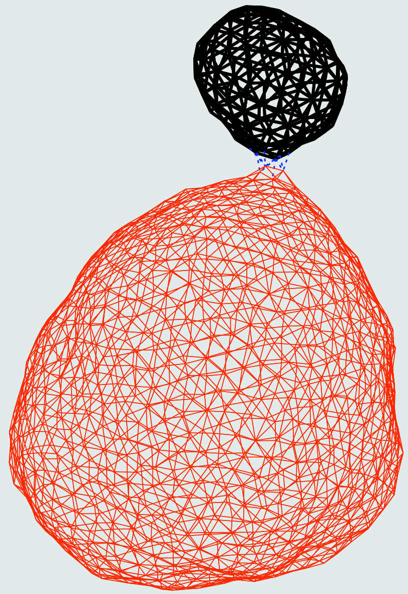
Shapes for fixed spontaneous curvature and increasing line tension λ:



$\lambda/k_BT = 1.5$



$\lambda/k_BT = 3.0$



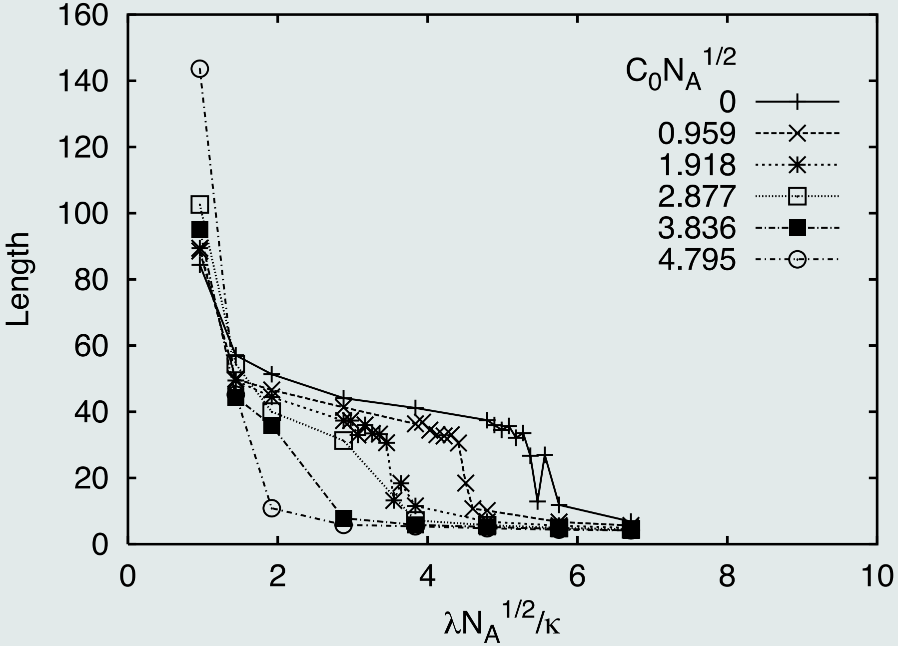
$\lambda/k_BT = 5.0$

Kohyama, Kroll, Gompper, Phys. Rev. E (2003)

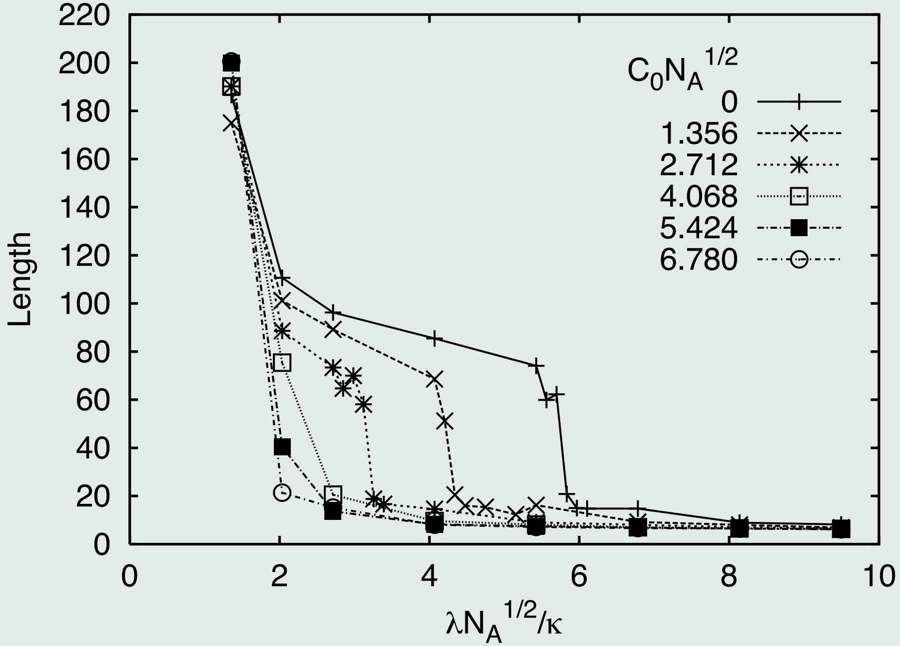
Phase Behavior for Crystalline Domains

Length of domain boundary:

$N_A = 92$



$N_A = 184$

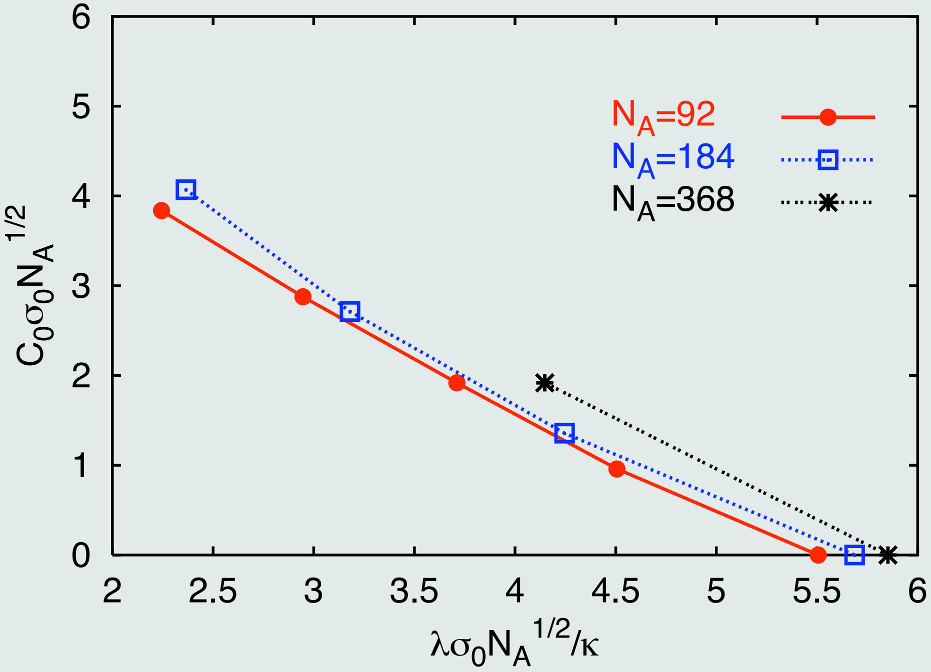


Kohyama, Kroll, Gompper, Phys. Rev. E (2003)

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

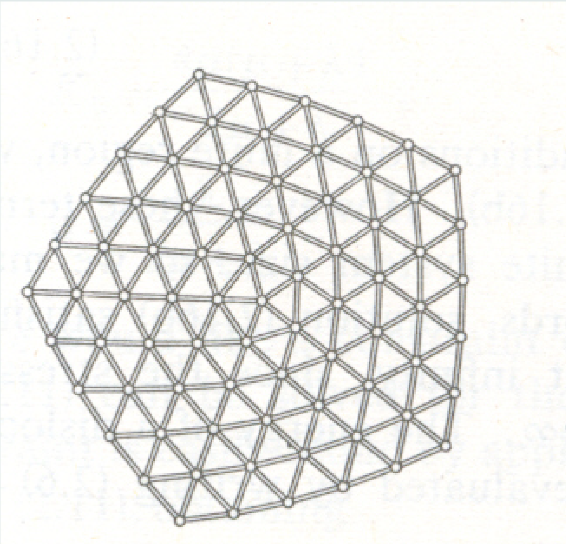
$\Gamma(R)$	N	R/σ
3.39 ± 0.02	92	6.18
3.45 ± 0.03	184	8.74
3.68 ± 0.05	368	12.4

Defects in Flexible Membranes: Buckling

For flexible membranes, buckling reduces elastic energy.

