ME 470: Mechanics of Soft and biological matter.

LECTURE 11: VESICLE SHAPE.

CONTENTS

- MODE ANALYSIS
- HETEROGENEOUS VESICLE
- NUMERICAL METHODS

4.9. VESICLE SHAPE

GOAL: WHAT IS EQUILIBRIUM SHAPE OF VESICLE UNDER DIFFERENT CONDITIONS?

$$U_{min} = \frac{1}{2} k_b \iint (2H)^2 dA + k_g \iint K_G \, dA \Rightarrow \delta U_{min} = 0$$

MINIMIZE?
- → MODE ANALYSIS (FEW PARAMETERS)
- → SHAPE EXPANSION (MANY PARAMETERS)
- → VARIATIONAL CALCULUS (∞ PARAMETERS)
- → NUMERICAL METHODS

4.9.1. MODE ANALYSIS

IDENTIFY EASY-TO PARAMETRIZE "CARICATURES" OF VESICLE SHAPES, DETERMINE U_{tot} AS FUNCTION OF EXTERNAL PARAMETER. HERE

REDUCED VOLUME.
$$v = \frac{V_{vesicle}}{V_{\text{SPHERE OF EQUAL AREA}}}$$

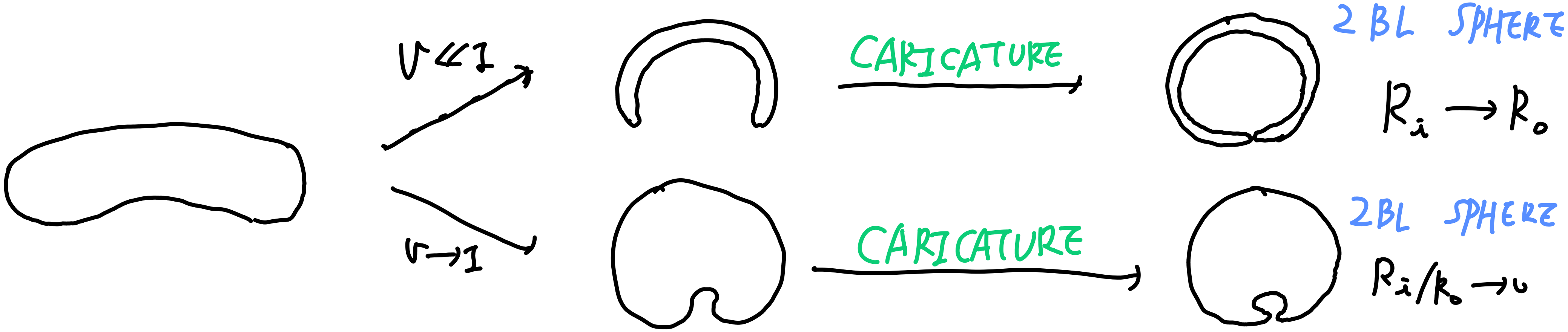
(b/c $A = \text{CONST}$ NO STRETCH, $U_{tot} = U_{bend}$)

