Mechanics of Lipid Membrane

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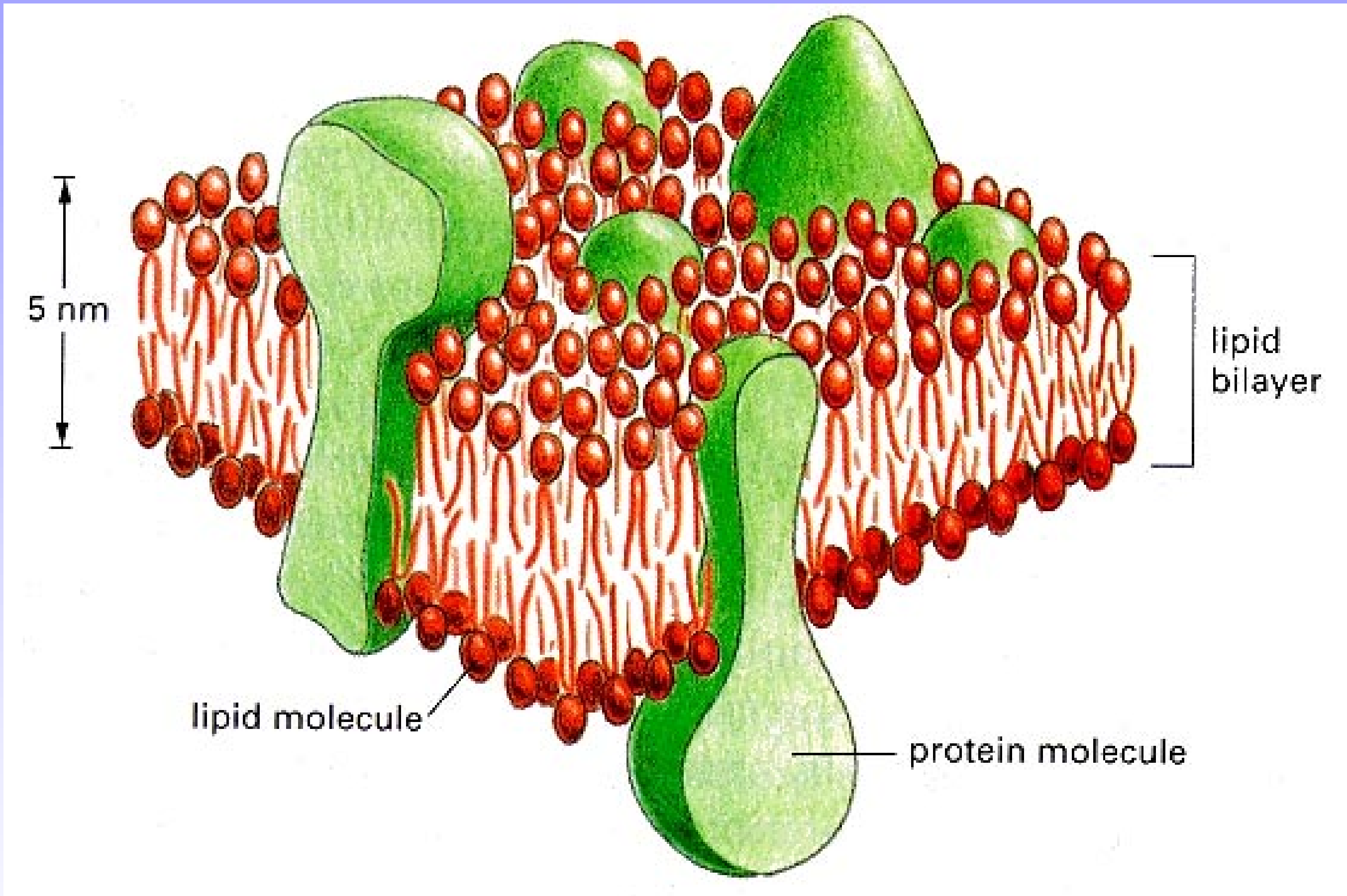
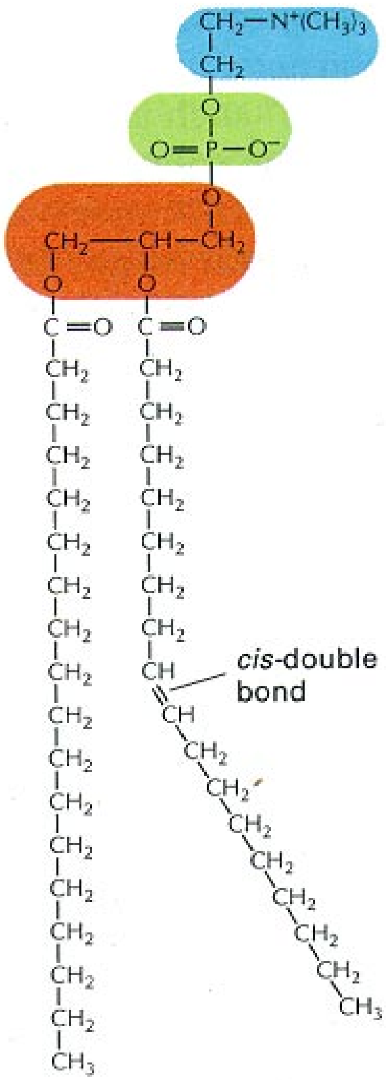
Lipid Membranes



Singer & Nicolson's Mosaic Model (1972)



Partition & Transport

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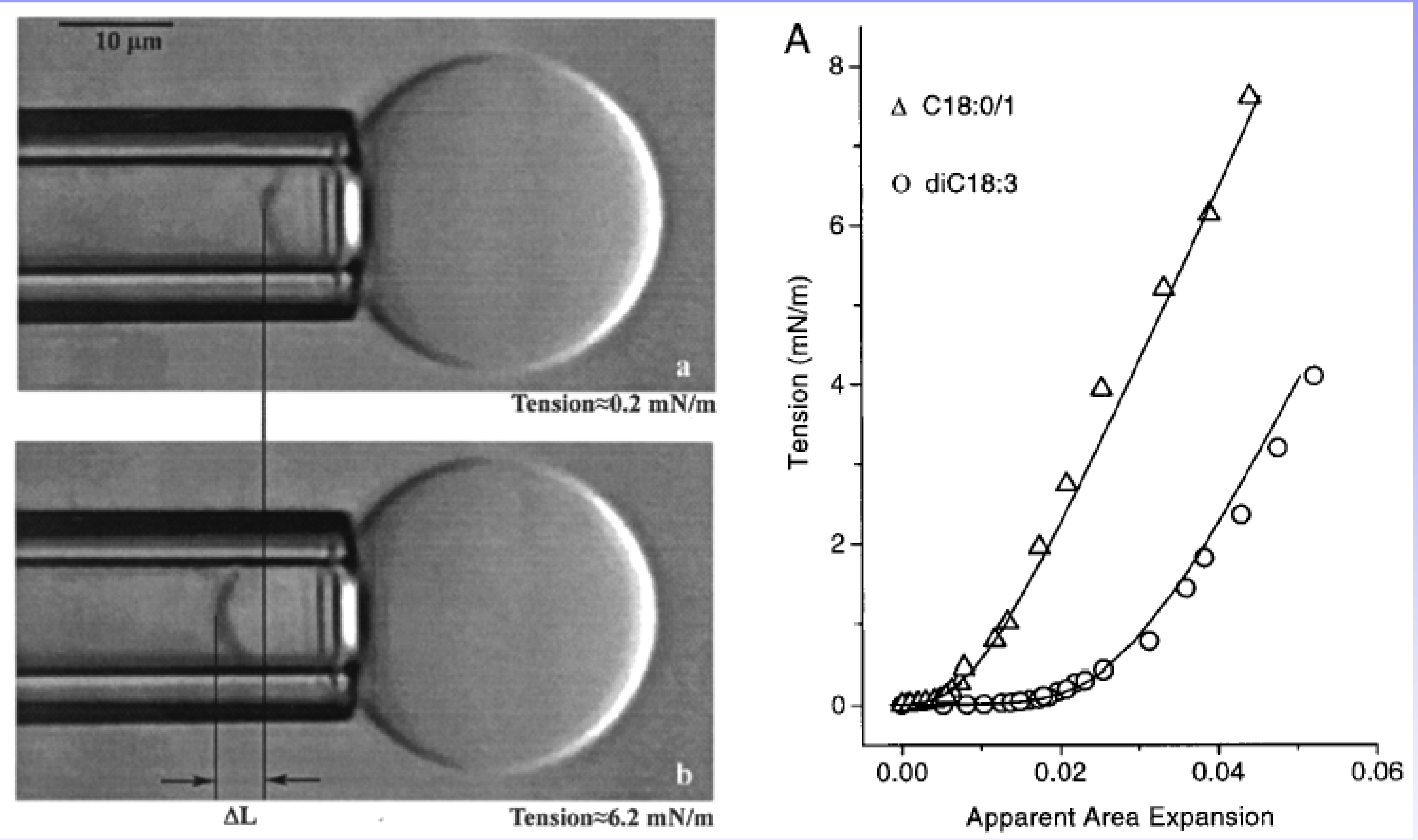
Lipid Bilayers

