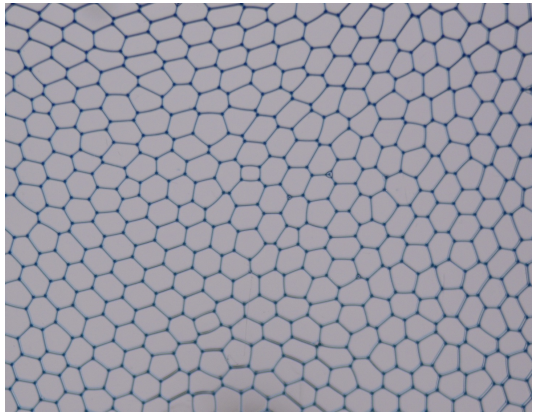
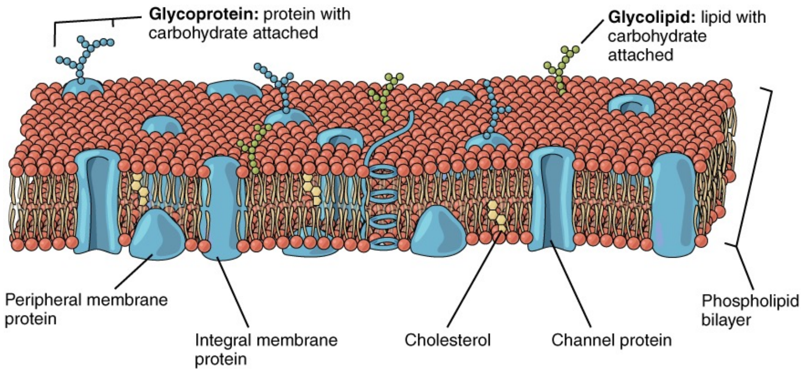
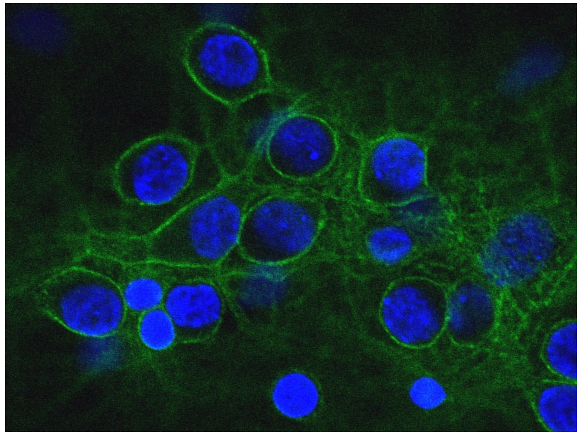
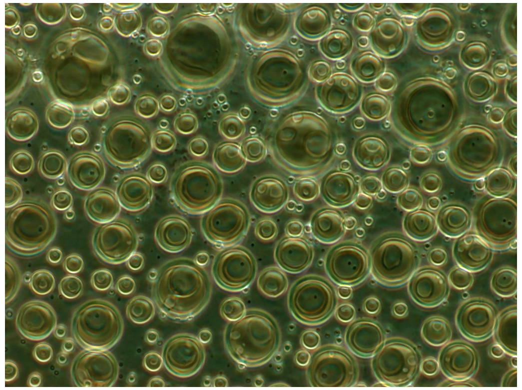
ME470: Mechanics of Soft and Biological Matter
Lecture14: Review