MORE EXPLICITLY, $V_{\text{VESICLE}} = V$

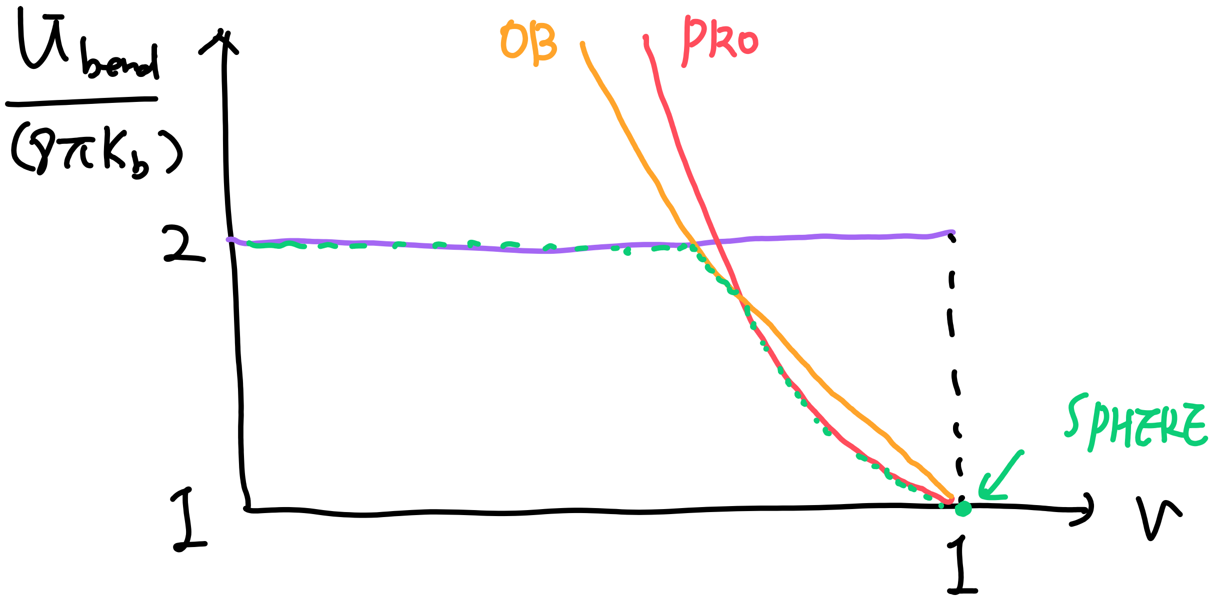
$$V_{sph} = \frac{4\pi}{3} R^3 \underset{\substack{\uparrow \\ (A=4\pi R^2)}}{=} \frac{4\pi}{3}\left(\frac{A}{4\pi}\right)^{3/2} = \frac{A^{3/2}}{6\cdot\sqrt{\pi}} \Bigg) \Rightarrow v = 6\sqrt{\pi}\,\frac{V}{A^{3/2}}$$

$v \longrightarrow 1 \Rightarrow$ SPHERE

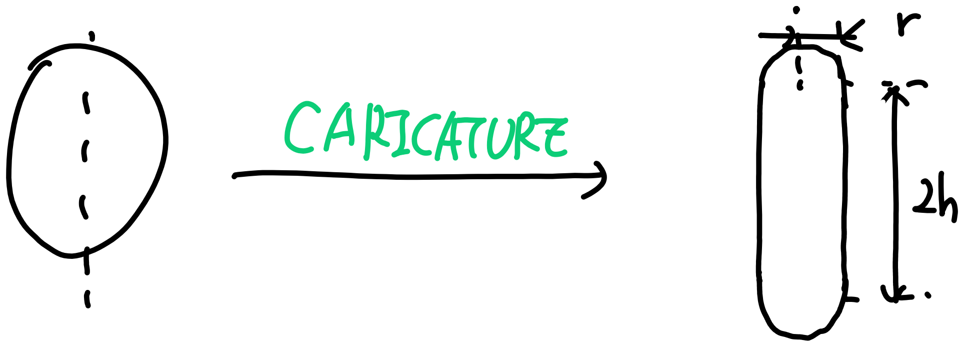
(1) "RBC STOMATOCYTES"



$\Rightarrow U_{bend}(v) = 2 \cdot 8\pi K_b$ [NEGLECT CONSTANT K_G CONTRIBUTION, $g=0$ ALWAYS]



(2) " PROLATE SPHEROIDS



SPHEROCYLINDER

$$V = \frac{4\pi r^3}{3} + \pi r^2 \cdot 2h = \frac{4\pi}{3} r^3 \left(1 + \frac{3}{2}\frac{h}{r}\right)$$

$$A = 4\pi r^2 + 2\pi r \cdot 2h = 4\pi r^2 \left(1 + \frac{h}{r}\right)$$

$$\Rightarrow v = 6\sqrt{\pi} \cdot \frac{\frac{4\pi}{3} r^3 \left(1 + \frac{3}{2}\frac{h}{r}\right)}{(4\pi r^2)^{3/2} \cdot \left(1 + \frac{h}{r}\right)^{3/2}} = \frac{1 + \frac{3}{2}\cdot\frac{h}{r}}{\left(1 + \frac{h}{r}\right)^{3/2}}$$

$$U_{bend} = 8\pi K_b + \frac{1}{2} K_b \cdot \left(\frac{1}{r}\right)^2 \cdot 2\pi r \cdot 2h = 8\pi K_b \left(1 + \frac{h}{4r}\right)$$