- Amphiphilic molecules
  spontaneously form bilayers in aqueous solution
- Lipid bilayer is a two-dimensional fluid
  flexible, thermal fluctuation important
- Fluidity depends on bilayer's composition
  packing ability, lateral diffusion, phase separation
- Lipid bilayer is asymmetrical
  spontaneous curvature

Structure difficult to determine experimentally – (freeze-fracture/etch electron microscopy, NMR, X-ray, neutron, EPR)



Elastic bending modulus ~ 10^{-19} J

~ 100 $K_B T$

E. Evans et al (2000)

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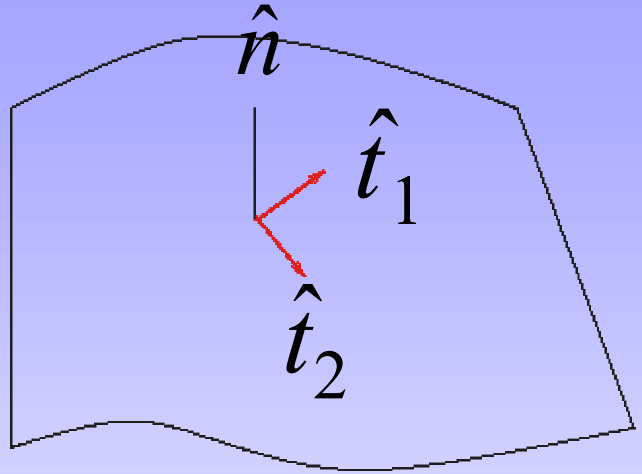
Elastic Bending



Mean curvature:

$$H = C_1 + C_2 = \frac{1}{R_1} + \frac{1}{R_2}$$

Gaussian curvature:

$$K = C_1 C_2$$

Helfrich elastic bending energy:

$$F_1 = \int d^2r \left[\frac{\kappa_1}{2}(H - H_0)^2 + \kappa_2 K \right]$$

Helfrich (1970)

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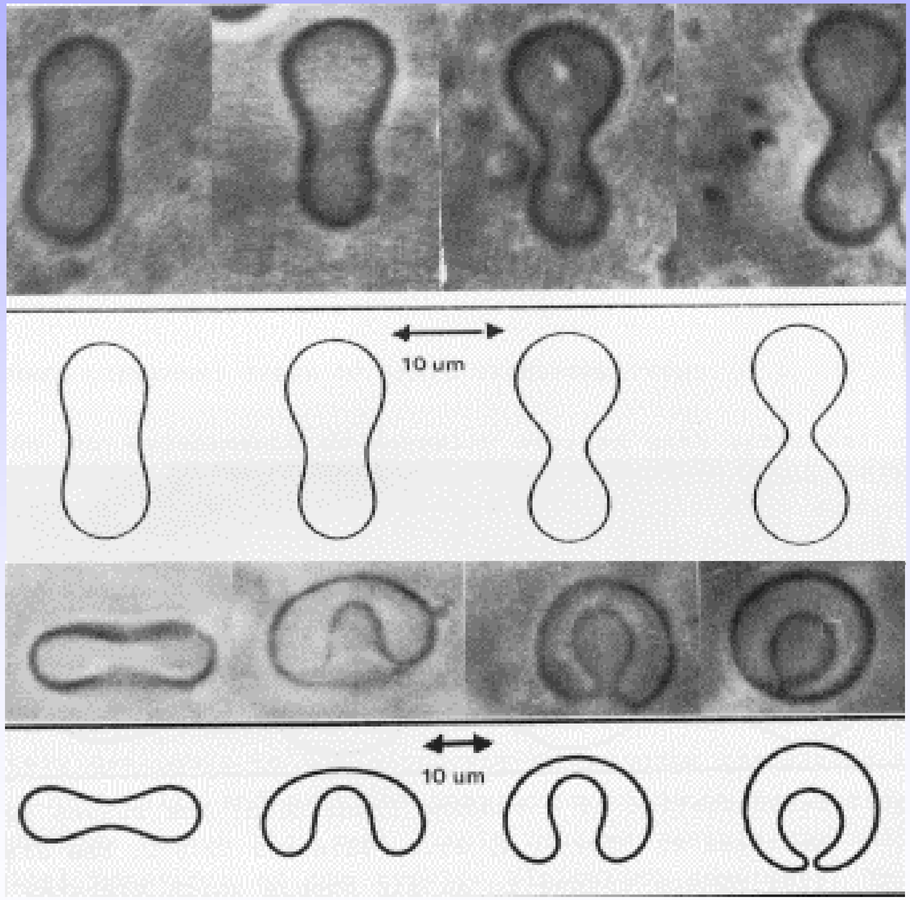
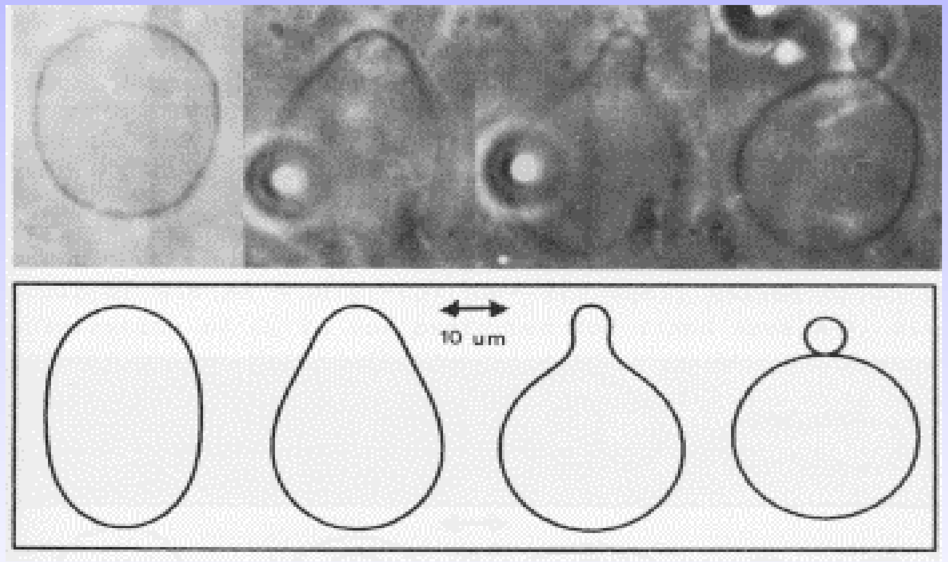
Elastic Bending

+ area constraint & volume constraint

$$\delta (F_1 + \gamma A + pV) = 0$$





Kerndl et al., (1991)

