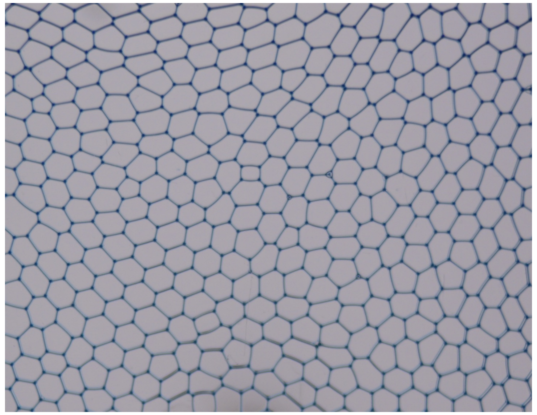
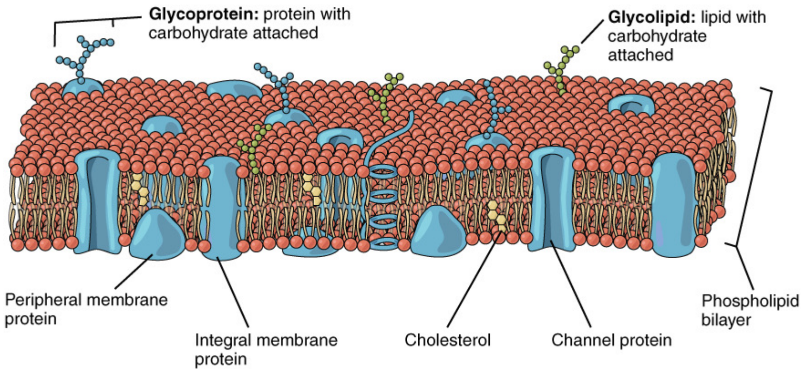
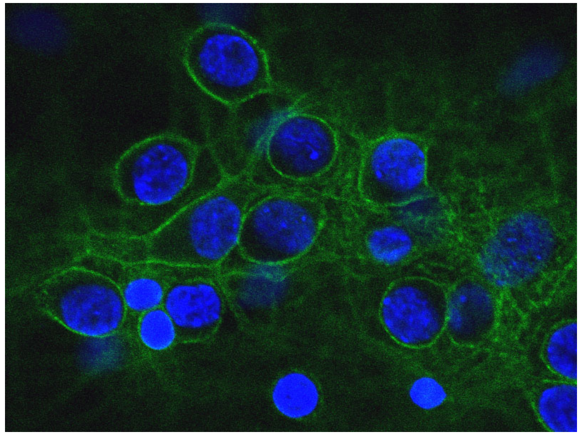
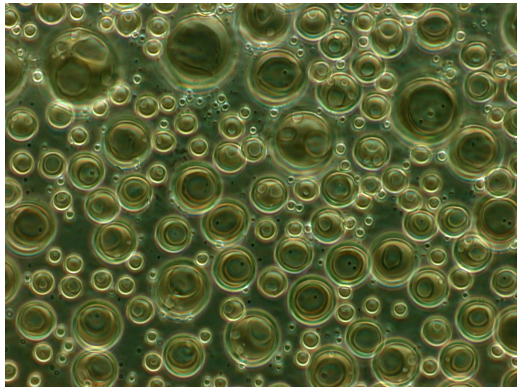
ME470: Mechanics of Soft and Biological Matter
Lecture9: Bilayer Mechanics









Red Blood Cells

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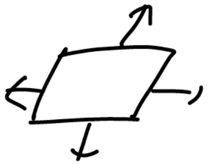
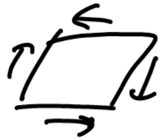
Bilayer

Membrane as 2D continuum materials

(1) stretch/compression 

(2) shear 

(3) bending 

(1) $K_A^{bl} = 2K_A^{mono} = 2(k+1)\gamma \sim 0.1 - 0.2\ J/m^2$

(can be increased by the presence of more than one molecules, e.g. $K_A^{RBC} \approx 0.45 J/m^2$, cholesterol is present)