$\rightarrow U_{bend}(v)$

ASYMPTOTE: $\quad v \longrightarrow 1. \qquad \left(\frac{h}{r} \to 0\right)$

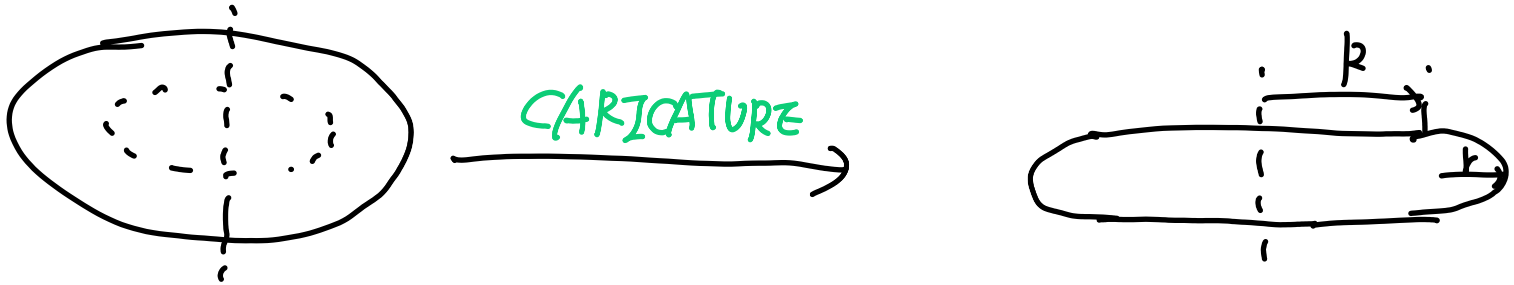
$$\Rightarrow \quad v \simeq 1 - \frac{3}{8}\left(\frac{h}{r}\right)^2 + H.O.T \quad \Rightarrow \quad \frac{h}{r} = \left[\frac{8}{3}(1-v)\right]^{1/2}$$

$$\Rightarrow \quad U_{bend} \simeq 8\pi k_b \left(1 + \frac{\sqrt{2}}{2\sqrt{3}} \cdot \sqrt{1-v}\right)$$

$$v \to 0 \quad \left(\frac{h}{r} \gg 1\right) \qquad v \simeq \frac{\frac{3}{2} \cdot \frac{h}{r}}{\left(\frac{h}{r}\right)^{3/2}} = \frac{3}{2}\left(\frac{r}{h}\right)^{1/2} \Rightarrow \frac{h}{r} = \frac{9}{4v^2}$$

$$\Rightarrow \quad U_{bend} \simeq 8\pi k_b \cdot \frac{1}{4} \cdot \frac{9}{4v^2} = \frac{9\pi}{2} k_b \cdot \frac{1}{v^2}$$

(3) "OBLATE SPHEROID"



"PANCAKE"

$$U_{bend} \simeq \frac{1}{2}K_b\left(\frac{1}{R}+\frac{1}{r}\right)^2 \cdot \pi r \cdot 2\pi R = \pi^2 K_b\, R r \cdot \left(\frac{1}{R}+\frac{1}{r}\right)^2$$

$$V = \pi R^2 \cdot 2r + \frac{\pi r^2}{2} \cdot 2\pi R = 2\pi r R^2 \left(1 + \frac{\pi r}{2R}\right)$$

$$A = 2\pi R^2 + \pi r \cdot (2\pi R) = 2\pi R^2 \left(1 + \pi \cdot \frac{r}{R}\right)$$

$$\Rightarrow \quad v = 6\sqrt{\pi} \cdot \frac{2\pi R^2 \cdot \left(1+\frac{\pi r}{2R}\right)}{(2\pi R^2)^{3/2}\left(1+\pi\frac{r}{R}\right)^{3/2}} = \frac{6}{\sqrt{2}} \cdot \frac{r}{R} \cdot \frac{1+\frac{\pi r}{2R}}{\left(1+\frac{\pi r}{R}\right)^{3/2}}$$