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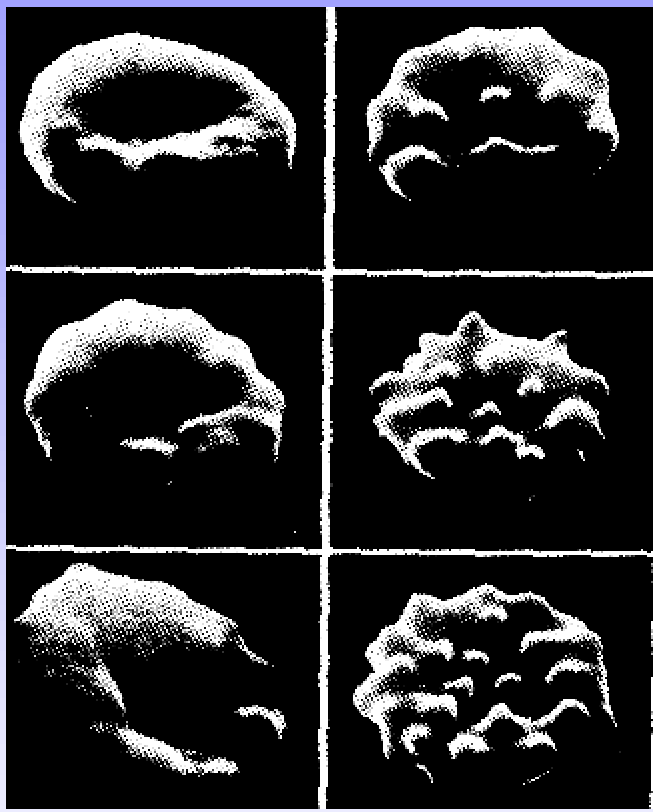
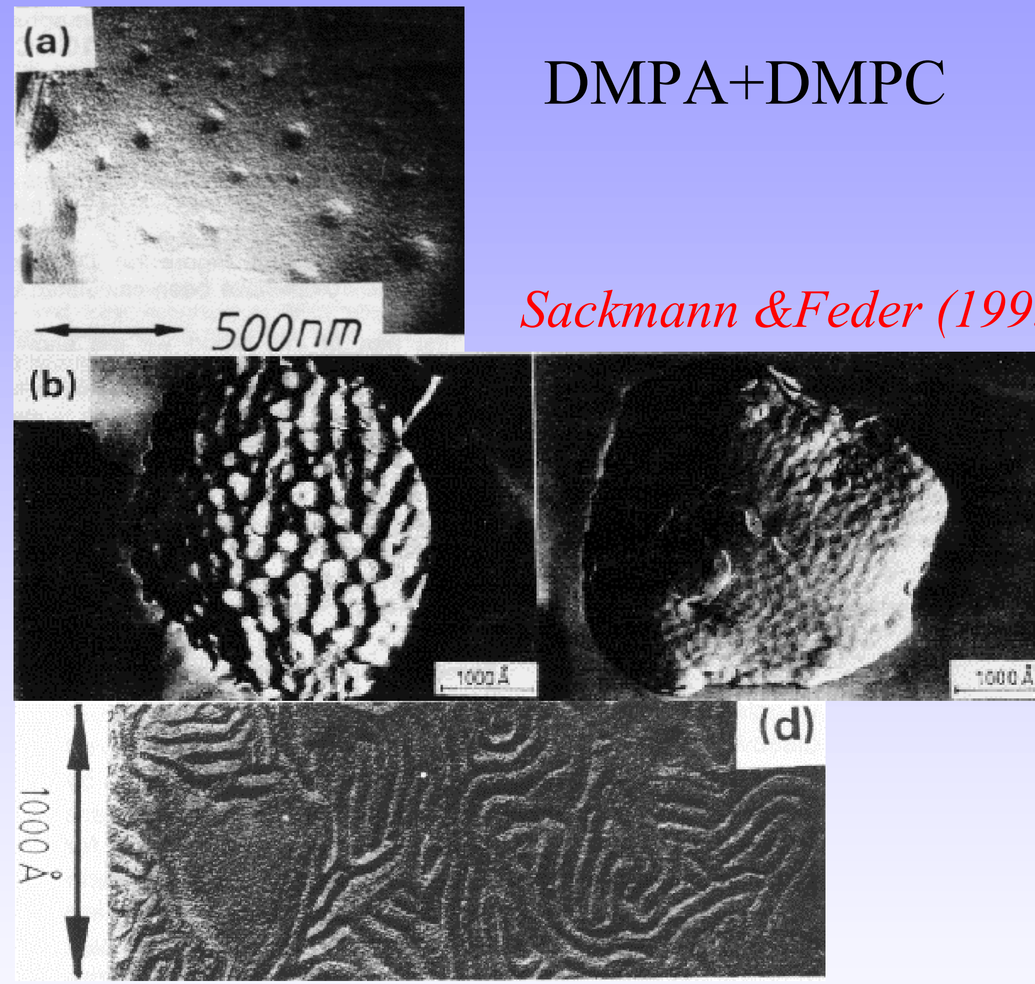
Real plasma membranes are mixtures of different lipids



Sheetz & Singer (1974)



DMPA+DMPC

Sackmann &Feder (1995)

Echinocytosis: related to chemical environment (PH) change

Suggesting coupling between local curvature and phase separation

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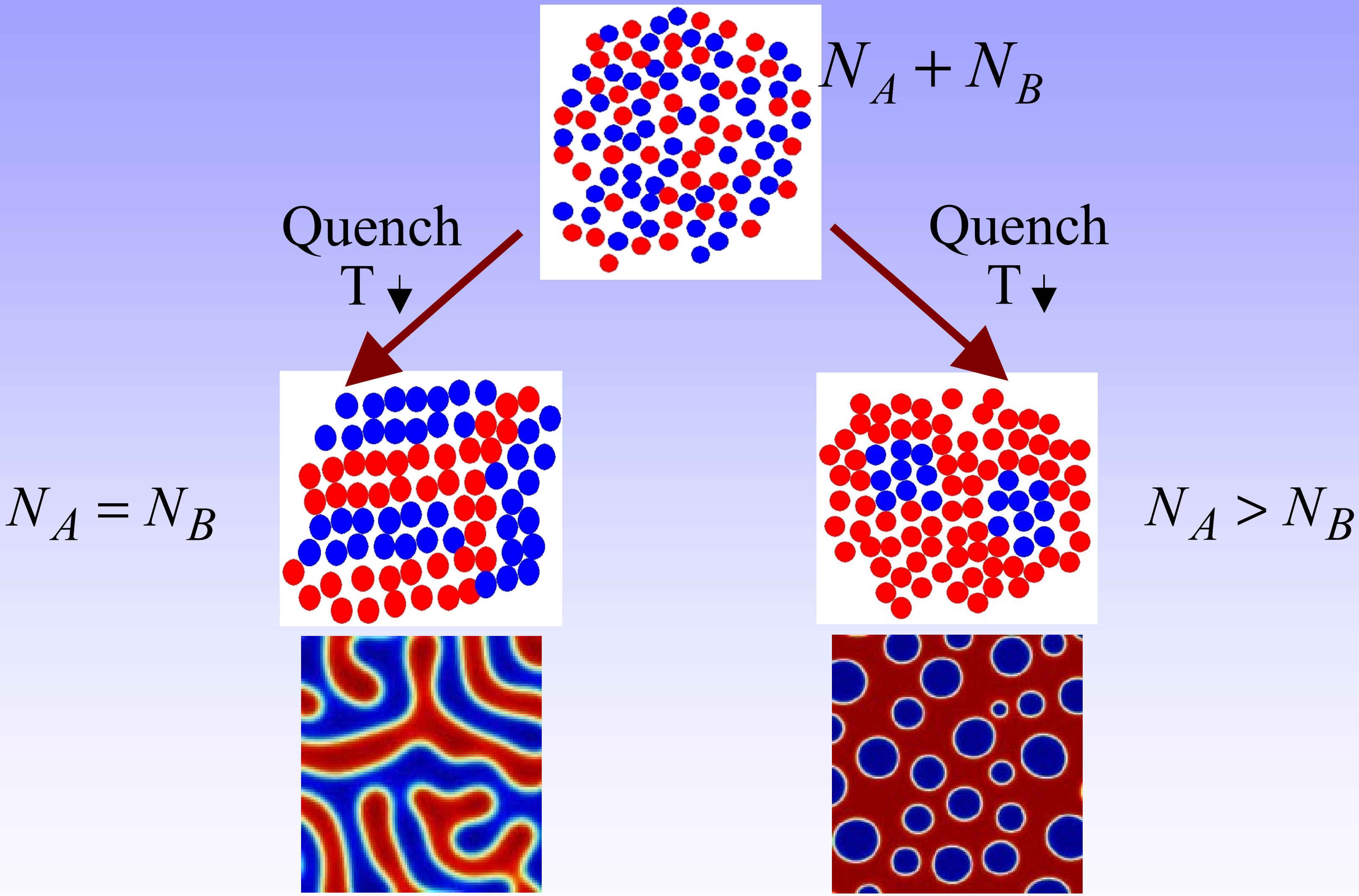
Phase Separation