Bilayer

- (2) In most biological/physiological situations, $\mu_A = 0$, PL molecules are liquid in plane
- (3) motivation: analogous to beam, bend a plate in one direction

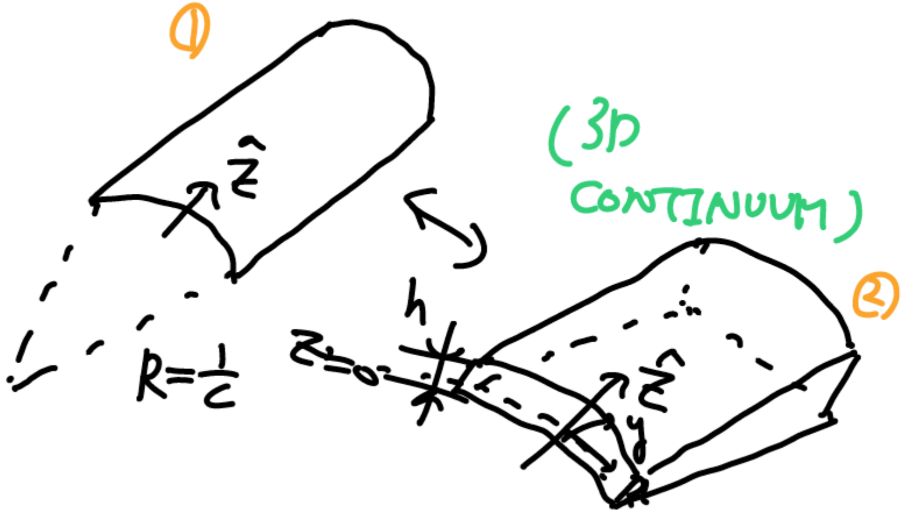
1. $U_b = \frac{1}{2} k_b \int c^2 dA$

Bending modulus for 2D membrane

2. $U_b = \frac{1}{h} \int_{-h/2}^{h/2} U_b(z) dz$

$$U_b(z) = \frac{1}{2} K_A \int \varepsilon_{ll}^2 \, dA$$

$$\varepsilon_{ll} = \varepsilon_{xx} = \frac{z}{R}$$



Bilayer

$$U_b = \frac{1}{2h} K_A \int_{-h/2}^{h/2} \int \left(\frac{z}{R}\right)^2 dA dz = \frac{1}{2}\left(\frac{h^2 K_A}{12}\right) \int c^2 dA$$

$$\boxed{k_b = \frac{1}{12} h^2 K_A}$$

Estimate: $K_A \sim 0.1 J/m^2$ $h \sim 4nm$

$$k_b \sim 30 k_B T$$

$k_b = 30 k_B T$, a little larger than measurement, because bilayer is not a continuum sheet. Another interpretation as two freely gliding monolayer yields, $k_b = K_A h^2/48$

Bilayer

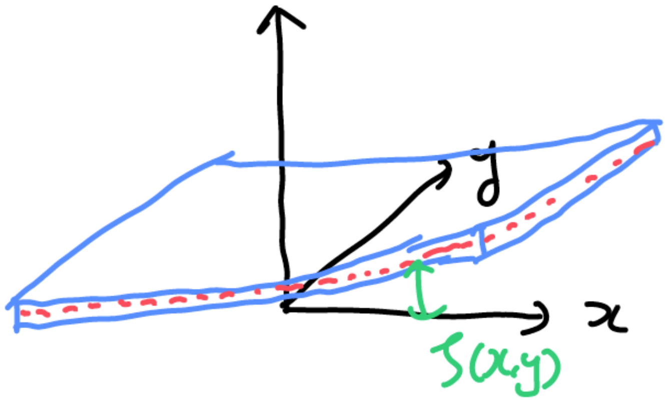
Polymer brush theory, with steric interactions

$$k_b \approx \frac{1}{24} h^2 K_A$$

Close to experiment ($k_b^{PL} \sim 10 - 20 k_B T$)