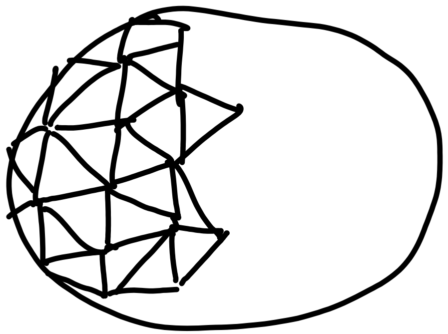
LIMIT $v \to 0$: $\quad v = \frac{6}{\sqrt{2}} \cdot \frac{r}{R} + \text{H.O.T}$

$$U_{bend} \xrightarrow{v \to 0} \pi^2 K_b \frac{R}{r} = \frac{6\pi^2}{\sqrt{2}} K_b \cdot \frac{1}{v}$$

4.9.2. NUMERICAL COMPUTATION.

ONE CAN DISCRETIZE SURFACE AS A COLLECTION OF TRIANGES

⇒ MESHING THE SURFACE.



· IMPLEMENT DIFFERENT ENERGY CONTRIBUTION. – BENDING

· ALSO, IMPOSE CONSTRAINTS USING LAGRANGE MULTIPLIER. – REDUCED VOLUME, SURFACE AREA

⇒ FROM INITIAL CONFIGURATION, MINIMIZE ENERGY USING ANNEALING ALGORITHM (STEEPEST DESCENT, CONJUGATE GRADIENT)

4.9.3 VARIATIONAL ANALYSIS

UP TO NOW, WE MINIMIZE $\mathcal{U}$ w.r.t A FINITE NUMBER OF PARAMETERS β_i

$$d\mathcal{U}=0 \iff \frac{\partial \mathcal{U}}{\partial \beta_i}=0 \quad \forall i$$

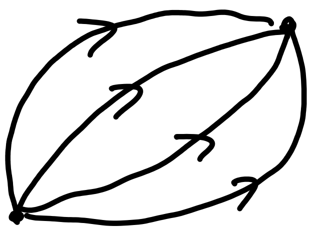
BUT, IN GENERAL, MINIMIZATION w.r.t SHAPE HAS ∞LY MANY DEGREES OF FREEDOM:

$\mathcal{U}$ IS A FUNCTIONAL OF THE SHAPE, WHICH ITSELF IS A FUNCTION OF COORDINATES. e.g) $\zeta(x,y)$

HERE, $\mathcal{U}_{bend}[H, K_G] = \mathcal{U}_{bend}(\zeta_x, \zeta_y, \zeta_{xx}, \zeta_{xy}, \zeta_{yy})$

WE NEED A METHOD FOR SYSTEMATIC MINIMIZATION OF FUNCTIONALS

! VARIATIONAL CALCULUS. (EULER-LAGRANGE MECHANICS)



POINT OBJECT MOVES FROM $\vec{x}_0$ TO $\vec{x}_1$ IN $[t_0, t_1]$ UNDER INFLUENCE OF A CLASSICAL POTENTIAL $U(\vec{x})$

$\Rightarrow$ MINIMIZATION PRINCIPLE : MINIMIZING FUNCTIONAL

ACTION

$$S \equiv \int_{t_0}^{t_1} \mathcal{L} \, dt$$

EL DENSITY

CLASSICAL MECHANICS.

$$\mathcal{L} = T - U = \frac{1}{2} m \cdot \dot{\vec{x}}^2 - U(\vec{x}) = \mathcal{L}(\vec{x}, \dot{\vec{x}})$$

KINETIC ENERGY

POINT MASS

THEOREM S IS MINIMUM IF AND ONLY IF $\mathcal{L}$ SATISFIES

$$\boxed{\vec{\nabla}_{\vec{x}} \mathcal{L} - \frac{d}{dt} \vec{\nabla}_{\dot{\vec{x}}} \mathcal{L} = 0}$$

EULER-LAGRANGE FORMULA

$\Rightarrow$ HERE: $-\vec{\nabla} U - \frac{d}{dt}(m\dot{\vec{x}}) = 0 \iff [m\ddot{\vec{x}} = -\nabla U = F]$

WHY DOES EL MINIMIZE S? CHECK IF VALUE OF S IS STATIONARY FOR A GIVEN PATH $\vec{x}(t)$!