Sangwoo Kim

MESOBIO – IGM – STI – EPFL

Red Blood Cells

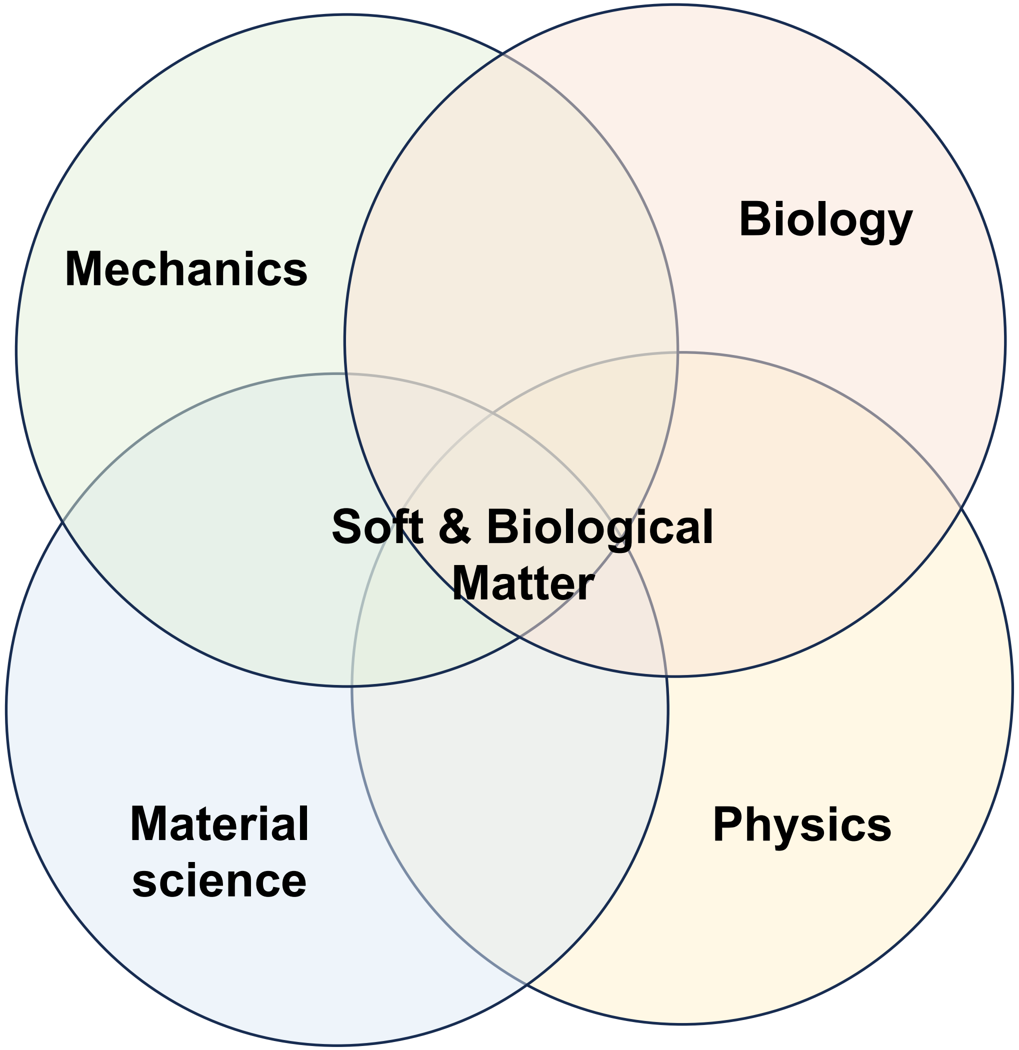
Motivation

Soft and Biological Matter

- Polymer melts/solutions
- Foams, emulsions, suspensions
- Granular materials
- Rubber
- Cells
- Tissues, Organs
- Membrane, vesicles

Many, but not all, soft and biological matter

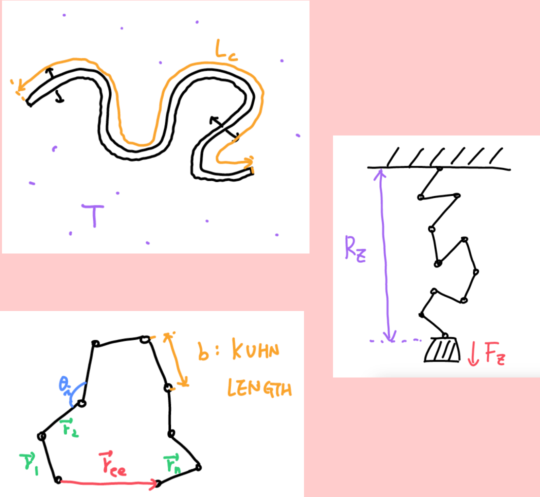
- Are viscoelastic/viscoplastic
- Are self-organized
- Show “slow” relaxation of strain
- Show entropic effects (thermal fluctuations)



Course Contents

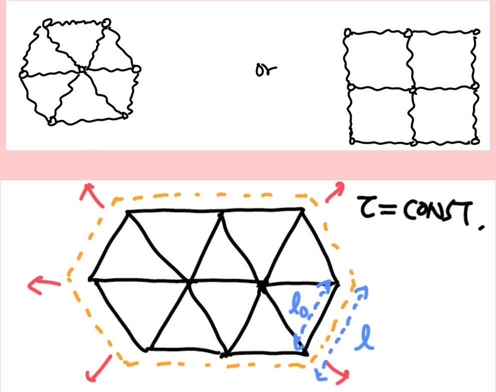
Objective: a comprehensive understanding of theoretical (and computational) modeling of soft and biological matter, emphasis on biological system