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

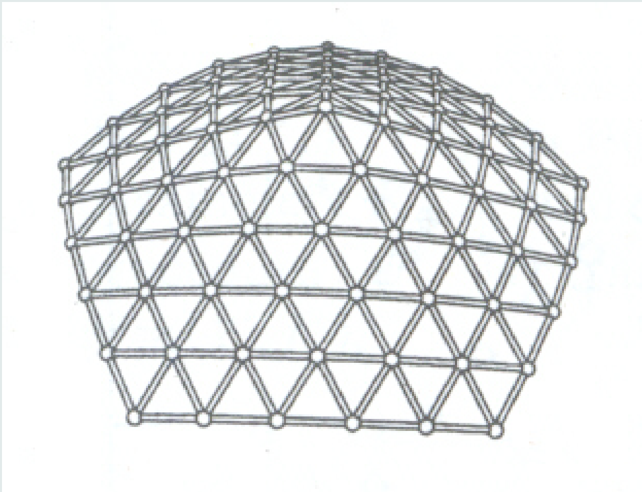
Stretching



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

versus

Buckling



$$E_b = s\kappa \ln(R/a)$$

Buckling favorable for R larger than bucking radius

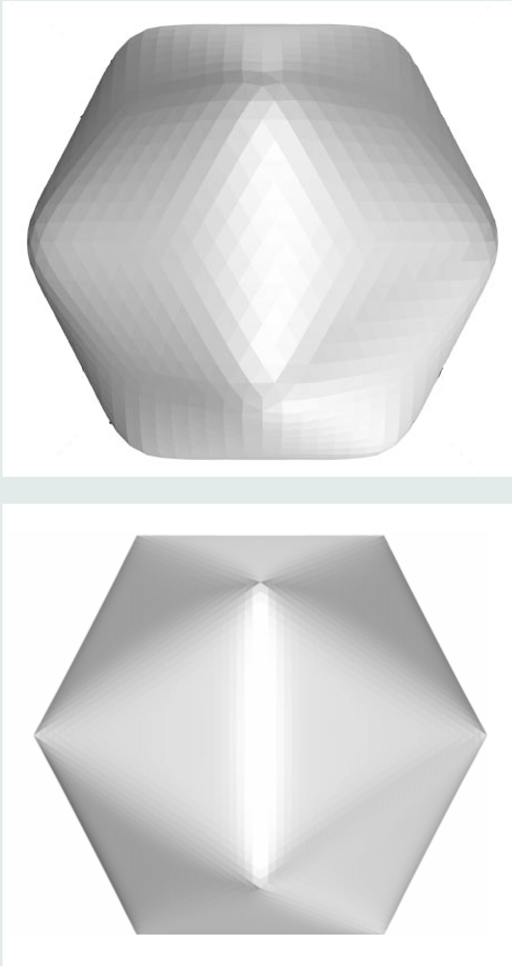
$$R_b = 10 \left(\frac{\kappa}{K_0 s} \right)^{1/2}$$

Seung & Nelson, Phys. Rev. A (1988)

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: $\Gamma(R) \sim \ln(R/a)$



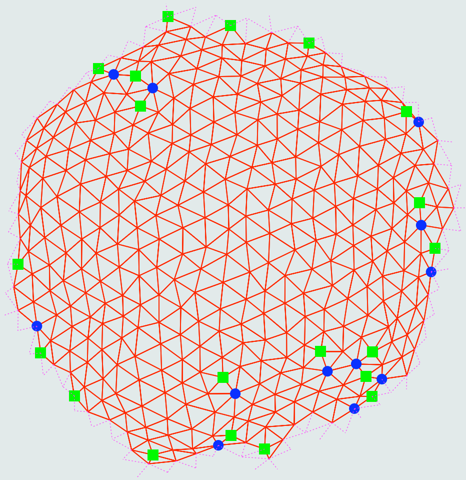
Lidmar et al., Phys. Rev. E (2003)

Conclusion:

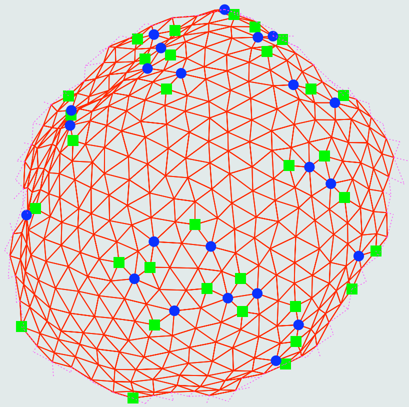
- Budding of crystalline domains qualitatively different than for fluid domains!

Bud Formation Dynamics

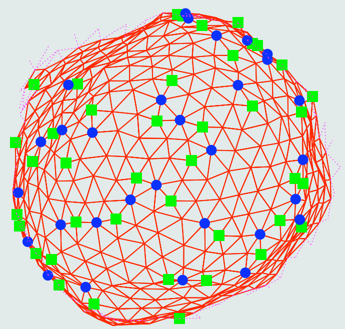
(Top view — embedding fluid membrane not shown)