$$S[\vec{x}] = \int_{t_0}^{t_1} \mathcal{L}(\vec{x}, \dot{\vec{x}})\, dt$$

VARIATION. $\delta S = S[\vec{x} + \vec{\varepsilon}] - S[\vec{x}]$

ARBITRARY EXCEPT $\vec{\varepsilon}(t_0) = \vec{\varepsilon}(t_1) = 0$

$$= \int_{t_0}^{t_1} \left(\mathcal{L}(\vec{x}+\vec{\varepsilon}, \dot{\vec{x}}+\dot{\vec{\varepsilon}}) - \mathcal{L}(\vec{x},\dot{\vec{x}}) \right) dt$$

EXPAND

$$= \int_{t_0}^{t_1} \left(\cancel{\mathcal{L}(\vec{x},\dot{\vec{x}})} + \vec{\varepsilon}\cdot\vec{\nabla}_{\vec{x}} \mathcal{L}(\vec{x},\dot{\vec{x}}) + \dot{\vec{\varepsilon}}\,\vec{\nabla}_{\dot{\vec{x}}} \mathcal{L}(\vec{x},\dot{\vec{x}}) - \cancel{\mathcal{L}(\vec{x},\dot{\vec{x}})} \right) dt$$

$$\delta S = \int_{t_0}^{t_1} \vec{\varepsilon}\cdot\vec{\nabla}_{\vec{x}} \mathcal{L}(\vec{x},\dot{\vec{x}})\, dt$$

INTEGRATION BY PART

$$+ \cancelto{0}{\left[\vec{\varepsilon}\cdot\vec{\nabla}_{\dot{\vec{x}}} \mathcal{L}(\vec{x},\dot{\vec{x}}) \right]_{t_0}^{t_1}} - \int_{t_0}^{t_1} \vec{\varepsilon}\cdot \frac{d}{dt}\vec{\nabla}_{\dot{\vec{x}}} \mathcal{L}(\vec{x},\dot{\vec{x}})\, dt$$

$$= \int_{t_0}^{t_1} \underset{\substack{\uparrow \\ \text{ARBITRARY}}}{\vec{\varepsilon}} \cdot \underbrace{\left[\vec{\nabla}_{\vec{x}} \mathcal{L}(\vec{x},\dot{\vec{x}}) - \frac{d}{dt}\vec{\nabla}_{\dot{\vec{x}}} \mathcal{L}(\vec{x},\dot{\vec{x}}) \right]}_{\text{MUST BE ZERO} \Rightarrow \text{EL}} dt \overset{!}{=} 0$$

GENERALIZATION TO MEMBRANES OR PLATES:

$$\mathcal{U}_{min} = \iint f(\varsigma, \varsigma_x, \varsigma_y, \varsigma_{xx}, \varsigma_{xy}, \varsigma_{yy})\,dx\,dy$$

$$\Rightarrow \boxed{\frac{\partial f}{\partial \varsigma} - \frac{d}{dx}\cdot\frac{\partial f}{\partial \varsigma_x} - \frac{d}{dy}\cdot\frac{\partial f}{\partial \varsigma_y} + \frac{d^2}{dx^2}\cdot\frac{\partial f}{\partial \varsigma_{xx}} + \frac{d^2}{dy^2}\cdot\frac{\partial f}{\partial \varsigma_{yy}} + \frac{d^2}{dx\,dy}\cdot\frac{\partial f}{\partial \varsigma_{xy}} = 0}$$

FOR MINIMAL ENERGY FUNCTIONAL. $\quad U_b = \frac{1}{2}K_b \iint (\varsigma_{xx}+\varsigma_{yy})^2\,dx\,dy$

LAPLACIAN OPERATOR

$$\Rightarrow K_b\left[\frac{d^2}{dx^2}(\varsigma_{xx}+\varsigma_{yy}) + \frac{d^2}{dy^2}(\varsigma_{xx}+\varsigma_{yy})\right] = k_b\vec{\nabla}^2\cdot(\vec{\nabla}^2\varsigma) = k_b\vec{\nabla}^4\varsigma = 0$$

BIHARMONIC OPERATOR

$$\boxed{K_b\vec{\nabla}^4\varsigma - \sigma = 0}$$

PLATE EQUATION.