Part 1



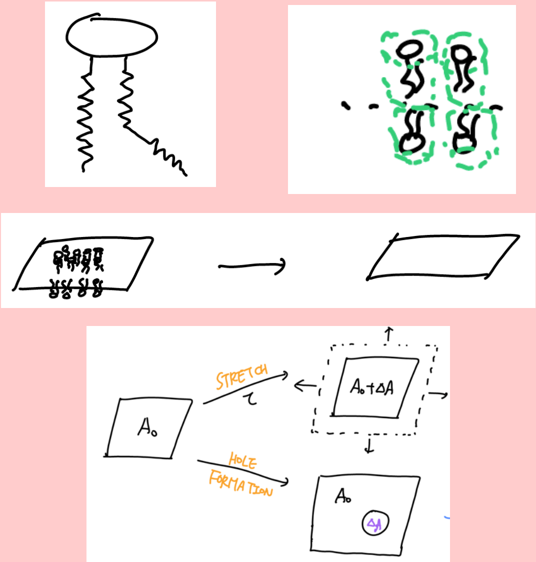
Mechanics of 1D elements

Part 2



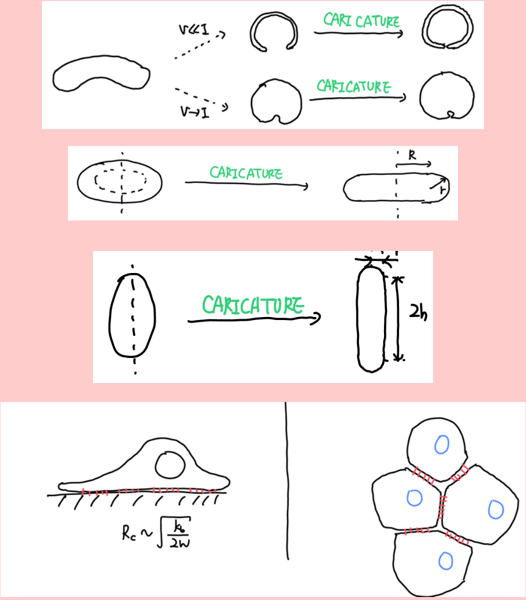
Mechanics of 2D network

Part 3



Mechanics of membranes

Part 4



Mechanics of cells and tissues

Relation between external load and deformation

3D homogeneous isotropic linear elastic materials

$$\boxed{\sigma_{ik} = 2\mu\left(\varepsilon_{ik} - \frac{1}{3}\varepsilon_{ll}\delta_{ik}\right) + K\varepsilon_{ll}\delta_{ik}}$$

Shear modulus Bulk modulus

2D homogeneous isotropic linear elastic materials

$$\boxed{\tau_{ij} = 2\mu_A\left(\varepsilon_{ij} - \frac{1}{2}\varepsilon_{ll}\delta_{ij}\right) + K_A\varepsilon_{ll}\delta_{ij}}$$

Area shear modulus Area stretch modulus

⇨ We mainly used strain energy formalism $u = \frac{1}{2}\sigma_{ik}\varepsilon_{ik}$

Part 0: Review – Continuum Thermodynamics

Use different energy functionals

u is minimal for $ds = 0,\ d\varepsilon_{ik} = 0$

h is minimal for $ds = 0,\ d\sigma_{ik} = 0$ $\quad h = u - \sigma_{ik}\varepsilon_{ik}$

f is minimal for $dT = 0,\ d\varepsilon_{ik} = 0$ $\quad f = u - Ts$

g is minimal for $dT = 0,\ d\sigma_{ik} = 0$ $\quad g = u - Ts - \sigma_{ik}\varepsilon_{ik}$

Statistical Mechanics

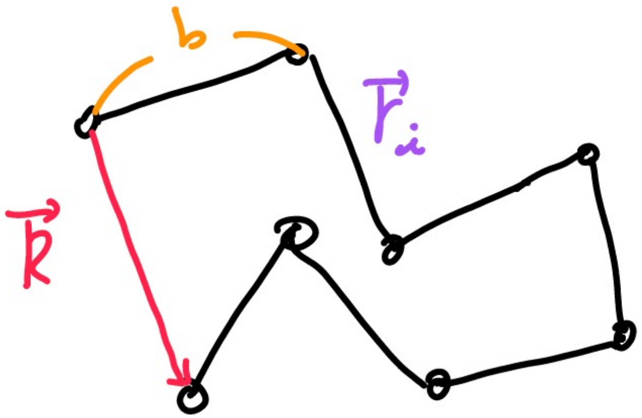
Entropy: $S = k_b \ln \Omega$

Canonical ensemble: $Prob(E_A) = \frac{1}{Z} e^{-\beta E_A}$ $\quad Z = \sum_{E_A} e^{-\beta E_A}$