Consider concentrations instead of single molecules

Phase & Shape

$$F = \int dS \left[\frac{\kappa_1}{2} (H - H_0)^2 + \kappa_2 K + \frac{\xi}{2} g^{ij} \varphi_{,i} \varphi_{,j} + V(\varphi) + \Lambda \varphi H \right]$$

Elastic bending

K term disappear for closed surfaces

H_0 is determined by membrane asymmetry

Phase separation

$$V(\varphi) = \frac{\alpha}{4} \varphi^4 - \frac{\beta}{2} \varphi^2$$

Coupling

bilinear coupling dictated by symmetry

$$dS = \det(g^{ij}) dX_i dX_j$$

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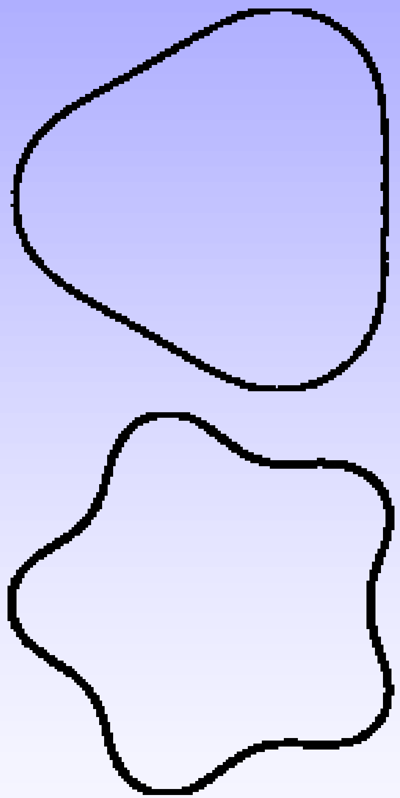
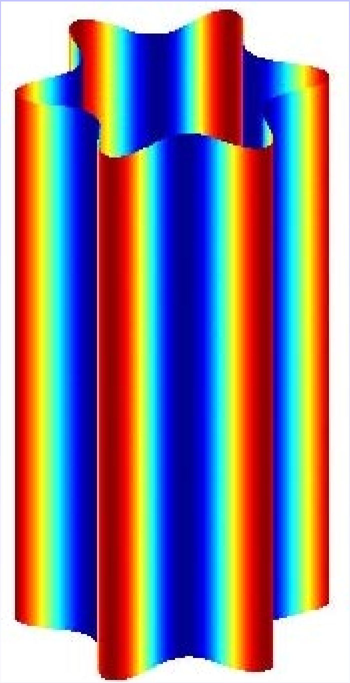
Equilibrium Phase and Shape



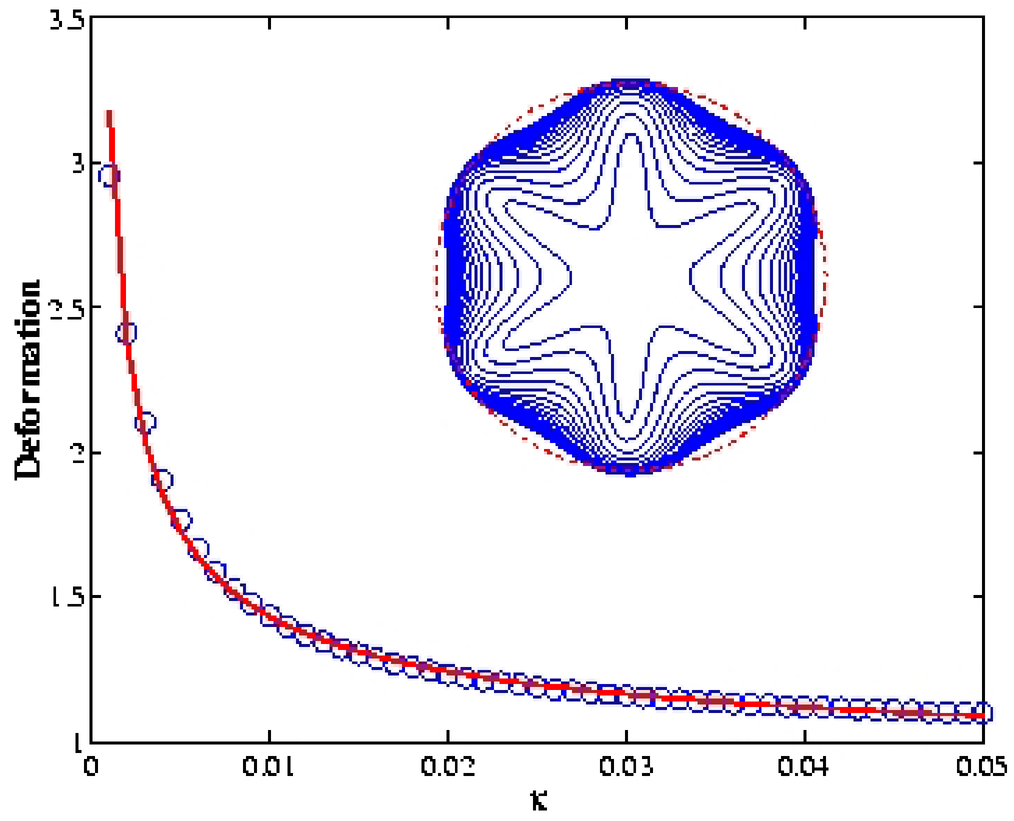


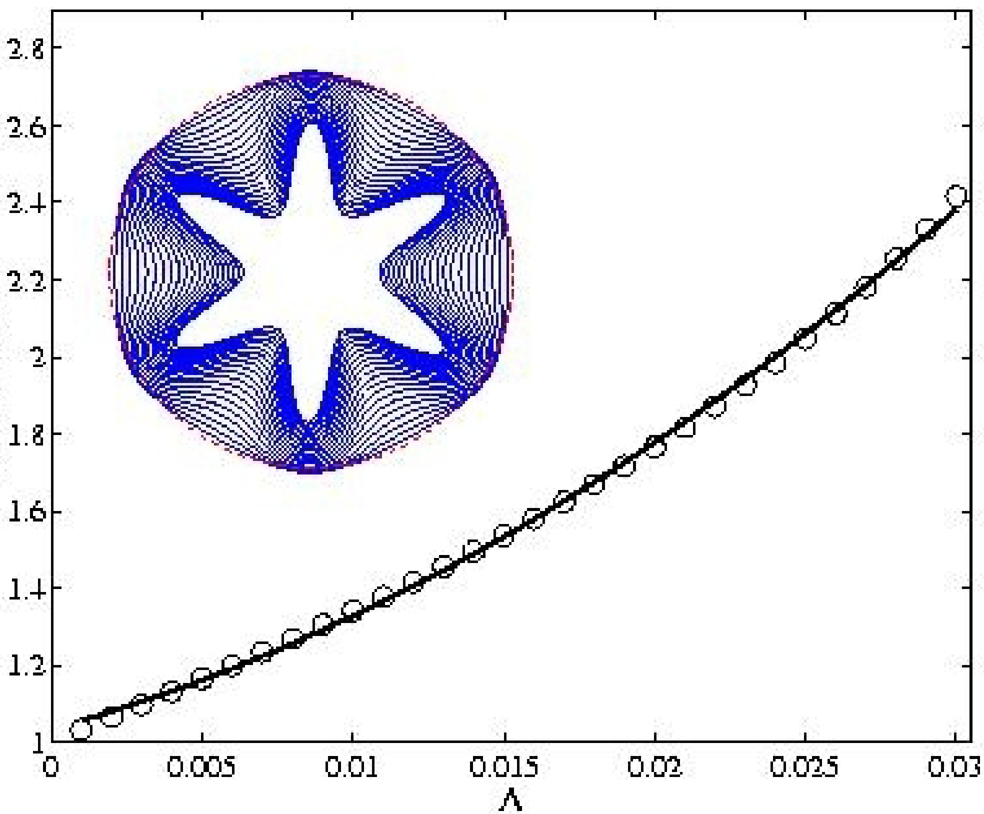
YJ et al. (2000)