More generally: bending deformation of 3D continuum thin plate with thickness, h

Limit of small deviation from flatness ⟺ XY plane



$$z_{plate} = \varsigma(x, y)$$

Neutral plane location

Bilayer

Thin plate: easy to bend, normal forces are small

$$\sigma_{ik} n_k = 0$$

@ surfaces, but this stress projection is approximately zero throughout thickness

$$\hat{n} = \hat{z}$$

To leading order (small deviation from flatness)

$$\Rightarrow \quad \sigma_{xz} = \sigma_{yz} = \sigma_{zz} = 0$$

Use

$$\sigma_{ik} = \frac{E}{1+\nu}\left(\varepsilon_{ik} + \frac{\nu}{1-2\nu}\varepsilon_{ll}\delta_{ik}\right)$$

$$\sigma_{xz} = 0 \quad \Rightarrow \quad \frac{\partial u_x}{\partial z} = -\frac{\partial u_z}{\partial x} = -\frac{\partial \varsigma}{\partial x}$$

$$\sigma_{yz} = 0 \quad \Rightarrow \quad \frac{\partial u_y}{\partial z} = -\frac{\partial u_z}{\partial y} = -\frac{\partial \varsigma}{\partial y}$$

$$\sigma_{zz} = 0 \quad \Rightarrow \quad 0 = \frac{E}{(1+\nu)(1-2\nu)}\left[(1-\nu)\varepsilon_{zz} + \nu\left(\varepsilon_{xx} + \varepsilon_{yy}\right)\right]$$

Bilayer

$$\Rightarrow \quad u_x = -z\frac{\partial \varsigma}{\partial x} \qquad u_y = -z\frac{\partial \varsigma}{\partial y}$$

$$\Rightarrow \quad \varepsilon_{xx} = -z\varsigma_{xx} \qquad \varepsilon_{yy} = -z\varsigma_{yy} \qquad \varepsilon_{xy} = -z\varsigma_{xy}$$

$$\Rightarrow \quad \varepsilon_{zz} = \frac{\nu}{1-\nu} z\left(\varsigma_{xx} + \varsigma_{yy}\right)$$

Use energy per volume:

$$u = \frac{1}{2}\sigma_{ik}\varepsilon_{ik} = \frac{E}{2(1+\nu)}\left(\varepsilon_{ik}^2 + \frac{\nu}{1-\nu}\varepsilon_{ll}^2\right)$$

$$\frac{\nu}{1-\nu}\varepsilon_{ll}^2 = \frac{\nu(1-2\nu)}{(1-\nu)^2} z^2\left(\varsigma_{xx} + \varsigma_{yy}\right)^2$$

Bilayer

$$u = \frac{E}{2(1+\nu)} z^2 \left[\frac{1}{1-\nu}\left(\varsigma_{xx} + \varsigma_{yy}\right)^2 + 2\left(\varsigma_{xy}^2 - \varsigma_{xx}\varsigma_{yy}\right)\right]$$

$$u_A = \int_{-h/2}^{h/2} u dz = \frac{1}{2}\left(\frac{Eh^3}{12(1-\nu^2)}\right)\left[\left(\varsigma_{xx} + \varsigma_{yy}\right)^2 + 2(1-\nu)\left(\varsigma_{xy}^2 - \varsigma_{xx}\varsigma_{yy}\right)\right]$$

$$\boxed{U_{b,plate} = \frac{1}{2}\left(\frac{Eh^3}{12(1-\nu^2)}\right)\iint \left[\left(\varsigma_{xx} + \varsigma_{yy}\right)^2 + 2(1-\nu)\left(\varsigma_{xy}^2 - \varsigma_{xx}\varsigma_{yy}\right)\right] \, dxdy}$$