0.1 million MCS



0.5 million MCS

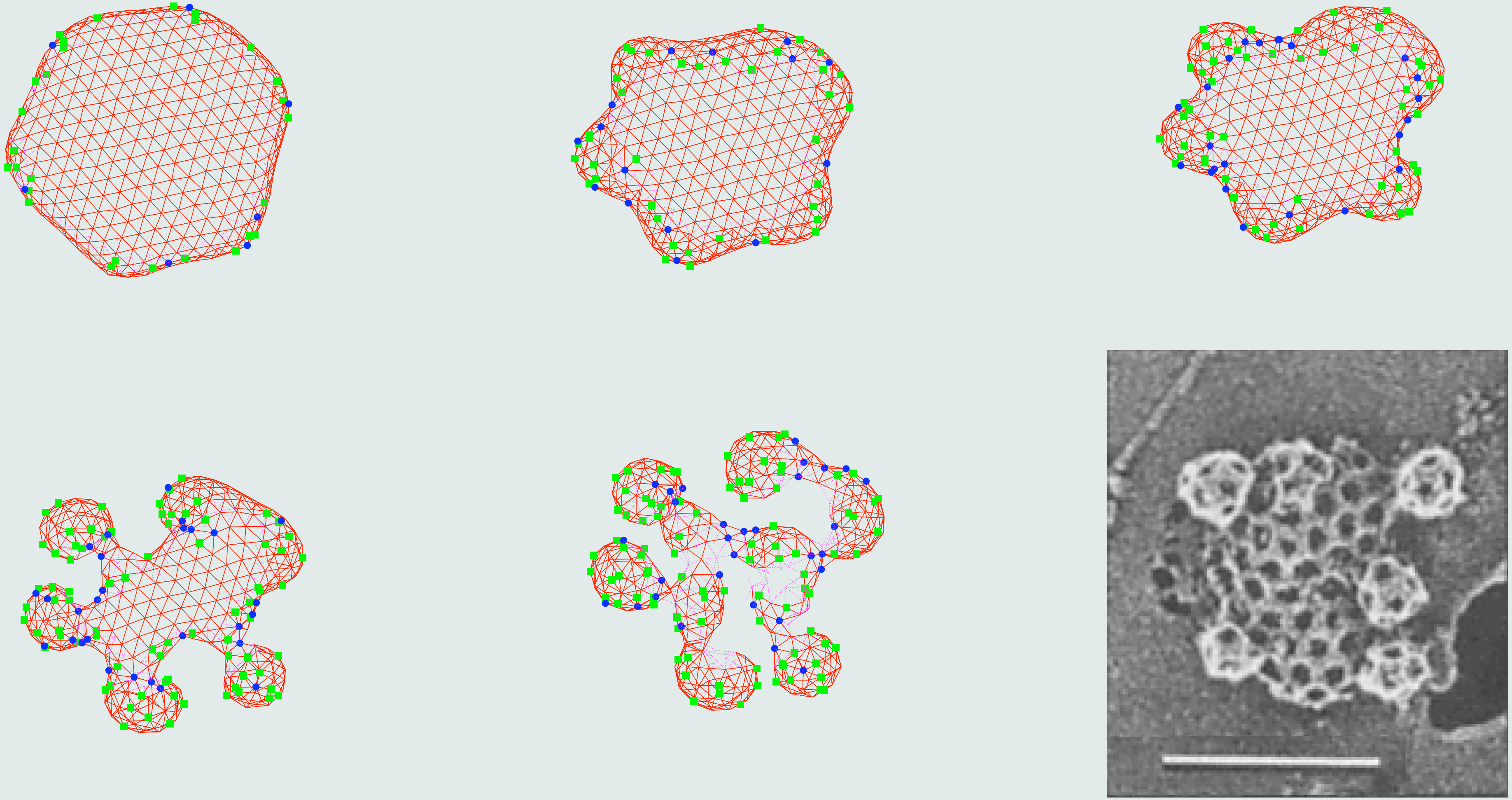


2.0 million MCS

- Defects are generated at boundary, diffuse into interior

Formation of Microcages

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



Kohyama, Kroll, Gompper, Phys. Rev. E (2003)

Summary & Outlook

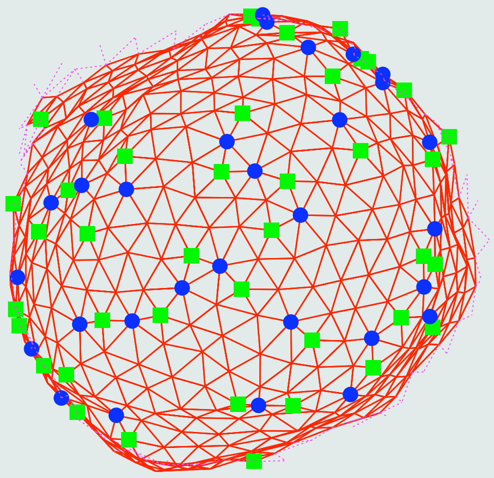
Budding of crystalline domains in fluid membranes:

- Defects generated at domain boundary, diffuse into interior.
- Line tension λ, 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?

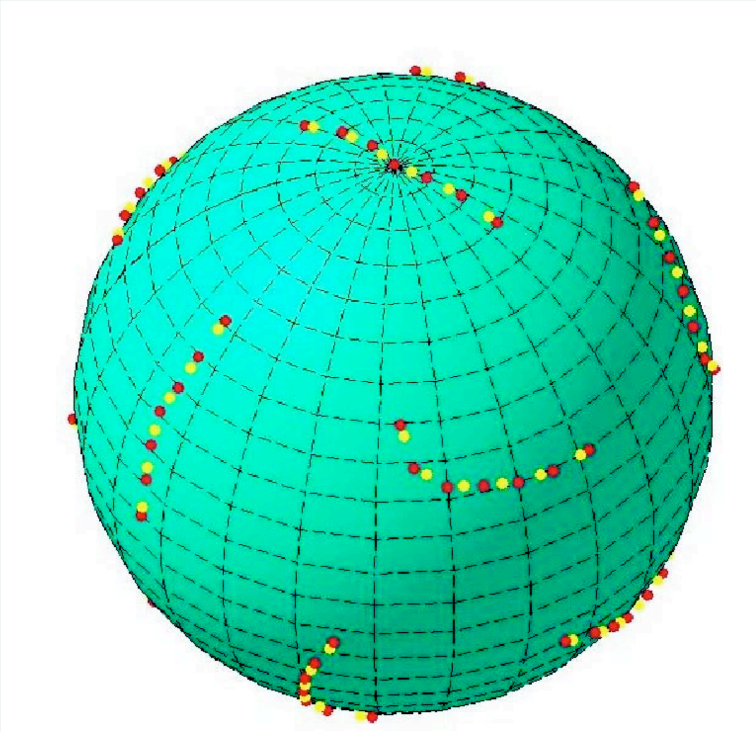
Defect Scars on Flexible Crystalline Vesicles



Defects on Crystalline Vesicles

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

Scar length inceases *linearly* with sphere radius R



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

Bausch, Bowick, Cacciuto, Dinsmore, Hsu, Nelson, Nikolaides, Travesset, Weitz, Science (2003)

What happens on flexible surfaces ??

Defects on Crystalline Vesicles

Flexible surfaces *without* defects:

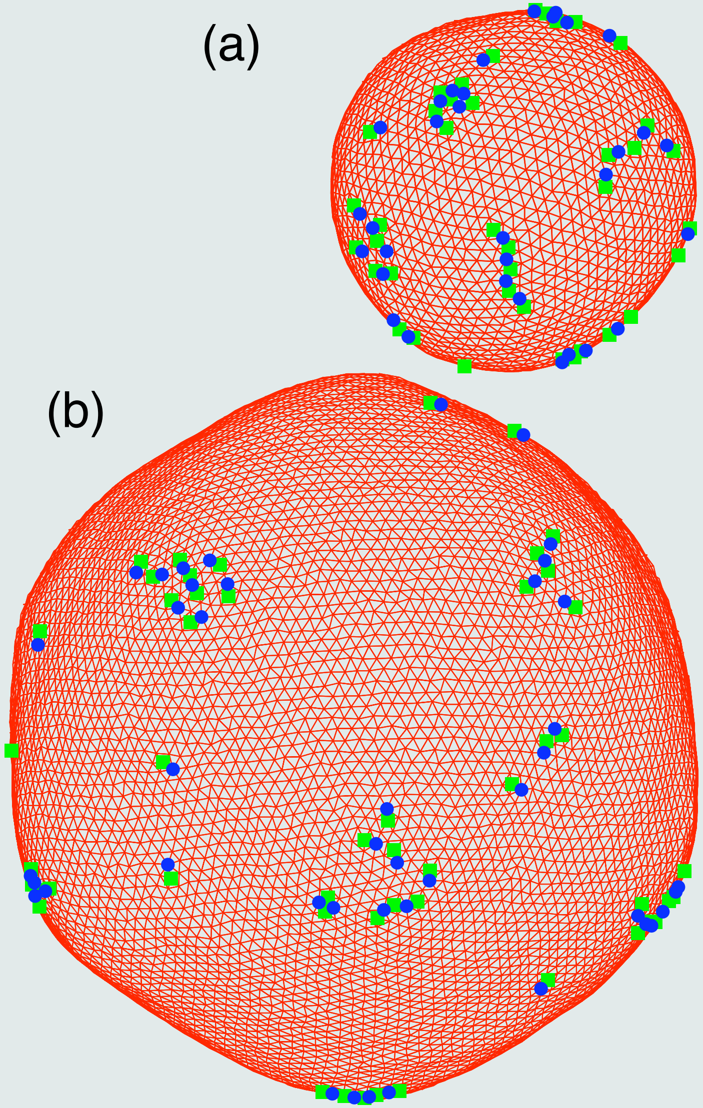
Faceting with increasing Föppl-von Kármán number $\gamma = K_0 R^2/\kappa$

