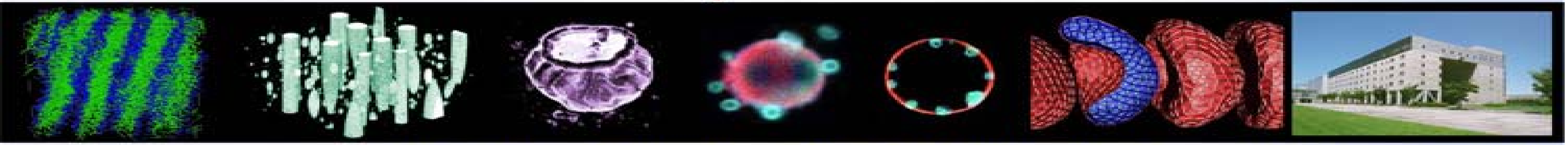
ISSP International Workshop on

Soft Matter Physics



Workshop - 1st week “Structural Rheology” 9-13 August, 2010

2nd week “Biomembranes and Vesicles” 23-27 August, 2010

Lipid membranes with free edges

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Outline

- Introduction
- Theretical analysis to an open lipid membrane with free edge(s)
- Numerical solutions
- Summary

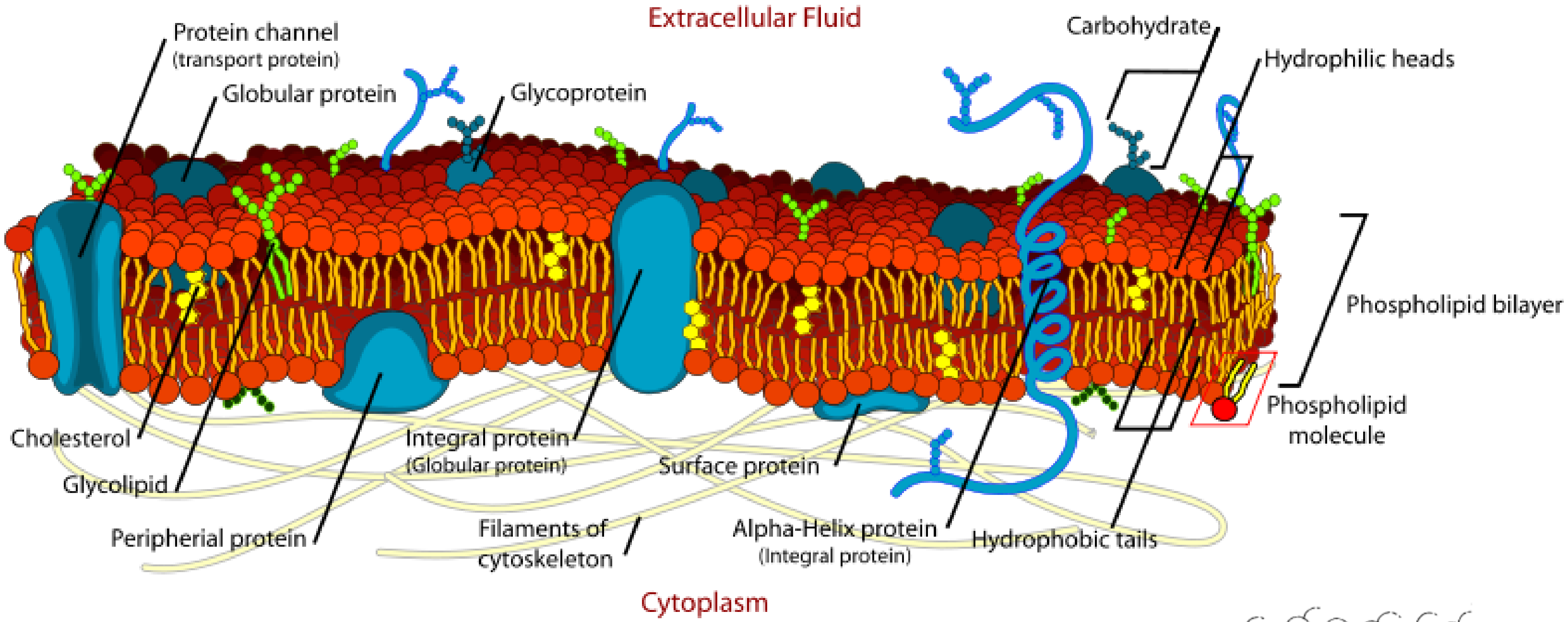
Introduction

- RBC

Human (normal): diameter 8μm, height 2 μm; biconcave discoid (why?)