Deformation

As a function of

elastic rigidity **coupling strength**





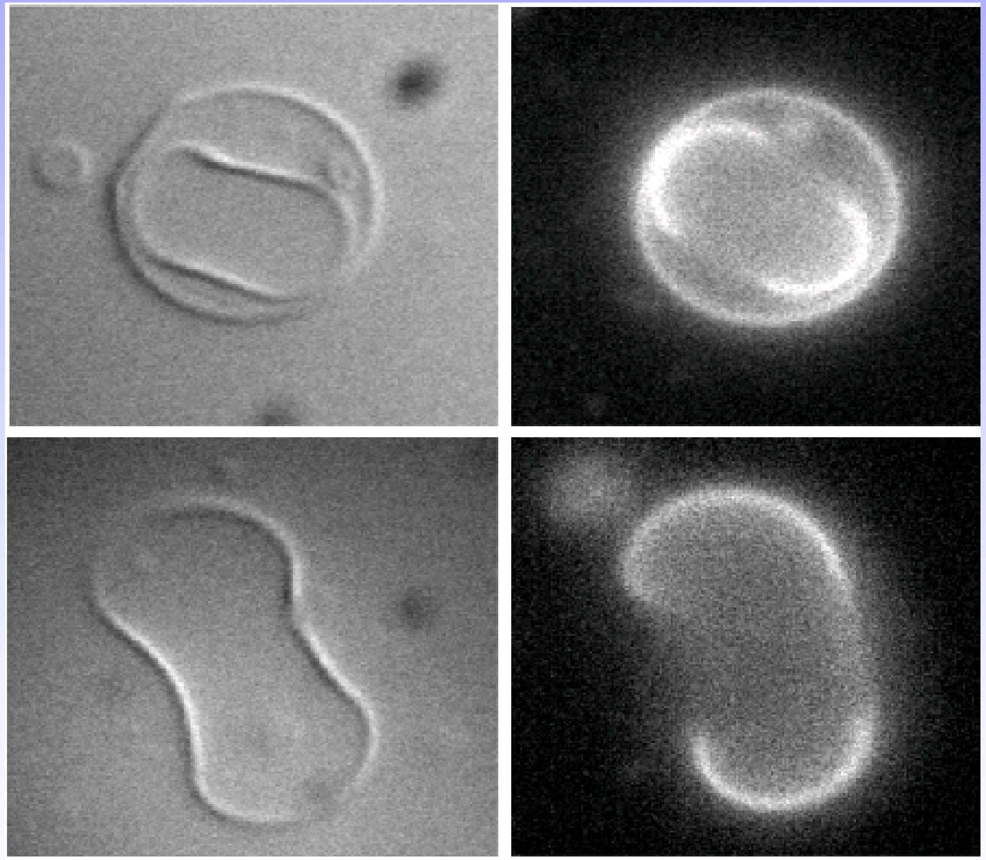
Composition & Curvature

Vesicles are DLPC/DPPG mixture, stained with 1:1000 AS dye; collected at 25^{o}C.

Non-spherical morphologies may be formed when the membrane components phase segregate.

Drastic changes in curvature result when the local structure is perturbed.

Fluid phase domains at regions of higher curvature.



P. Weiss et.al (2000)

PENNSTATE

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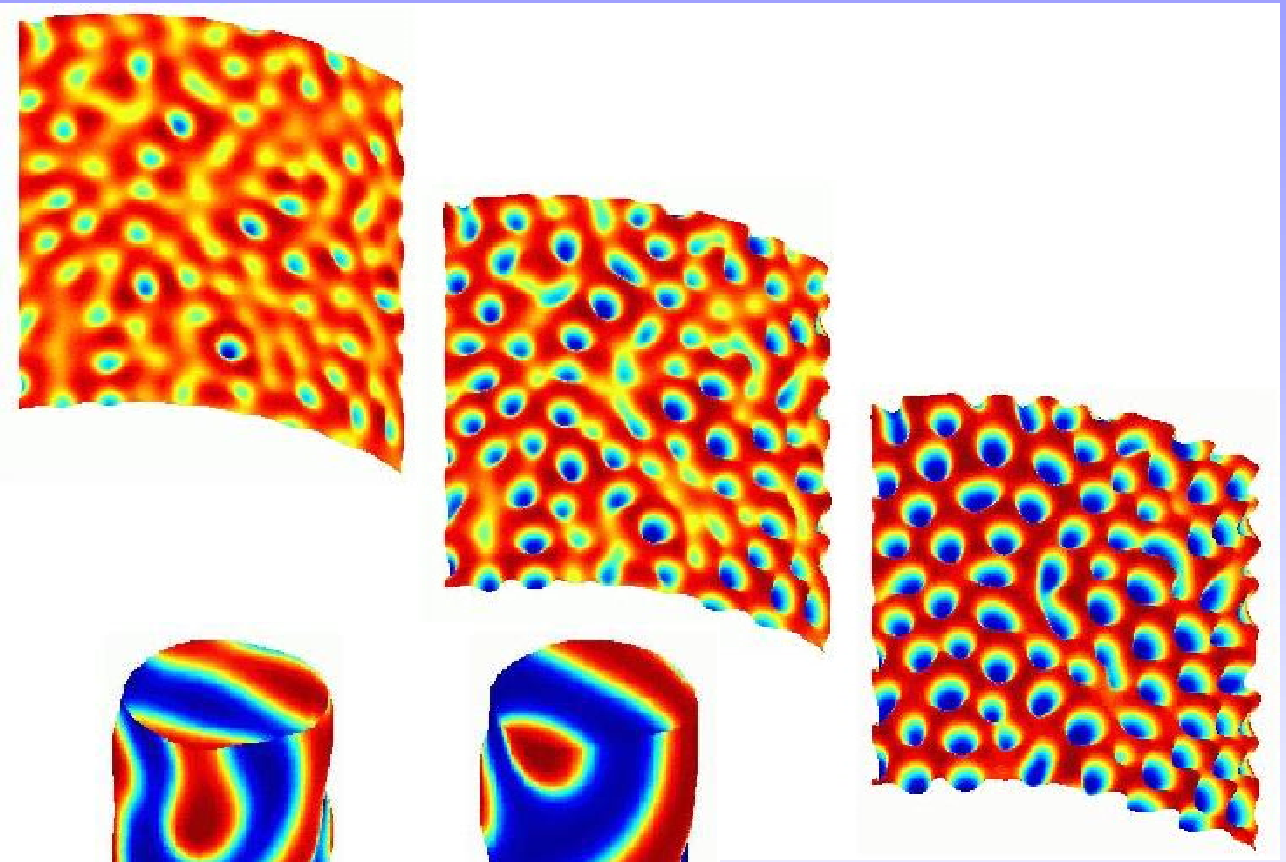
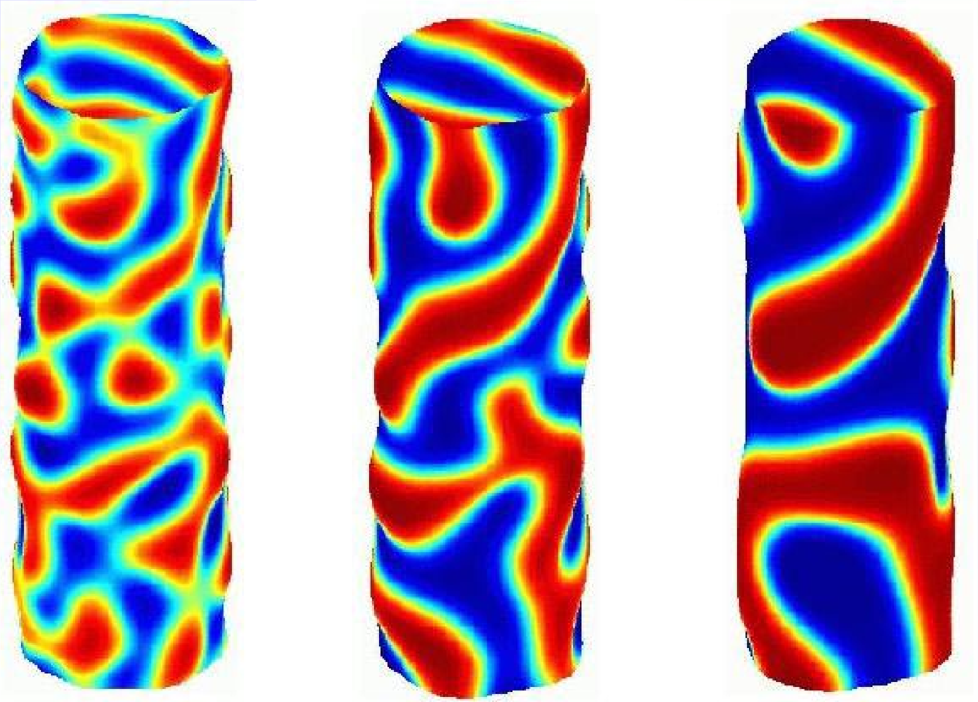
Time Evolution