Lobkovsky et al., Science **270** (1995);

Lidmar, Mirny, Nelson, Phys. Rev. E (2003)

Flexible surfaces *with* defects:

- Faceting still exists
- Defect scars get localized for “large” γ
- Scars get fuzzy at finite temeratures

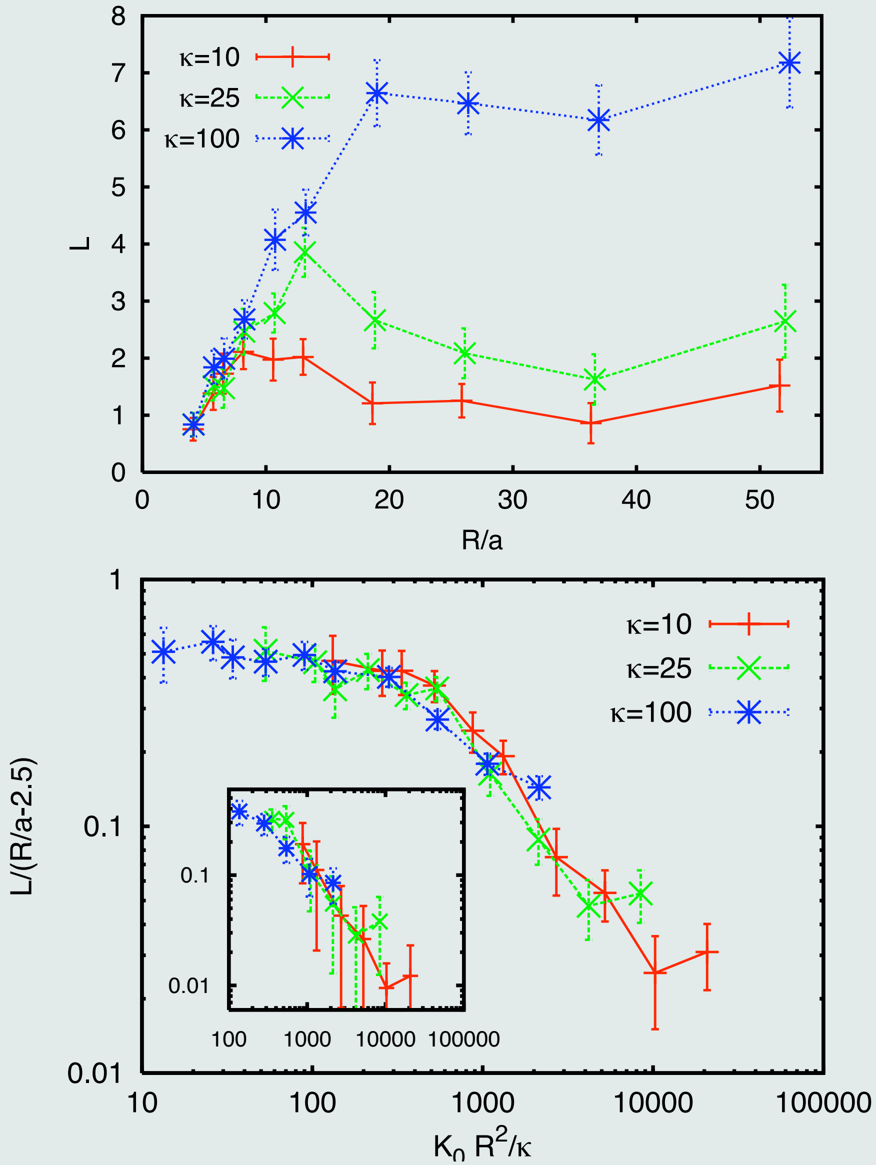


Kohyama & Gompper, Phys. Rev. Lett. (2007)

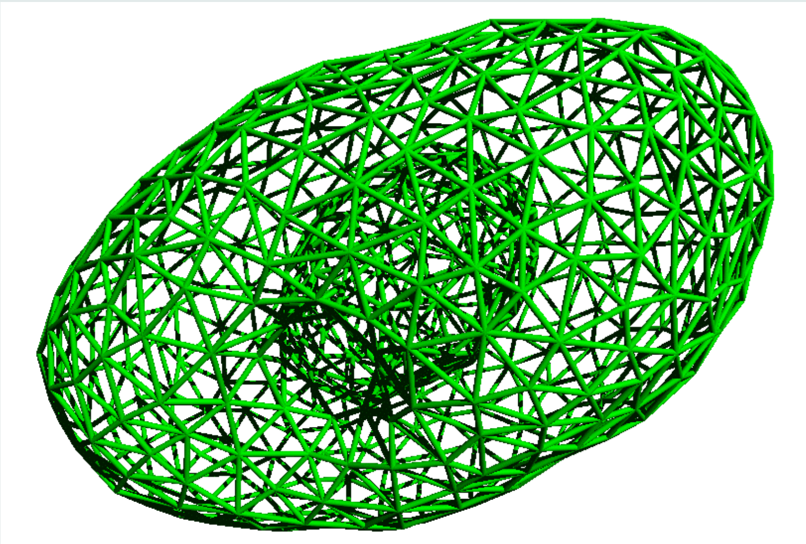
Defects on Crystalline Vesicles

- 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

Kohyama & Gompper, Phys. Rev. Lett. (2007)

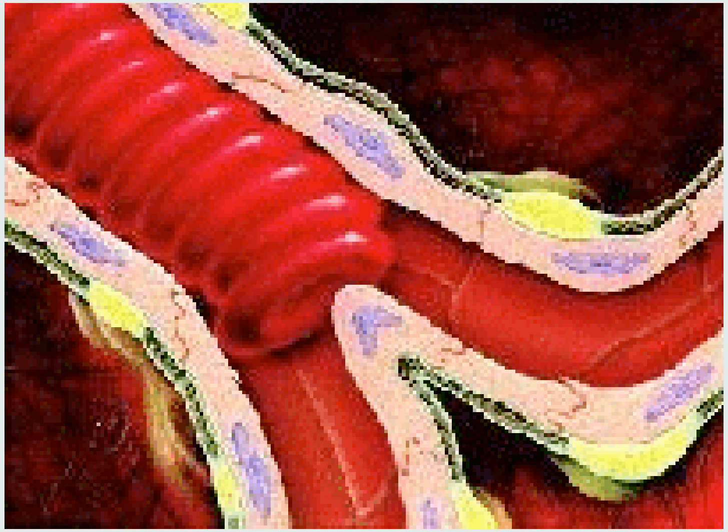


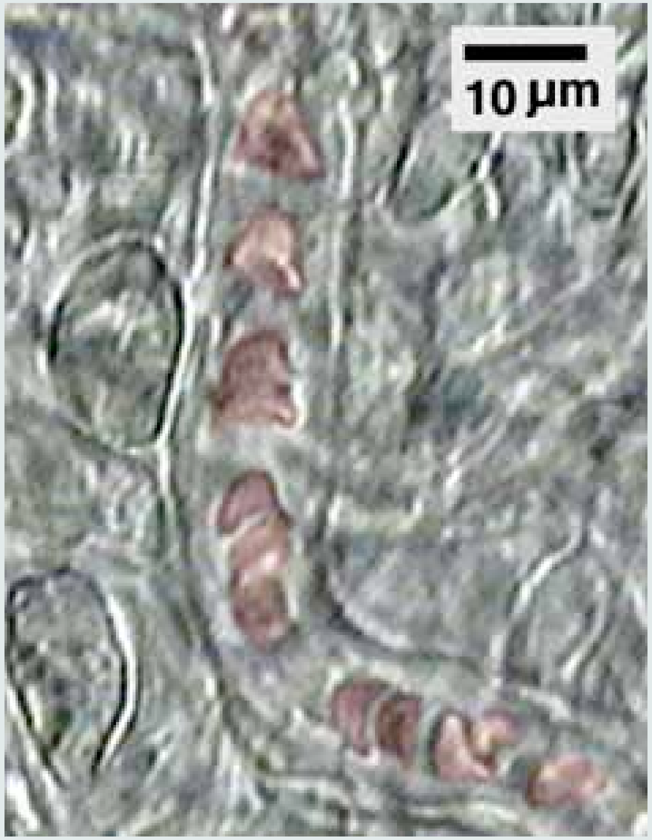
Hydrodynamics of Membranes and Vesicles



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)