Bending modulus, k_b

Differential Geometry of Membrane

Note: the bending modulus still has the 2D Poisson's ratio, so it does not directly translate into 2D elasticity

$$\frac{Eh^3}{12(1-\nu^2)}$$

Note: two deformation modes can respond differently in 2D mechanics

⇨ In general (for 2D object), write

$$\boxed{U_{b,plate} = \frac{1}{2} k_b \iint \left(\varsigma_{xx} + \varsigma_{yy}\right)^2 dA + k_G \iint \left(\varsigma_{xy}^2 - \varsigma_{xx}\varsigma_{yy}\right) dA}$$

Bending modulus

Gaussian bending modulus

Two bending moduli for two deformation modes:

Mean curvature: $H \equiv \frac{1}{2}\left(\varsigma_{xx} + \varsigma_{yy}\right)$

Gaussian curvature: $K_G \equiv \varsigma_{xx}\varsigma_{yy} - \varsigma_{xy}^2$

Differential Geometry of Membrane

These are approximate expressions, for small deviation from flatness

$$\boxed{U = \frac{1}{2} k_b \iint (2H)^2 dA + k_G \iint K_G \, dA}$$

Helfrich free energy

The expression is universal, while mean and Gaussian curvatures may have different expressions

e.g.) next order in ς_x, ς_y in "Monge patch, $\varsigma(x, y)$"

$$H = \frac{\left(1 + \varsigma_y^2\right)\varsigma_{xx} + \left(1 + \varsigma_x^2\right)\varsigma_{yy} - 2\varsigma_x \varsigma_y \varsigma_{xy}}{2\left(1 + \varsigma_x^2 + \varsigma_y^2\right)^{3/2}}$$

$$K_G = \frac{\varsigma_{xx}\varsigma_{yy} - \varsigma_{xy}^2}{\left(1 + \varsigma_x^2 + \varsigma_y^2\right)^2}$$

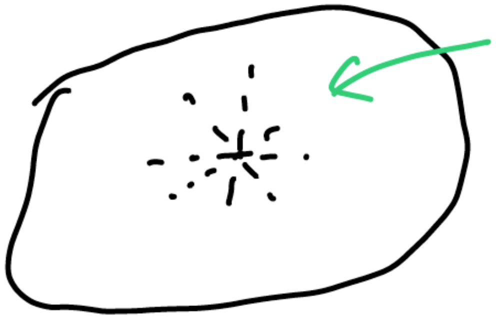
Differential Geometry of Membrane

Note: $[H] \equiv \frac{1}{m}$ $[K_G] = \frac{1}{m^2}$

Note: from elastic plate, would expect, $k_G = -(1-\nu)k_b < 0$

e.g. saddle point $\varsigma_{xx} = -\varsigma_{yy}$ ⇨ $U_b = k_G \iint \left(-\varsigma_{xy}^2 - \varsigma_{xx}^2\right) dA > 0$

More general definition of mean and Gaussian curvature:



∞LY MANY CURVATURES AT EVERY POINT

Most curved (smallest $R = R_1$)

Least curved (largest $R = R_2$)

⇨ Principle curvature $C_1 = \frac{1}{R_1}$ $C_2 = \frac{1}{R_2}$

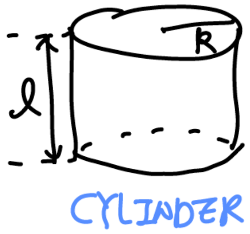
⇨ General definition:

$$\boxed{\begin{aligned} H &= \frac{1}{2}(C_1 + C_2) = \frac{1}{2}\left(\frac{1}{R_1} + \frac{1}{R_2}\right) \\ K_G &= C_1 C_2 = \frac{1}{R_1 R_2} \end{aligned}}$$

Differential Geometry of Membrane

e.g.)