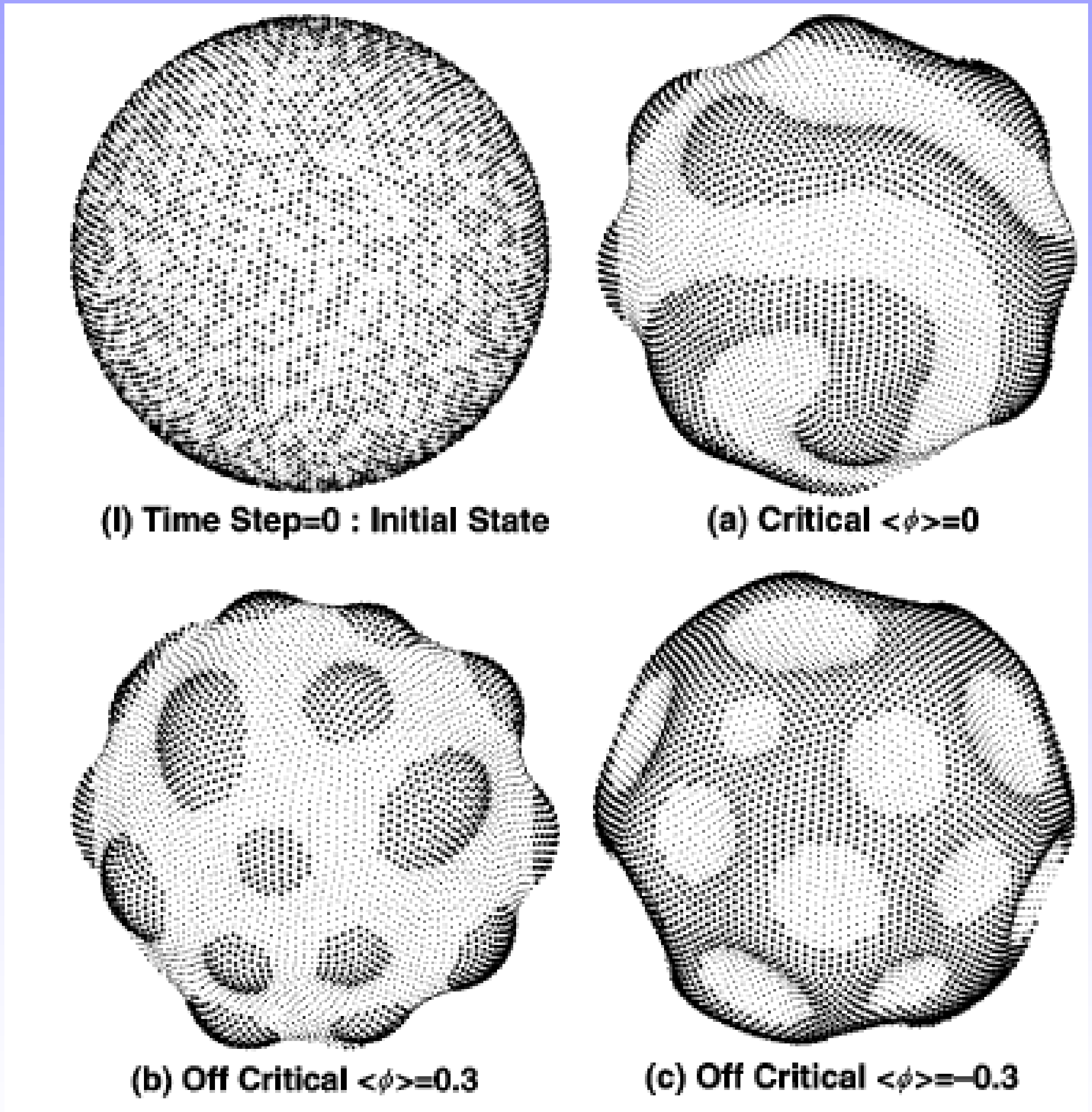
$$\frac{\partial \varphi}{\partial t} = \nabla^2 \frac{\delta F}{\delta \varphi}$$

$$\frac{\partial H}{\partial t} = -\frac{\delta F}{\delta H}$$





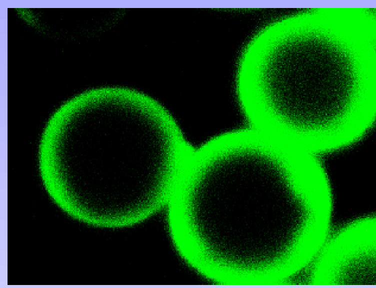
Evolution as a Function of Composition



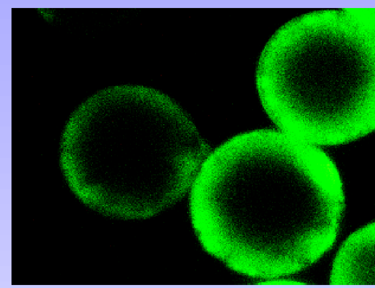
Taniguchi (1996)

Bead supported DPPC/DLPC mixture

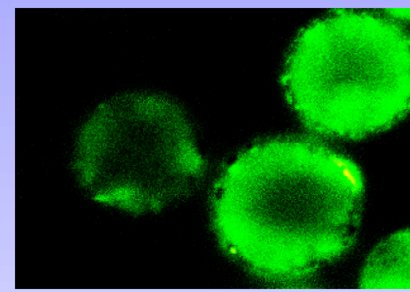
50°C Equilibrium



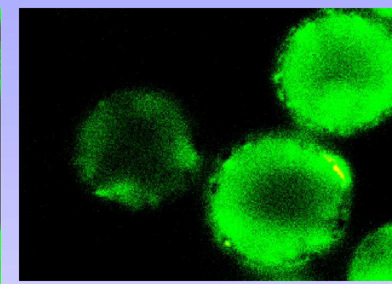
35°C -ΔH



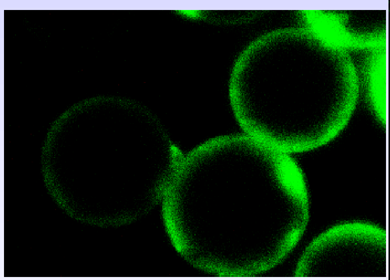
30°C -ΔH



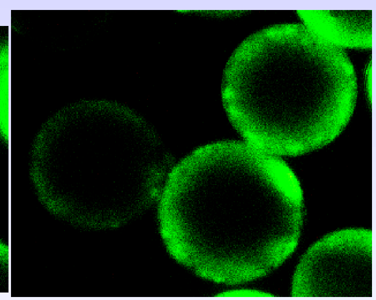
25°C -ΔH



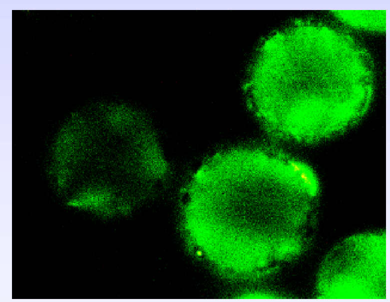
50°C +ΔH



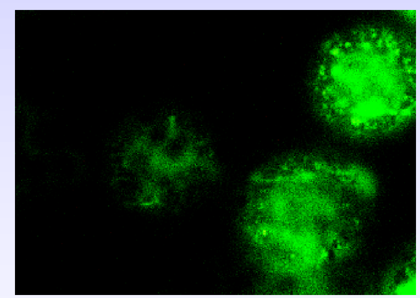
45°C +ΔH



40°C +ΔH



20°C -ΔH



T. Baranda

Evolution equation in dimensionless form:

$$\frac{\partial}{\partial t}\varphi(\vec{r},t) = -\nabla^2(\nabla^2\varphi + \varphi - \varphi^3) + \sqrt{\varepsilon}\,\eta(\vec{r},t) \quad (1)$$