$\longrightarrow$ **Mesoscale Simulation Techniques**

Basic idea:

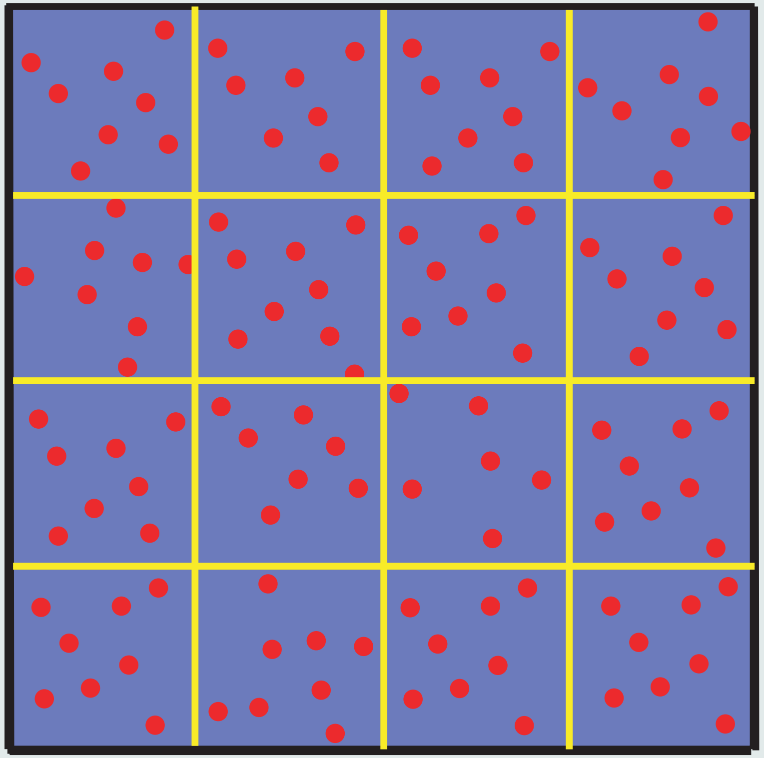
- drastically simplify dynamics on molecular scale
- respect conservation laws for mass, momentum, energy

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

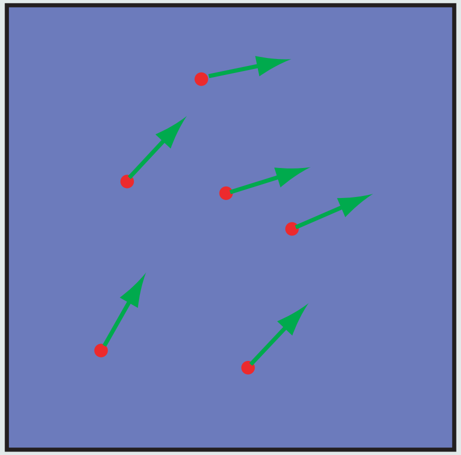
A. Malevanets and R. Kapral, J. Chem. Phys. **110** (1999)

A. Malevanets and R. Kapral, J. Chem. Phys. **112** (2000)

Mesoscale Flow Simulations: MPCD

Flow dynamics: Two step process

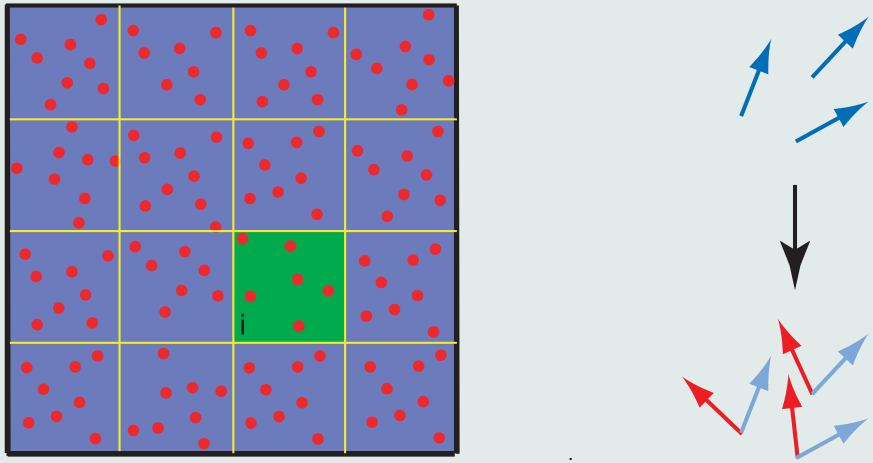
Streaming



- ballistic motion

$$\mathbf{r}_i(t+h) = \mathbf{r}_i(t) + \mathbf{v}_i(t)h$$

Collision



- mean velocity per cell

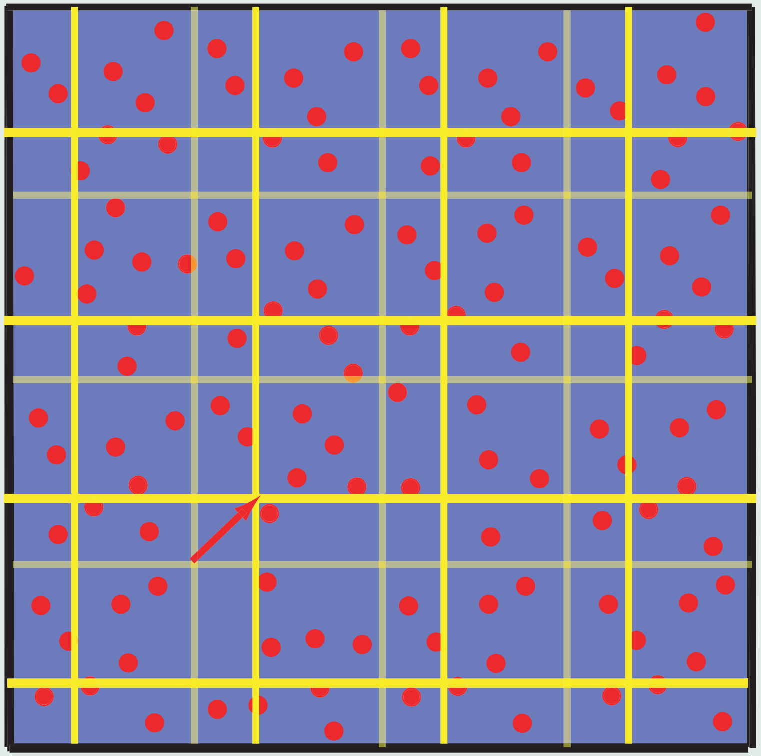
$$\bar{\mathbf{v}}_i(t) = \frac{1}{n_i}\sum_{j\in C_i}^{n_i} \mathbf{v}_j(t)$$

- rotation of relative velocity by angle α

$$\mathbf{v}_i' = \bar{\mathbf{v}}_i + \mathbf{D}(\alpha)(\mathbf{v}_i - \bar{\mathbf{v}}_i)$$