$$U_b = 8\pi k_b + 4\pi k_G$$



$$U_b = \pi k_b \left(\frac{l}{R}\right)$$

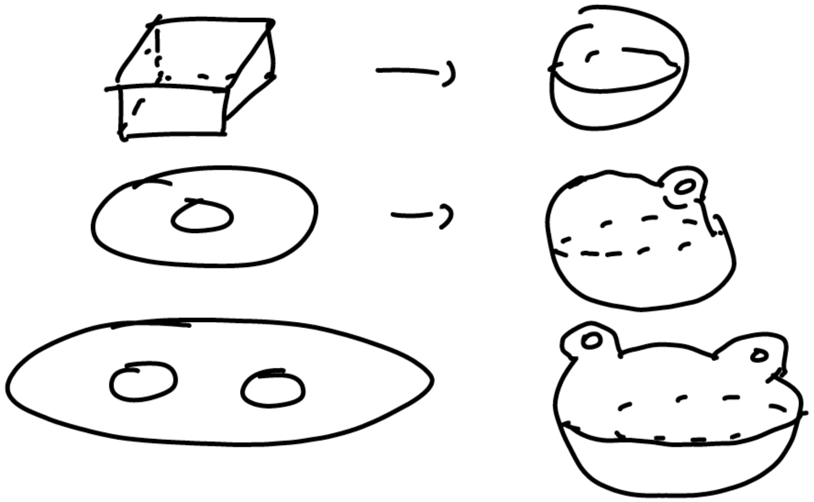
Gauss-Bonnet Theorem: for closed surface

$$\iint K_G dA = \oint K_G dA = 4\pi(1-g)$$

Where g is the topological genus of the surface

Differential Geometry of Membrane

$g =$ "Number of holes"



$g = 0$

$g = 1$

$g = 2$

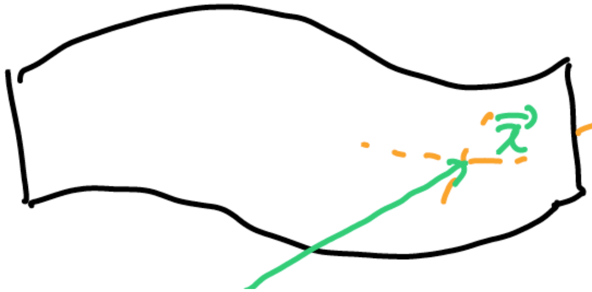
$\iint K_G dA$ is constant contribution to U_b, as long as g does not change

⇨ Can be neglected in finding equilibrium unless g changes

⇨ But also: k_G is very hard to measure

Differential Geometry of Membrane

General differential geometric formalism to compute H and K_G:



LOCAL COORDINATE SYSTEM $\vec{x}(u,v)$

First fundamental form:

$$E \equiv \left|\frac{\partial \vec{x}}{\partial u}\right|^2 \qquad F \equiv \frac{\partial \vec{x}}{\partial u} \cdot \frac{\partial \vec{x}}{\partial v} \qquad G \equiv \left|\frac{\partial \vec{x}}{\partial v}\right|^2 \qquad \Delta \equiv \sqrt{EG - F^2}$$

Second fundamental form:

$$e \equiv \frac{1}{\Delta}\left|\frac{\partial^2 \vec{x}}{\partial u^2} \cdot \left(\frac{\partial \vec{x}}{\partial u} \times \frac{\partial \vec{x}}{\partial v}\right)\right|^2$$

$$f \equiv \frac{1}{\Delta}\left|\frac{\partial^2 \vec{x}}{\partial u \partial v} \cdot \left(\frac{\partial \vec{x}}{\partial u} \times \frac{\partial \vec{x}}{\partial v}\right)\right|^2$$

$$g \equiv \frac{1}{\Delta}\left|\frac{\partial^2 \vec{x}}{\partial v^2} \cdot \left(\frac{\partial \vec{x}}{\partial u} \times \frac{\partial \vec{x}}{\partial v}\right)\right|^2$$

$\Rightarrow$

$$\boxed{H = \frac{eG - 2fF + gE}{2(EG - F^2)} \qquad K_G = \frac{eg - f^2}{EG - F^2}}$$