Local interaction energy at the surface of ***inclusions***

$$F_s = \int ds \left[h\varphi + \tfrac{1}{2} g\varphi^2 + \ldots\right]$$

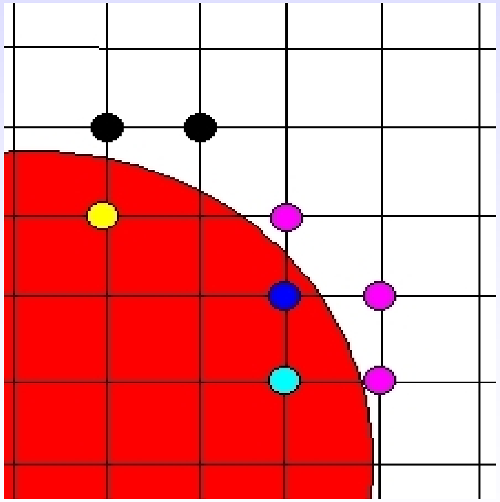
Boundary conditions:

No flux

$$\hat{n}\cdot\nabla(\nabla^2\varphi + \varphi - \varphi^3) = 0 \quad (2)$$

Surface equilibrium

$$\hat{n}\cdot\nabla\varphi + h + g\varphi = 0 \quad (3)$$



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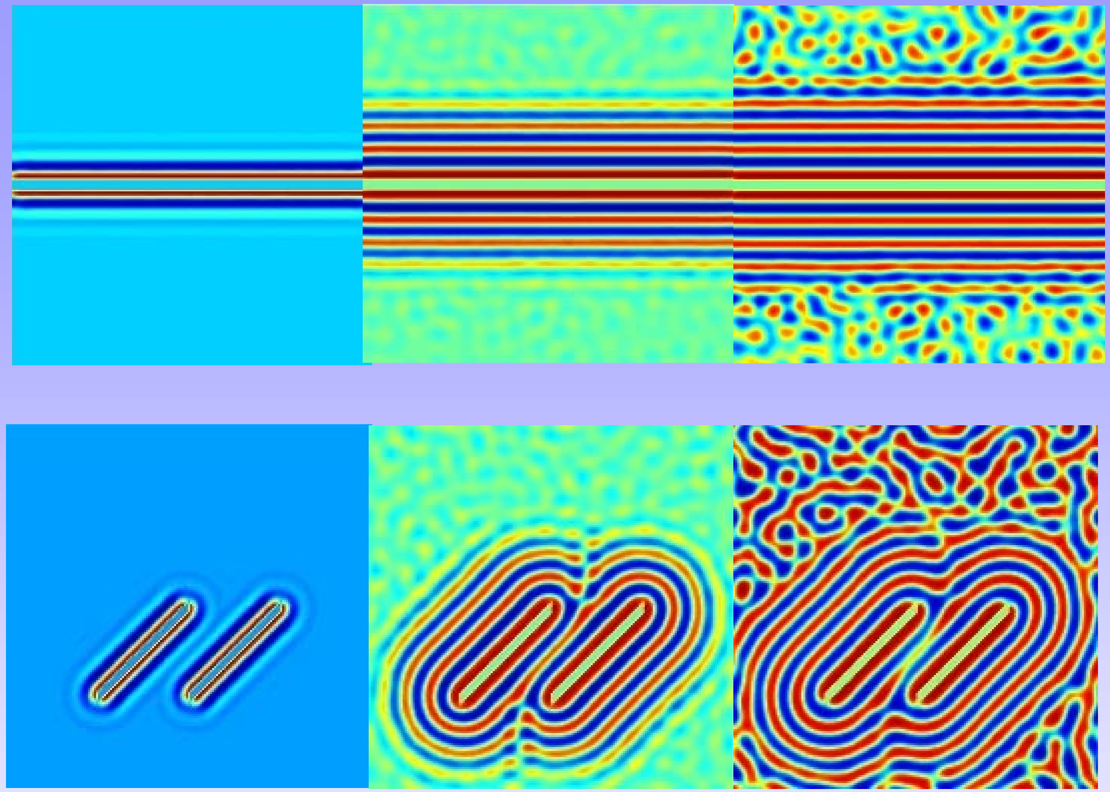
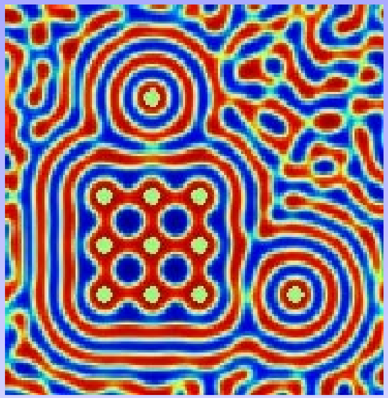
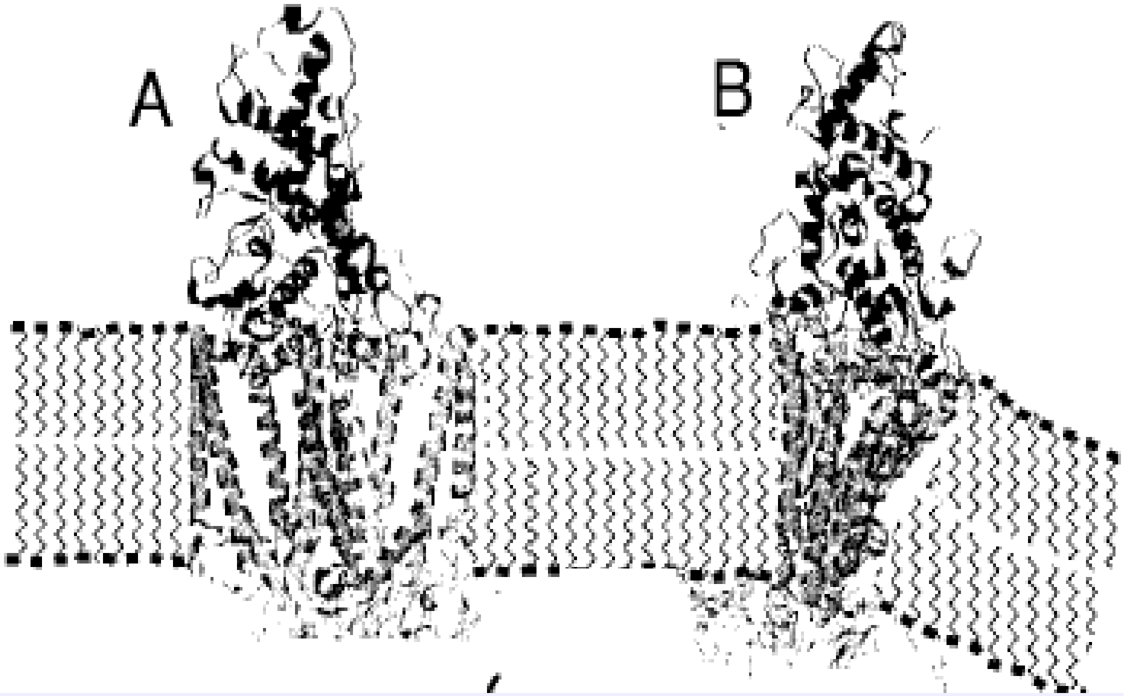