No inner cellular organelles. Shapes are determined by membranes.

- Cell membrane

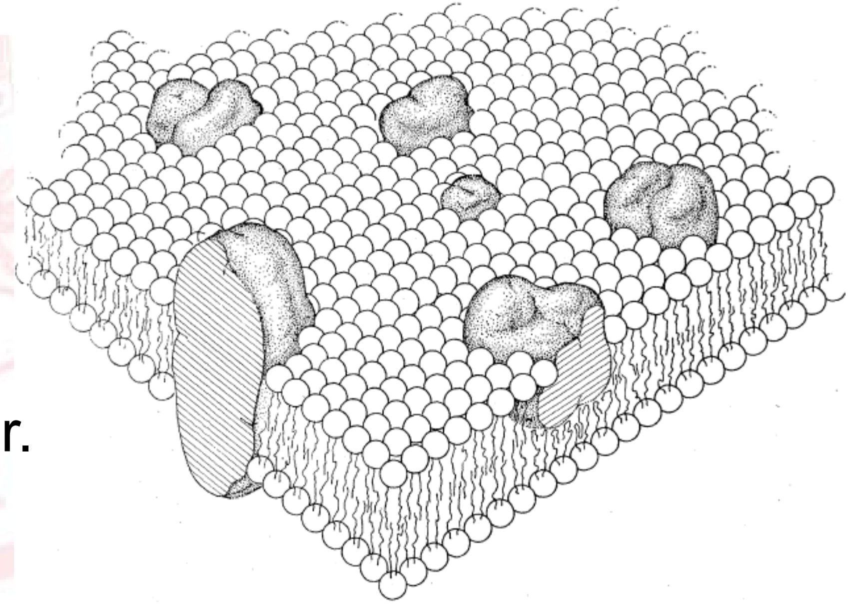


Fluid mosaic model

[Singer & Nicolson (1972) Science]

Shape determined mainly by lipid bilayer.

Lipid bilayer in liquid crystal phase



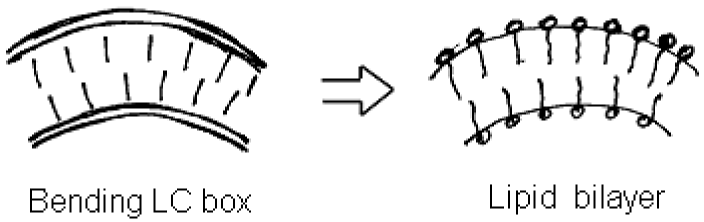
- Spontaneous curvature model [Helfrich (1973)]

$$g=\frac{k_c}{2}(2H+c_0)^2-\bar{k}K$$

Mean curvature

Gaussian curvature

spontaneous curvature

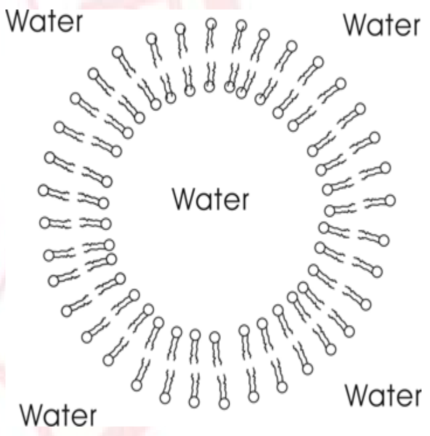


Analogy

- Shape equation of vesicles [Ou-Yang & Helfrich (1987)]

$$F=\int g\,dA+\lambda\int dA+\Delta p\int dV$$

$$\delta F=0$$



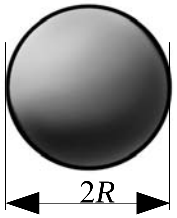
$$\Delta p-2\lambda H+2k_c\nabla^2 H+k_c(2H+c_0)(2H^2-c_0H-2K)=0$$