Mesoscale Flow Simulations: MPCD

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

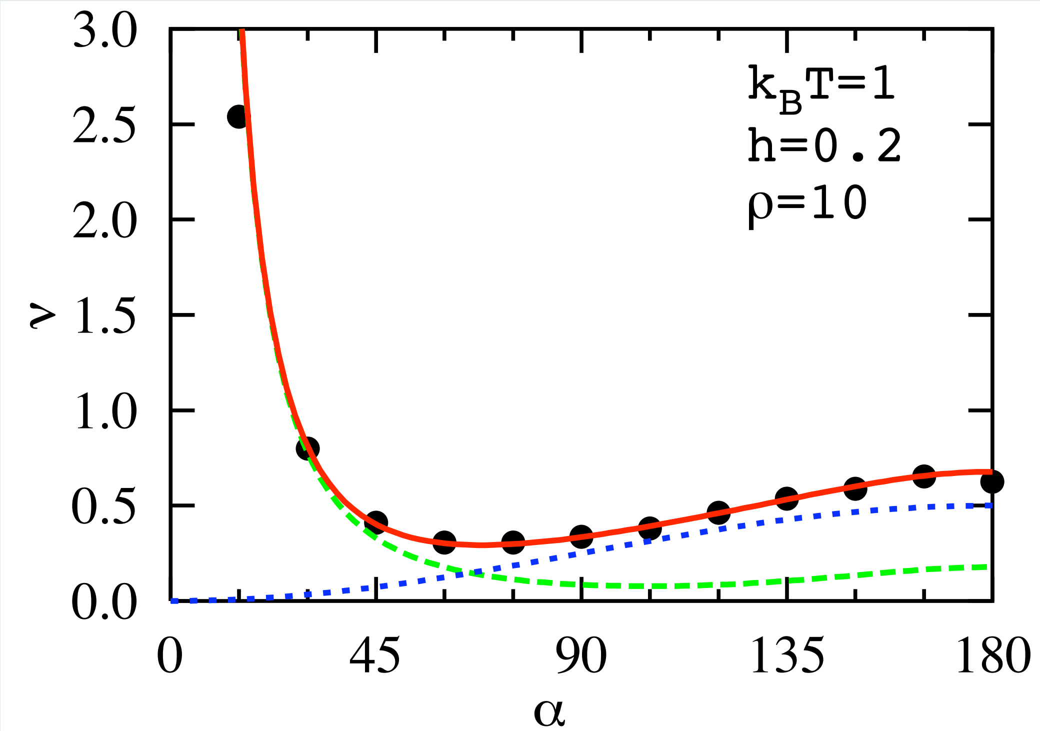


T. Ihle and D.M. Kroll, Phys. Rev. E **63** (2001)

.

MPCD: Viscosity

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



Analytical approximation from kinetic theory:

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

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

N. Kikuchi, C. M. Pooley, J. F. Ryder, J. M. Yeomans, J. Chem. Phys. **119** (2003)

T. Ihle, D. M. Kroll, Phys. Rev. E **67** (2003)

Membrane Hydrodynamics

Interaction between membrane and fluid:

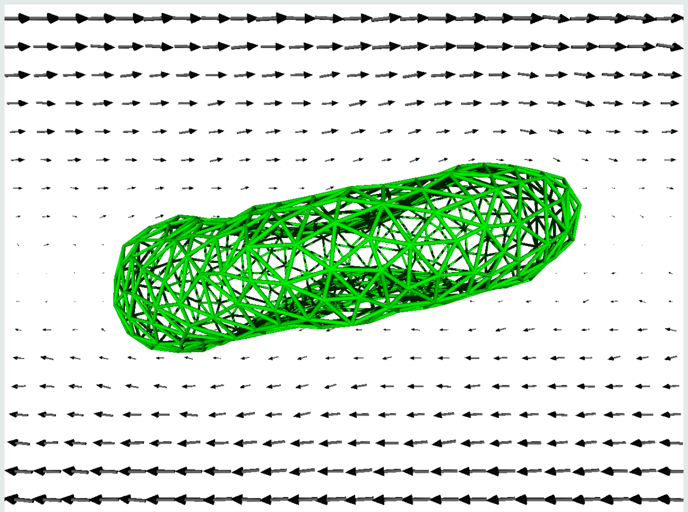
- Streaming step:

  bounce-back scattering of solvent particles on triangles

- Collision step:

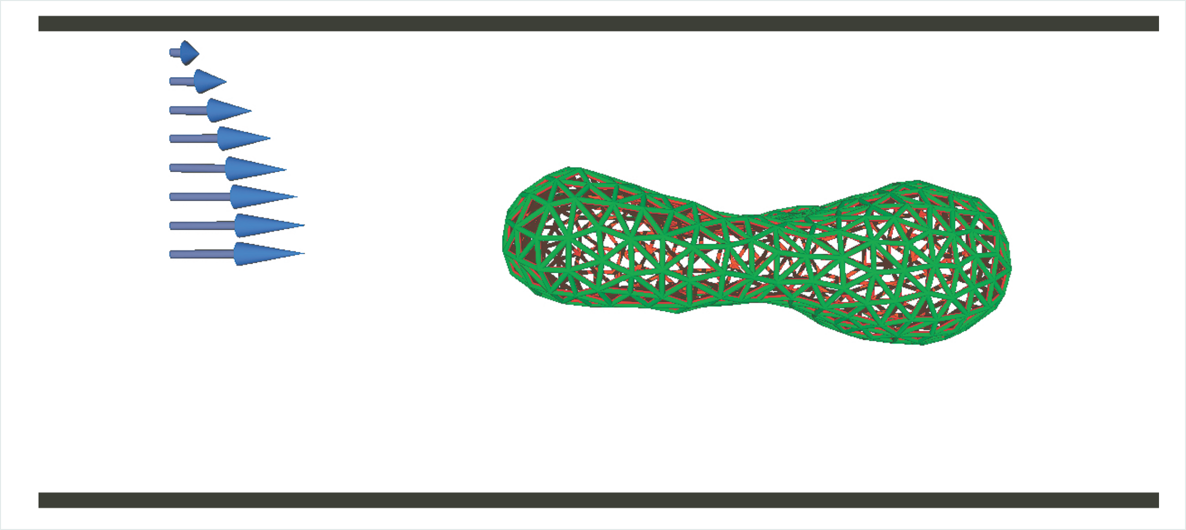
  membrane vertices are included in MPCD collisions

implies no-slip boundary conditions.