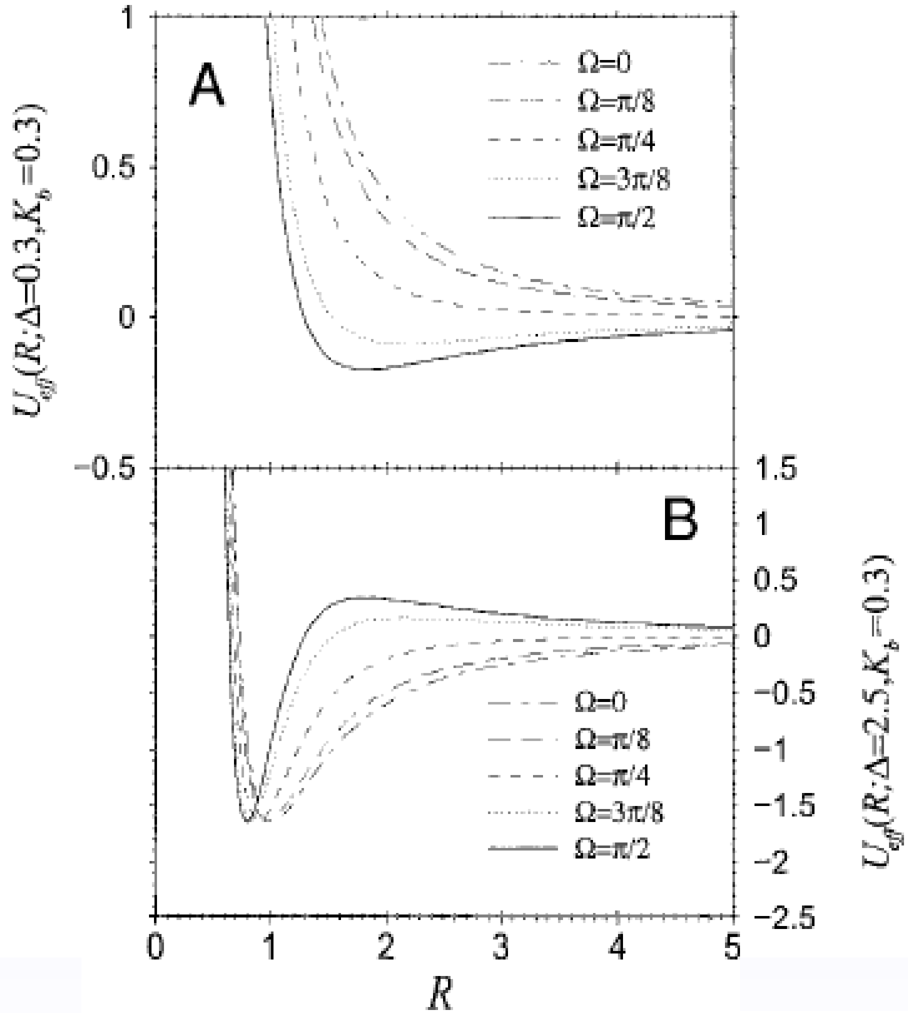


YJ & J. Douglas (2000)

- Extend of composition wave as a function of noise
- Interference of composition waves
- Stabilizing transient pattern
- Critical spacing/density

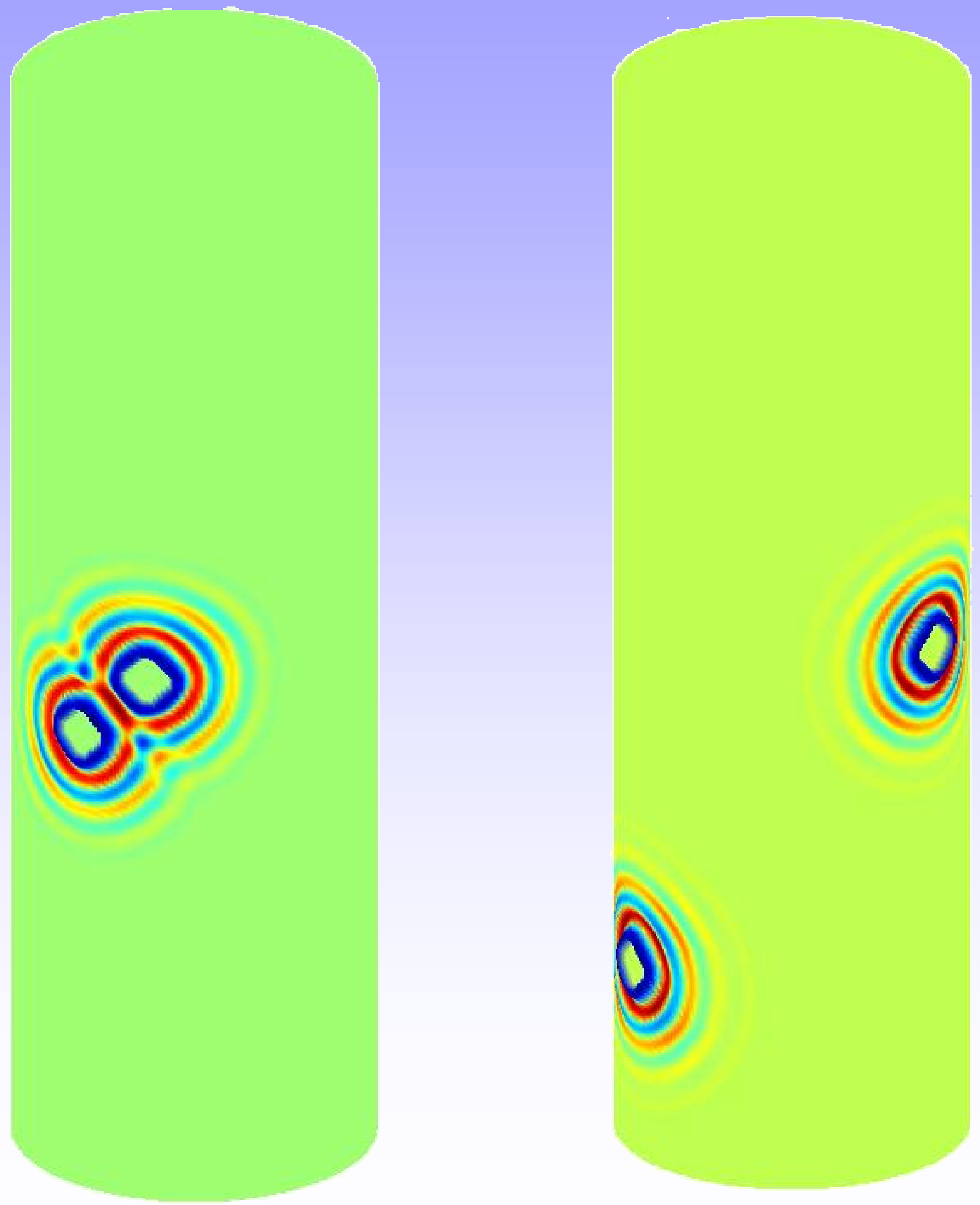
Membrane Bending-Mediated Protein Interactions





Chou et al. (2001)

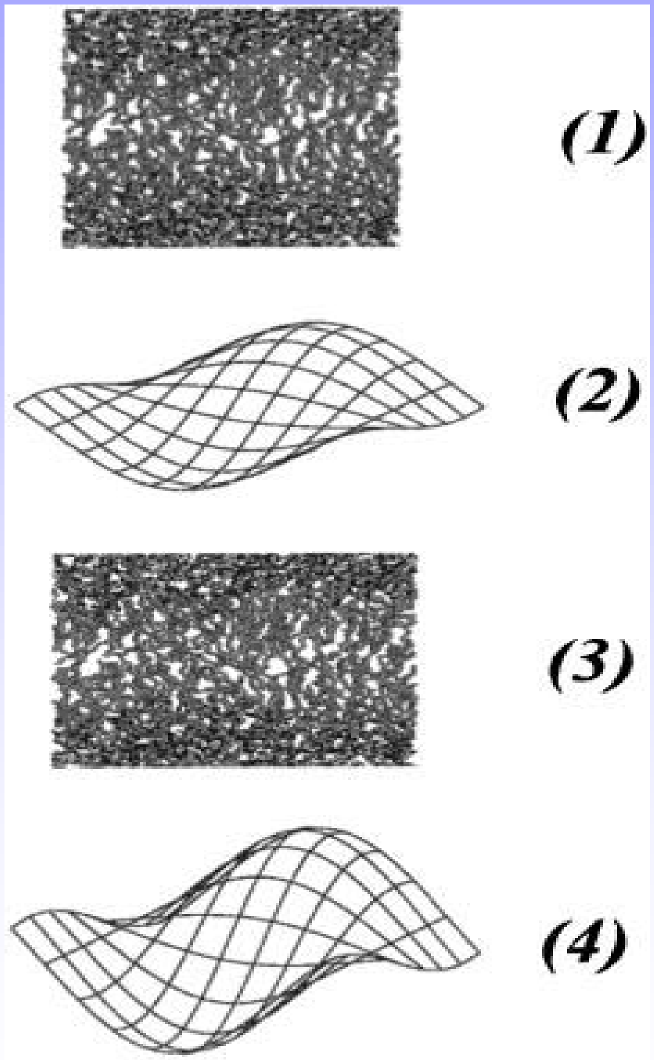
Bending elasticity + Phase Separation + Inclusions



Bridging MD & Continuum

Normal molecular dynamics for small scale membrane

Assume constitutive viscoelastic properties



Ayton et al (2001)