Describes the equilibrium shapes. called Shape equation

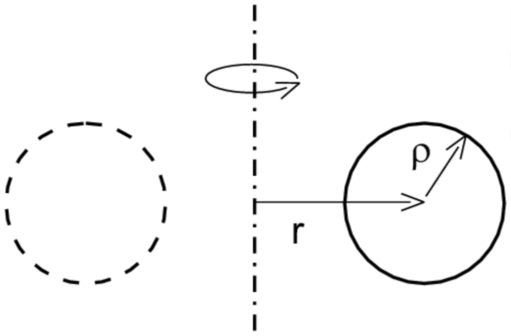
- Only 3 Analytical solutions (lipid vesicles)

Spherical surface

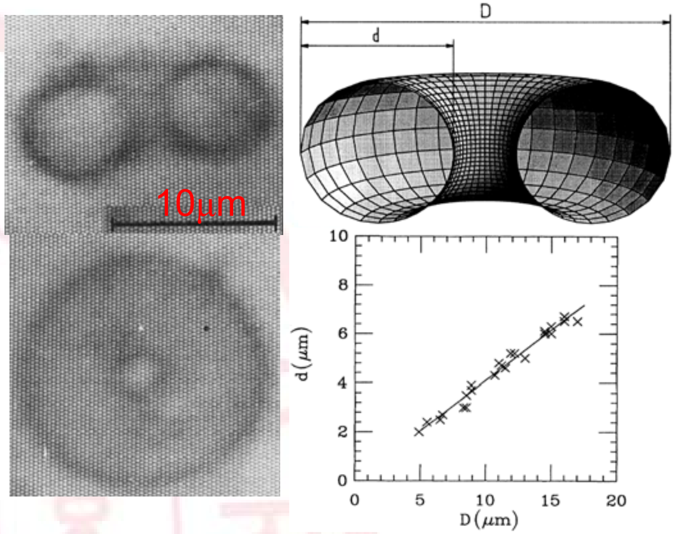
Shape equation=> $\Delta\, p R^2+(2\lambda+k_c c_0^2)R-2k_c c_0=0$



Torus [Ou-Yang (1990) PRA]



Shape equation=> $\frac{r}{\rho}=\sqrt{2}\Rightarrow\frac{D}{d}=\sqrt{2}+1\approx 2.4$

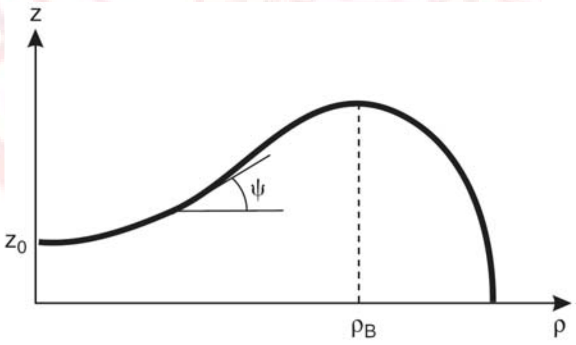


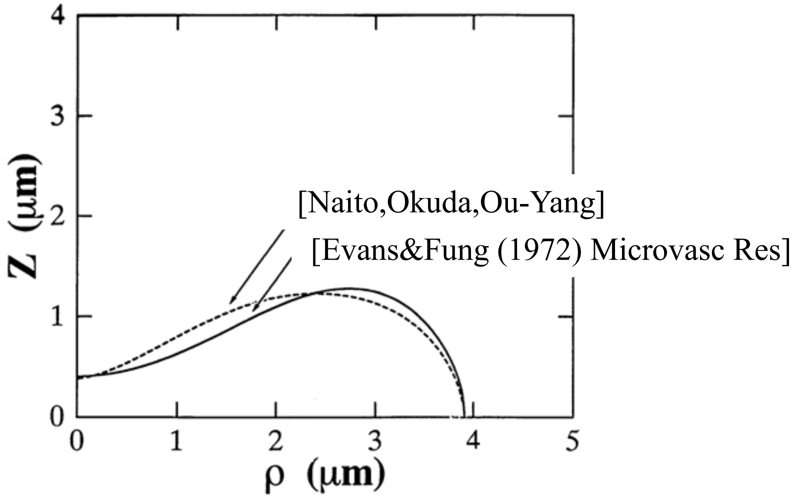
[Mutz-Bensimon (1991) PRA]