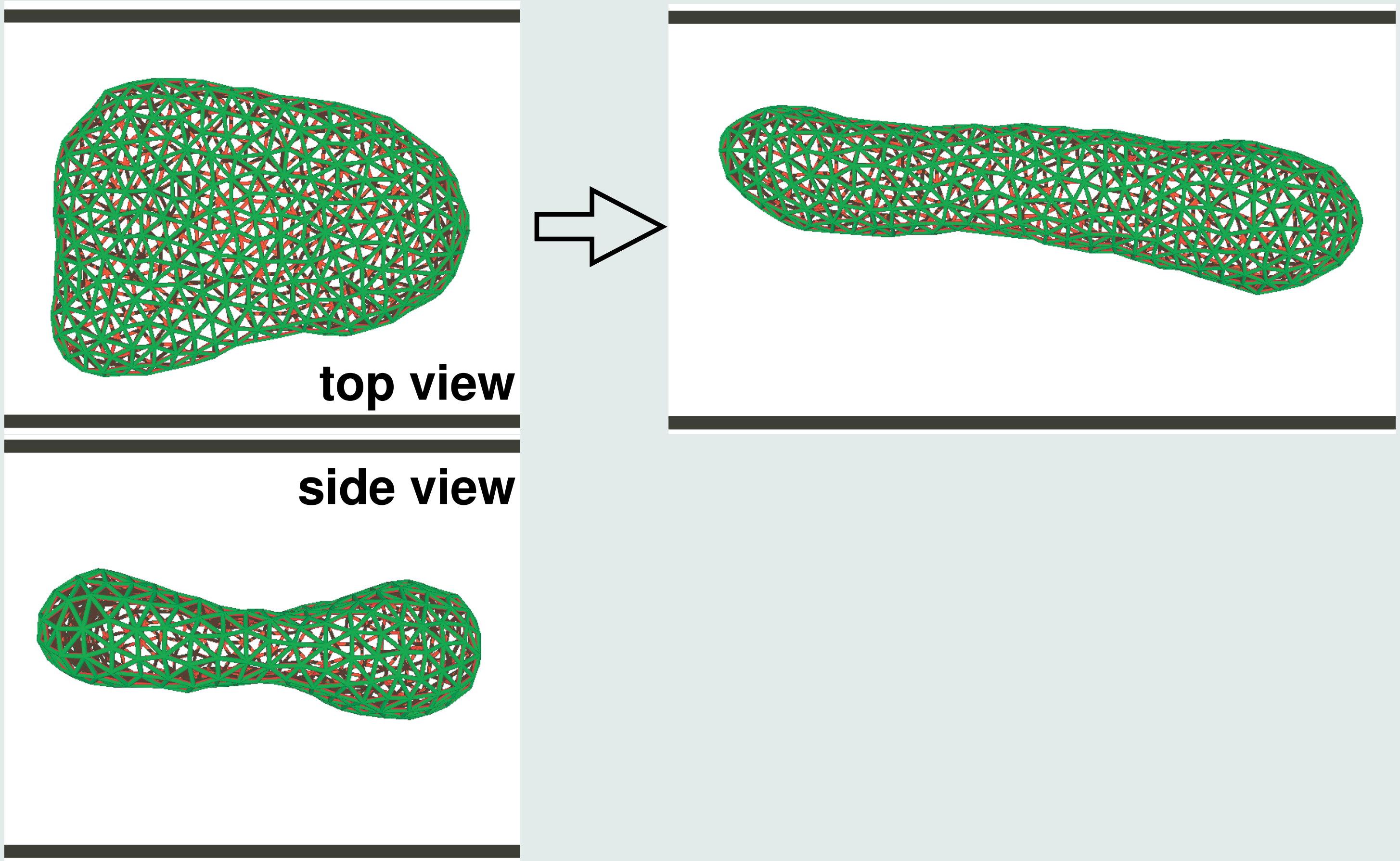


H. Noguchi and G. Gompper, Phys. Rev. Lett. **93**, 258102 (2004); Phys. Rev. E **72**, 011901 (2005)

Vesicle and Cells in Capillary Flow



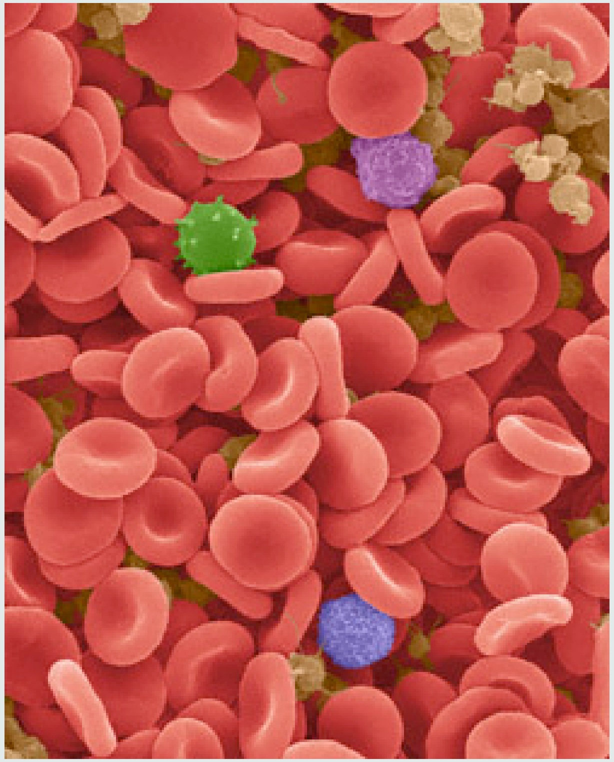
Capillary Flow: Fluid Vesicles

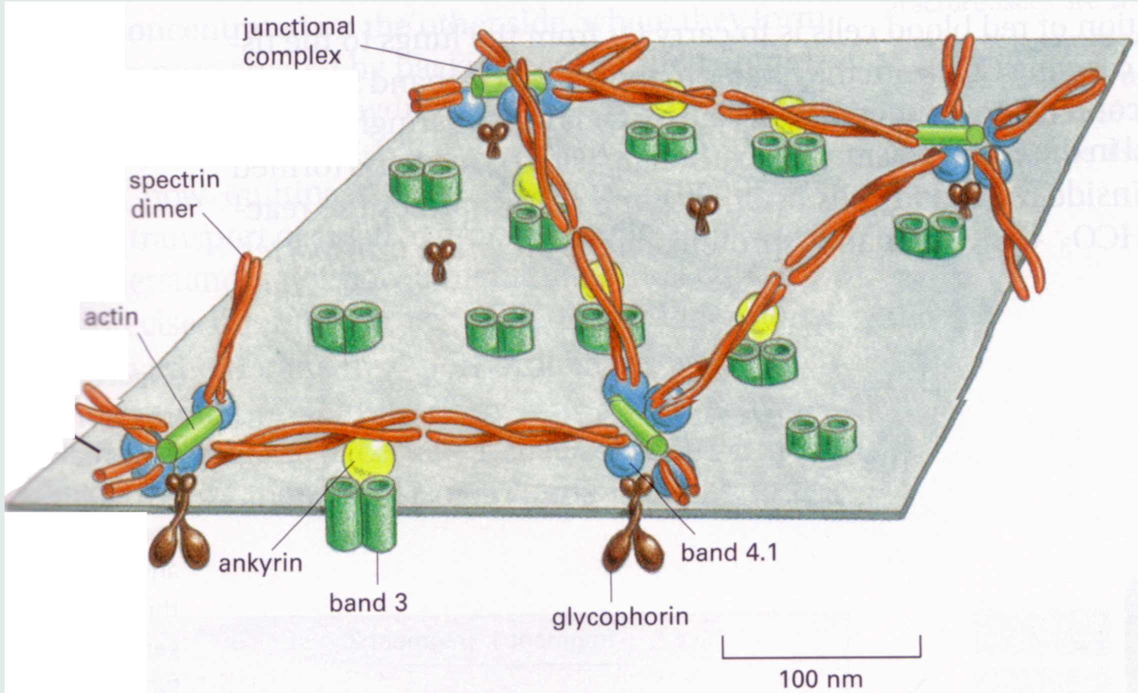


- small flow velocities: vesicle axis perpendicular to capillary axis $\longrightarrow$ no axial symmetry!
- discocyte-to-prolate transition with increasing flow