RBC[Naito,Okuda, Ou-Yang (1993) PRE]

Shape equation

$$\begin{cases}\sin\psi=c_0\rho\ln(\rho/\rho_B)\\ z=z_0+\int_0^{\rho}\tan\psi\, d\rho\end{cases}$$





- # Experiment: lipid vesicles opened by Talin

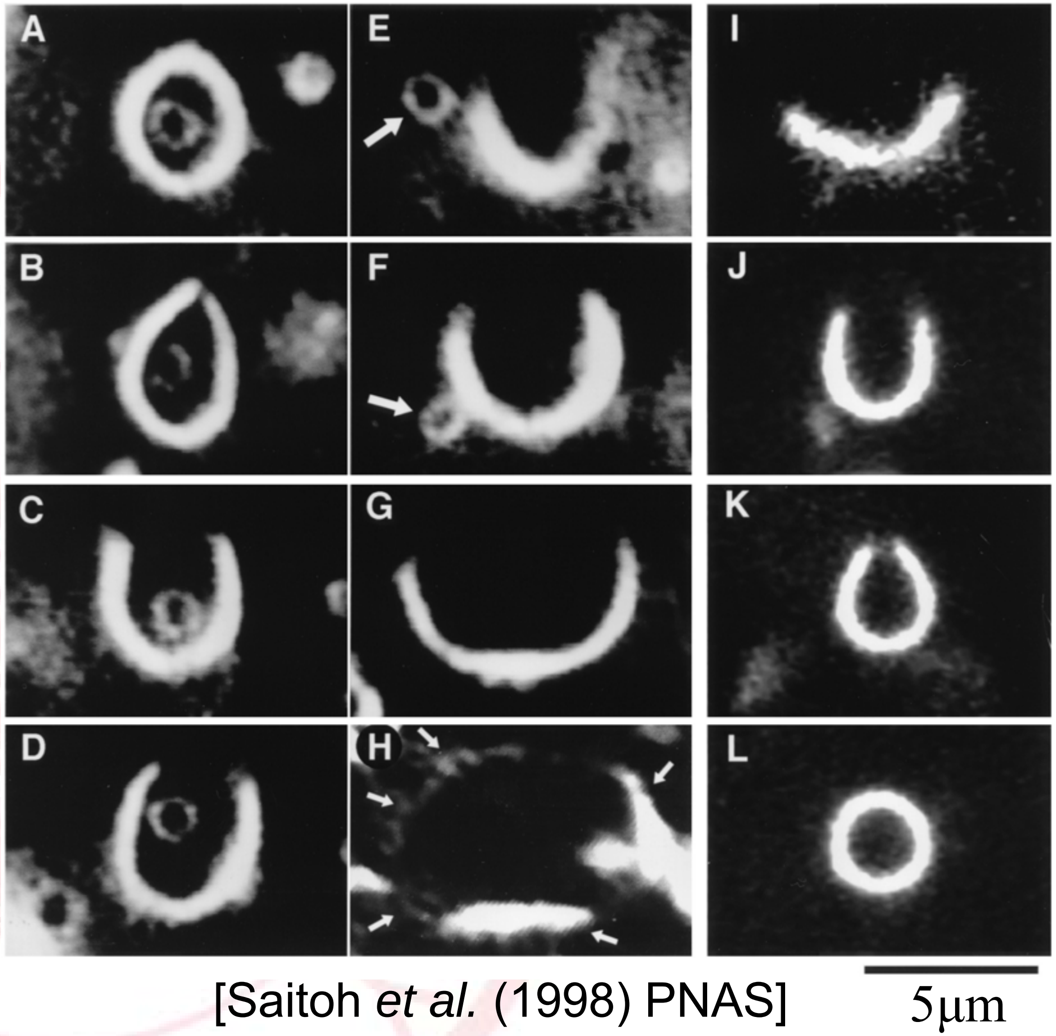
Experimental facts

(1) Talin opens the closed lipid vesicles

(2) Talin adheres to the free edge(s)

(3) The size of hole is enlarged with increasing the concentration of talin

(4) The process is partially reversible if decrease the concentration of talin



[Saitoh *et al.* (1998) PNAS]

- # Motivation of our work

(1) Can we derive the equation(s) to describe the equilibrium configurations of lipid membranes with free edges?

(2) Can we find analytical solutions?

(3) Numerical solutions to explain experimental results

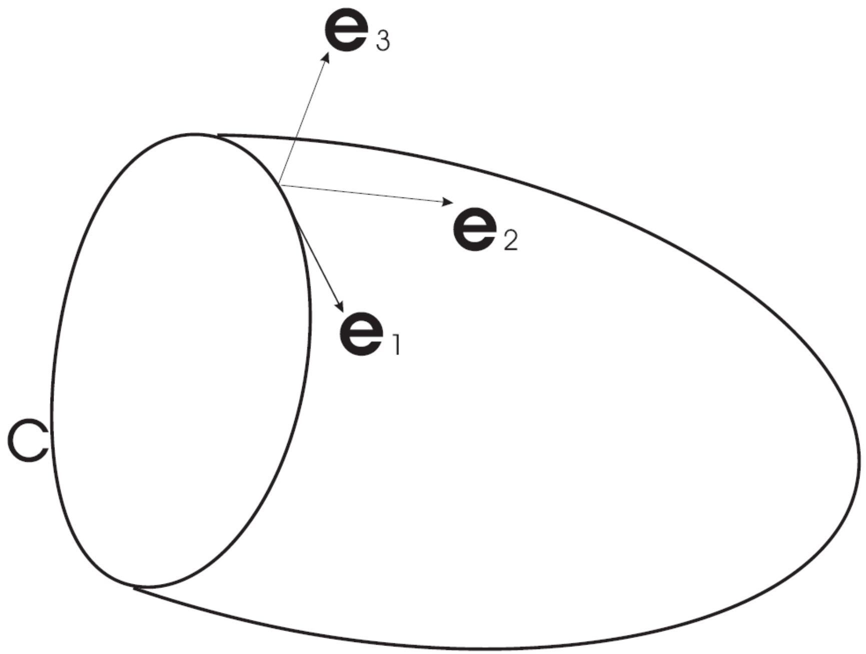
Theretical analysis to an open lipid membrane with free edge(s)

- Model

Free energy

$$F = \int G\, dA + \gamma \oint ds$$

$$G = \frac{k_c}{2}(2H + c_0)^2 + \bar{k}K + \lambda$$



Smooth surface with boundary curve C

Orthogonal moving frame

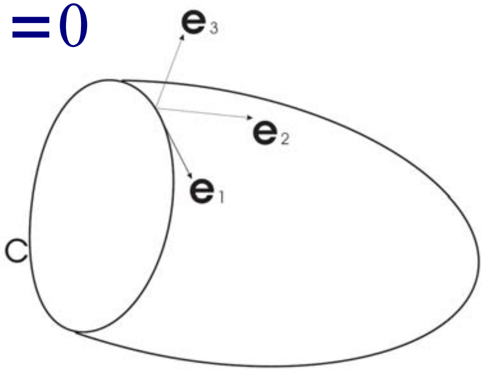
γ : Line tension, related to the concentration of talin in the experiment

$$\delta F = 0 \Rightarrow \text{shape equation} + \text{boundary conditions}$$

Governing equations

Shape equation: force balance in the normal direction

$$k_c(2H+c_0)(2H^2-c_0H-2K)-2\lambda H+2k_c\nabla^2 H=0$$



Boundary conditions (curve C satisfies...)

$$k_c(2H+c_0)+\bar{k}k_n=0$$

Moment balance equation of points in the edge along normal direction

$$-2k_c\frac{\partial H}{\partial \boldsymbol{e}_2}+\gamma k_n+\bar{k}\frac{d\tau_g}{ds}=0$$

Force balance equation of points in the edge around $\mathbf{e}_1$

$$\frac{k_c}{2}(2H+c_0)^2+\bar{k}K+\lambda+\gamma k_g=0$$

Force balance equation of points in the edge along $\mathbf{e}_2$

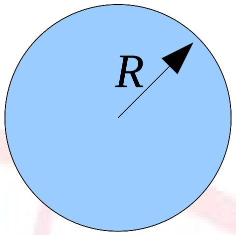
Note: above equations are also valid for an open membrane with more than one edges.