H. Noguchi and G. Gompper, Proc. Natl. Acad. Sci. USA **102** (2005)

Capillary Flow: Red Blood Cells



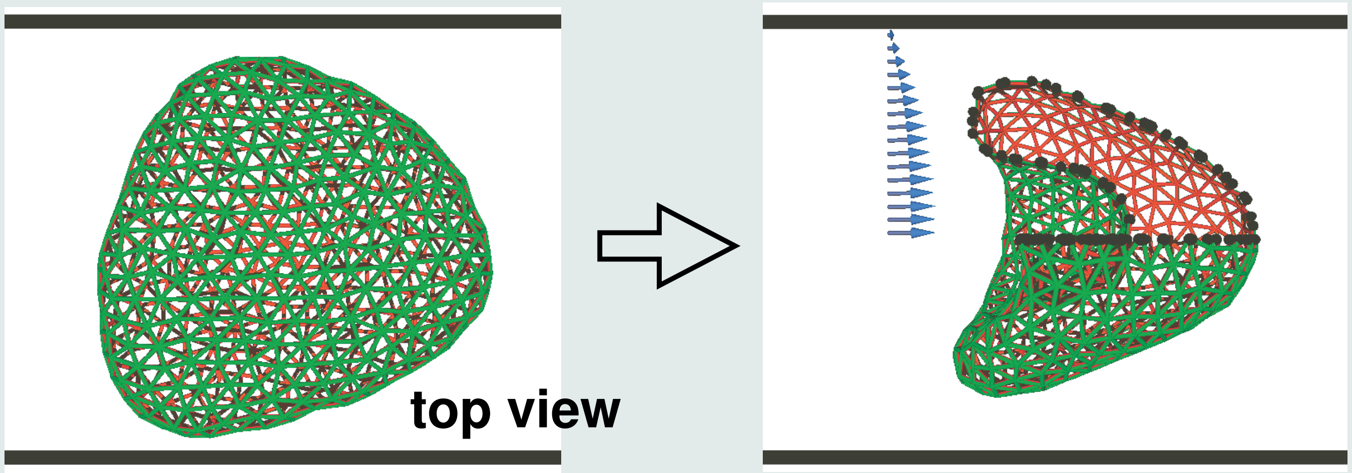


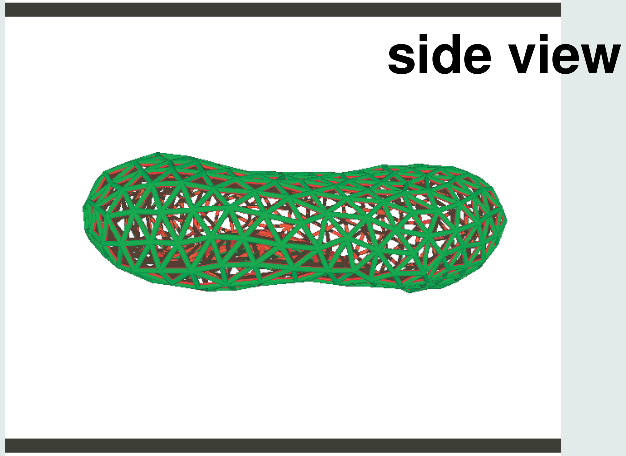
- Spectrin network induces shear elasticity μ of composite membrane
- Elastic parameters: $\kappa/k_BT = 50$, $\mu R_0^2/k_BT = 5000$

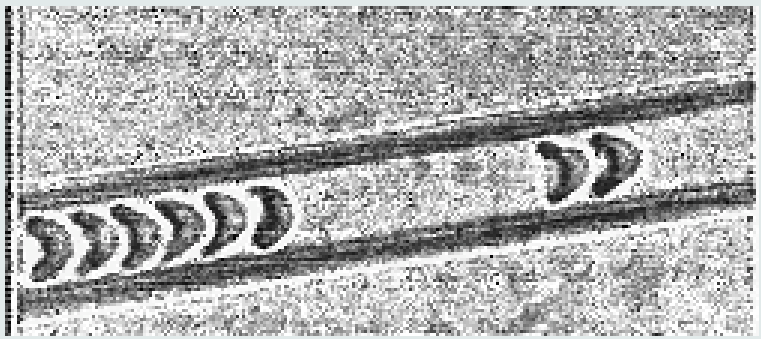
Capillary Flow: Elastic Vesicles

Elastic vesicle:

- curvature and shear elasticity
- model for red blood cells





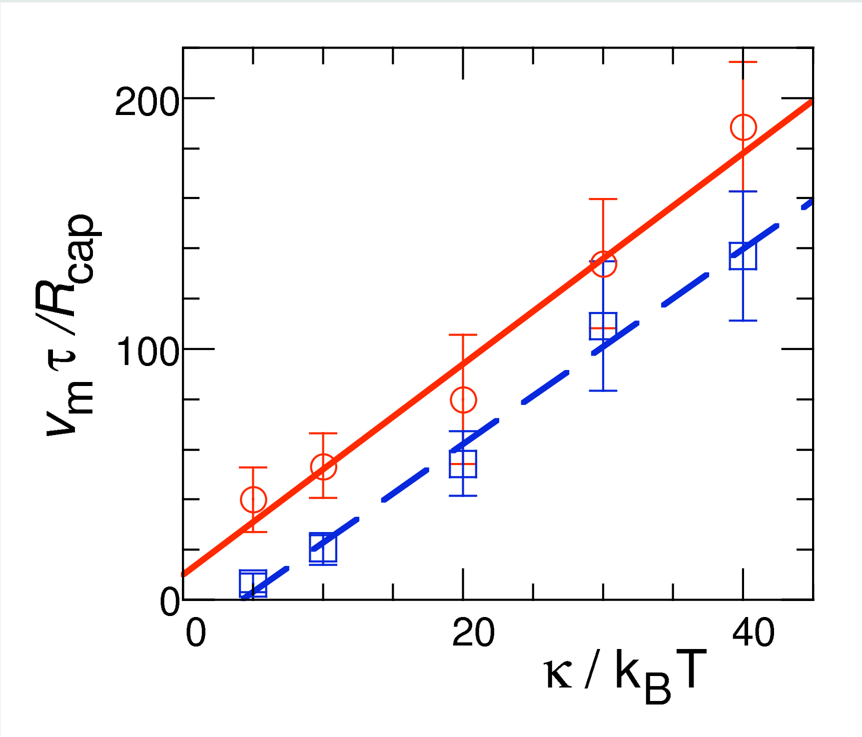


Tsukada et al., Microvasc. Res. **61** (2001)

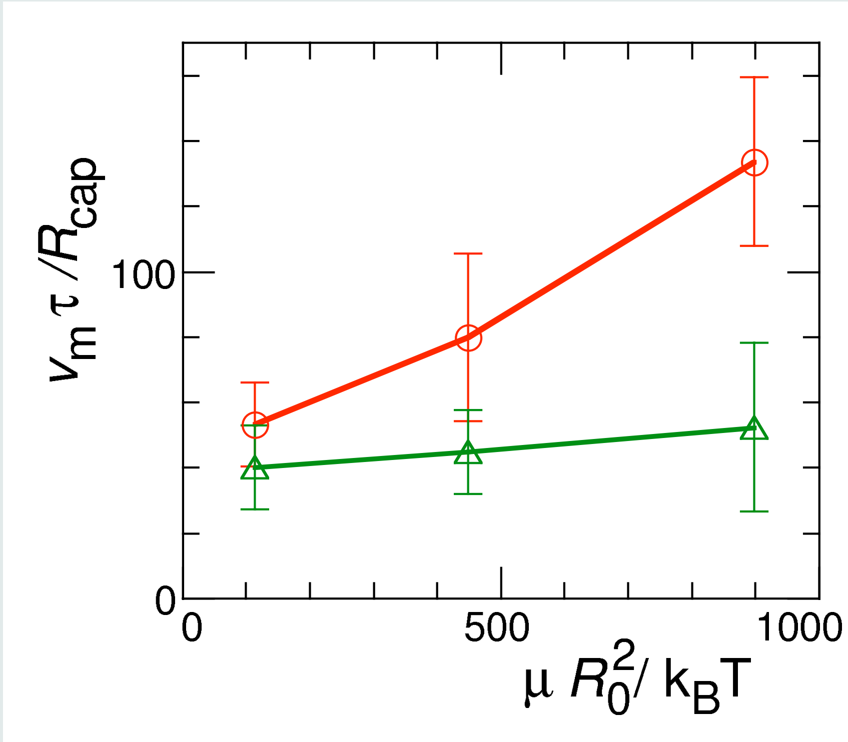
Capillary Flow: Elastic Vesicles

Shear elasticity suppresses prolate shapes (large deformations)

Flow velocity at discocyte-to-parachute transition



bending rigidity



shear modulus

Implies for RBCs: $v_{trans} \simeq 0.2 mm/s$ for $R_{cap} = 4.6 \mu m$

Outlook

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.

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