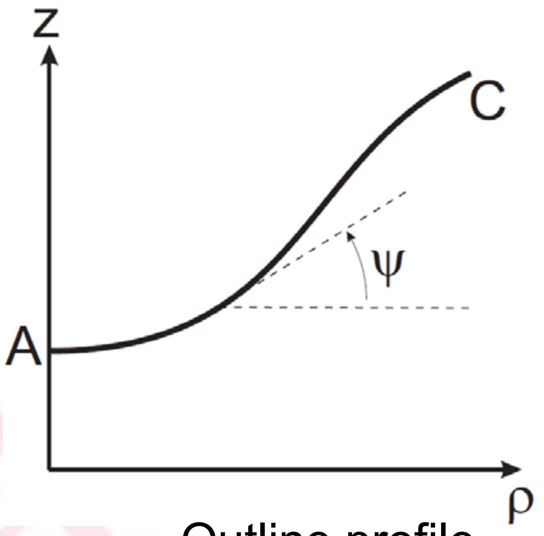
[Capovilla, Guven, Santiago (2002) PRE; Tu & Ou-Yang (2003) PRE]

- Analytical solutions

\# Trivial case: planar disk

$$\lambda R+\gamma=0$$





Outline profile

\# Axisymmetric nontrivial cases

Shape Eq=> $$(h-c_0)\left(\frac{h^2}{2}+\frac{c_0h}{2}-2K\right)-\tilde{\lambda}h+\frac{\cos\psi}{\rho}(\rho\cos\psi h')'=0$$

$$\text{where } h\equiv\sin\psi/\rho+(\sin\psi)' \text{ and } K\equiv\sin\psi(\sin\psi)'/\rho$$

BCs=> $$\begin{cases}\left[h-c_0+\tilde{k}\sin\psi/\rho\right]_C=0\\ \left[-\sigma\cos\psi h'+\tilde{\gamma}\sin\psi/\rho\right]_C=0\\ \left[\frac{\tilde{k}^2}{2}\left(\frac{\sin\psi}{\rho}\right)^2+\tilde{k}K+\tilde{\lambda}-\sigma\tilde{\gamma}\frac{\cos\psi}{\rho}\right]_C=0\end{cases}$$

$$\tilde{k}=\frac{\bar{k}}{k_c},\quad \tilde{\lambda}=\frac{\lambda}{k_c},\quad \tilde{\gamma}=\frac{\gamma}{k_c}$$

$\sigma=\pm1$: orientation of boundary curve

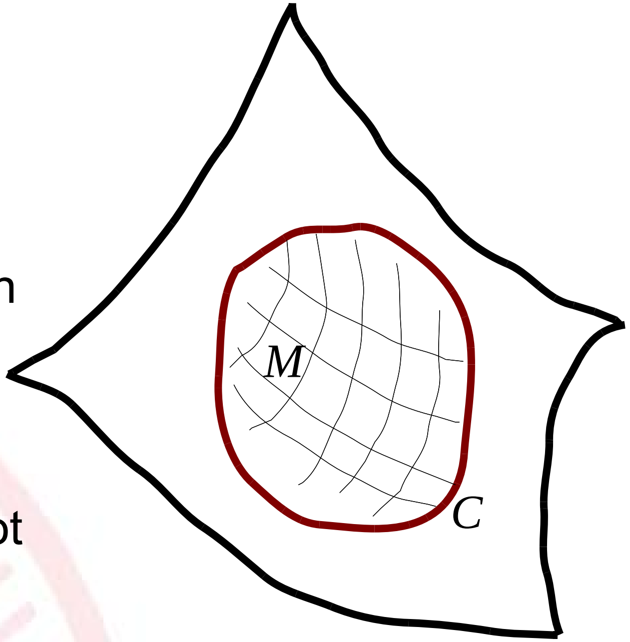
Note: shape Eq and BCs are highly nonlinear!

Procedure of finding analytical solutions:

(1) Find a surface satisfying the shape equation

(2) Find find a curve C on the surface satisfying the BCs

(3) The domain M enclosed by C on the surface is the solution



Key point:

For a given surface satisfying the shape equation, we may not always find a curve C on that surface satisfying the BCs.

Compatibility condition:

The shape equation is integrable, from which we arrive at the reduced shape Eq.

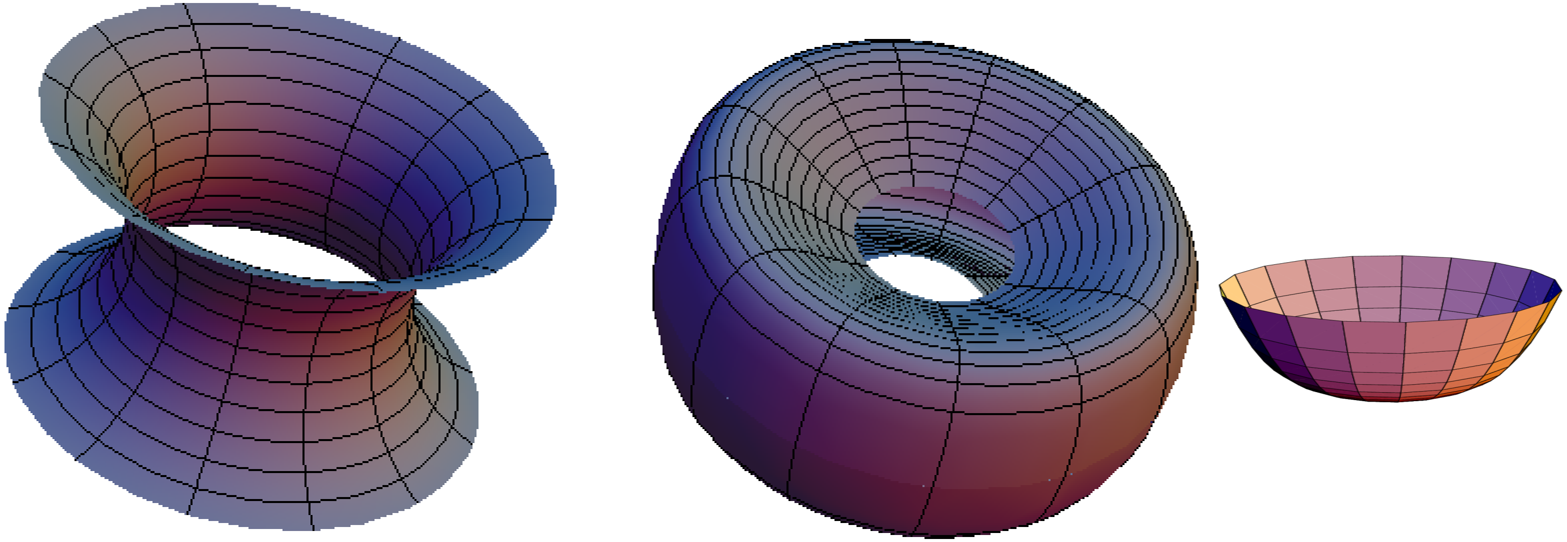
$$\cos\psi h' + (h-c_0)\sin\psi\psi' - \tilde{\lambda}\tan\psi + \frac{\eta_0}{\rho\cos\psi} - \frac{\tan\psi}{2}(h-c_0)^2 = 0 \quad \star$$

The points at the free edge should satisfy not only the reduced shape Eq but also three Bcs. Thus we derive

Compatibility condition: $\eta_0 = 0$

[Tu (2010) JCP]

Does there exist an axisymmetric open membrane being a part of a torus or a biconcave discoid?



Generation curves: $\sin\psi = \alpha\rho + \sqrt{2}, \alpha \neq 0$ $\qquad$ $\sin\psi = c_0 \rho \ln(\rho/\rho_B), c_0 \neq 0$

$$\Downarrow\star \qquad\qquad\qquad \Downarrow\star$$

$$\eta_0 = -\alpha \neq 0 \qquad\qquad \eta_0 = -2c_0 \neq 0$$

Compatibility condition is violated! Thus we have

Theorem 1. There is no axisymmetric open membrane being a part of torus generated by a circle expressed by $\sin\psi = \alpha\rho + \sqrt{2}$.

Theorem 2. There is no axisymmetric open membrane being a part of a biconcave discodal surface generated by a planar curve expressed by $\sin\psi = c_0 \rho \ln(\rho/\rho_B)$.

Does there exist an axisymmetric open membrane being a part of a constant mean curvature surface?

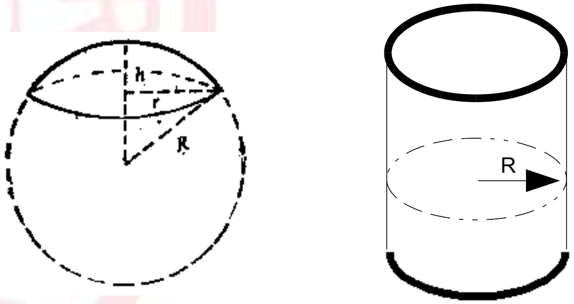
H=const. satisfies the Compatibility condition. Howerver, compatibility condition is necessary but not sufficient condition for existence of proper solutions.

In axisymmetric case, we can easily find that the shape equation and BCs cannot simultaneously be satisfied if H=const.

Theorem 3. There is no axisymmetric open membrane being a part of a constant mean curvature surface (including also spherical cap and short cylinder)

Direct consequence:

It is almost hopeless to find analytical solutions to the shape equation and BCs for lipid membranes with free edge(s).



(impossible!)

We have to invoke the numerical method!

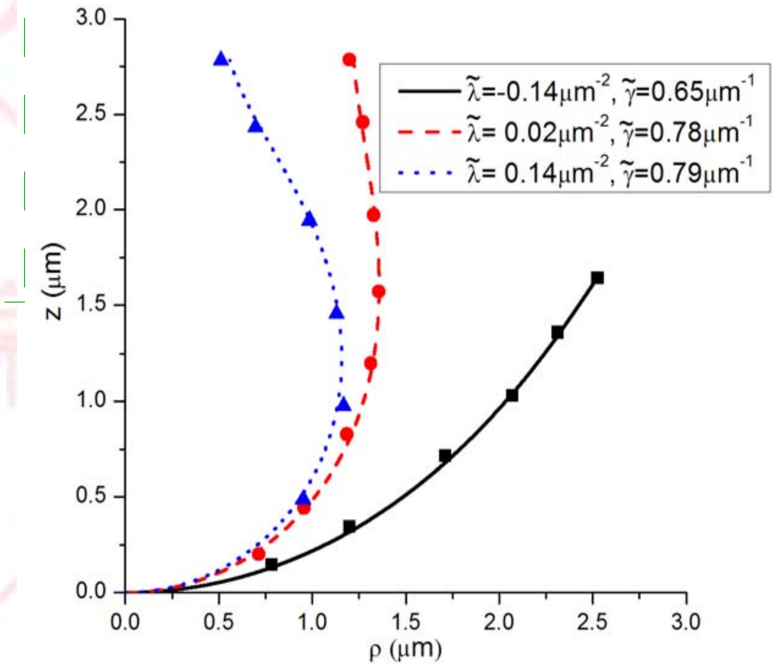
Axisymmetric Numerical solutions

Reduced SEq and BCs with the compatibility condition [Tu (2010) JCP]

SEq: $$\cos\psi h' + (h - c_0)\sin\psi\psi' - \tilde{\lambda}\tan\psi - \frac{\tan\psi}{2}(h - c_0)^2 = 0$$

2 BCs: $$\begin{cases} \left[h - c_0 + \tilde{k}\sin\psi/\rho\right]_C = 0 \\ \left[\frac{\tilde{k}^2}{2}\left(\frac{\sin\psi}{\rho}\right)^2 + \tilde{k}K + \tilde{\lambda} - \sigma\tilde{\gamma}\frac{\cos\psi}{\rho}\right]_C = 0 \end{cases}$$

Result from shoot method



Numerical results: solid, dash, dot lines

Experimental data: squares, circles, triangles

[Saitoh *et al.* (1998) PNAS]

Common parameters:

$$\tilde{k} = -0.122,\ c_0 = 0.4\,\mu\,\mathrm{m}^{-1}$$

Both results agree well with each other, which implies that line tension negatively correlate with the concentration of talin

[See also: Umeda et al.(2005)PRE based on the area difference model]

Summary

- Investigate lipid membranes with free edges based on Helfrich spontaneous curvature model
- Derive the shape equation and BCs
- Elucidate three theorems of nonexistence, which implies hopeless to find analytical solutions
- Numerical results are in good agreement with the experimental results.

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Thank you for your attention!