Part 1: 1D elements

- Stretching vs bending → Inextensible assumption
- Persistence length: $l_p = EI/k_BT$
    - competition between energetic influence and entropic influence
    - Stiff rod vs flexible filament

Ideal chain: polymer model in the flexible limit



$$\langle \vec{R} \rangle = 0 \qquad \langle R^2 \rangle = \langle \vec{R} \cdot \vec{R} \rangle = nb^2$$

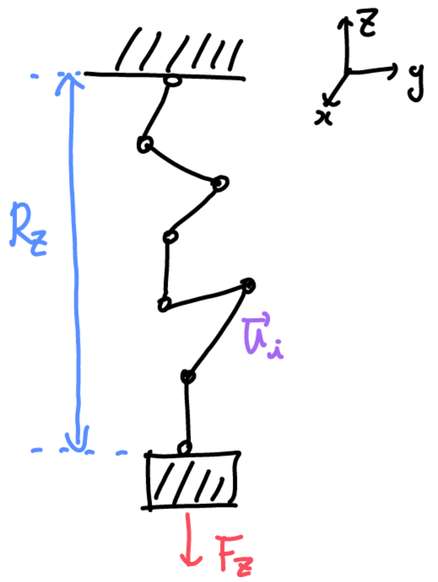
- n inextensible segments are joined by frictionless hinge
- Same as random walk → Gaussian distribution

$$\boxed{F = \left(\frac{3k_BT}{nb^2}\right) R}$$

k_{sp}: spring constant

Part 1: 1D elements

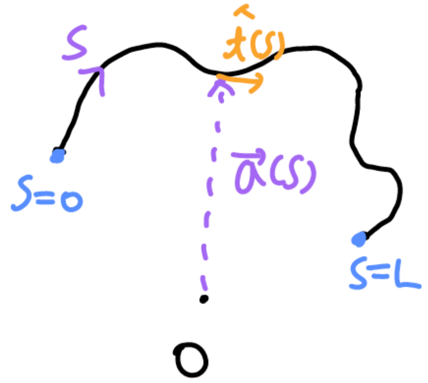
Freely jointed chain: realistic description at $R \sim L$



- n inextensible segments are joined by frictionless hinge with weight attached at the end
- Use canonical ensemble
- IC recovered for small F_z

$$\boxed{\langle R_z \rangle = nb\left[\coth\left(\frac{bF_z}{k_BT}\right) - \frac{k_BT}{bF_z}\right]}$$

Worm-like chain: continuous elastic curve in 3D

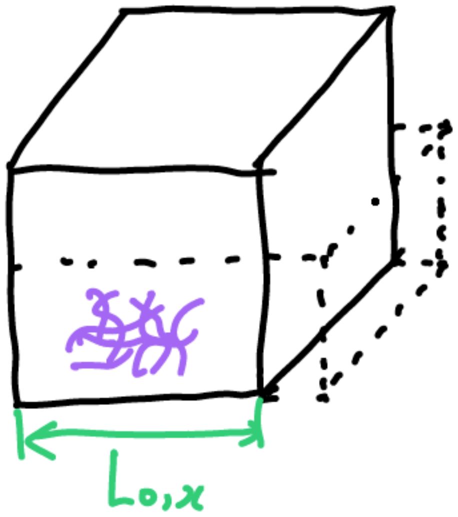


$$\boxed{F_z = \frac{k_BT}{l_p}\left[\frac{1}{4}\left(1 - \frac{\langle R_z \rangle}{L}\right)^{-2} - \frac{1}{4} + \frac{\langle R_z \rangle}{L}\right]}$$

$$\boxed{b = 2l_p}$$

EPFL Part 1: 1D elements

Bulk entropic materials: entangled entropic springs (disordered)



- Use affine deformation assumption
  - microscopic deformation=macroscopic deformation
- Consider free energy change for stretching

$$\boxed{\langle \Delta\Psi \rangle = \frac{k_B T}{2}\left(\lambda^2 + \frac{2}{\lambda^2} - 3\right)}$$

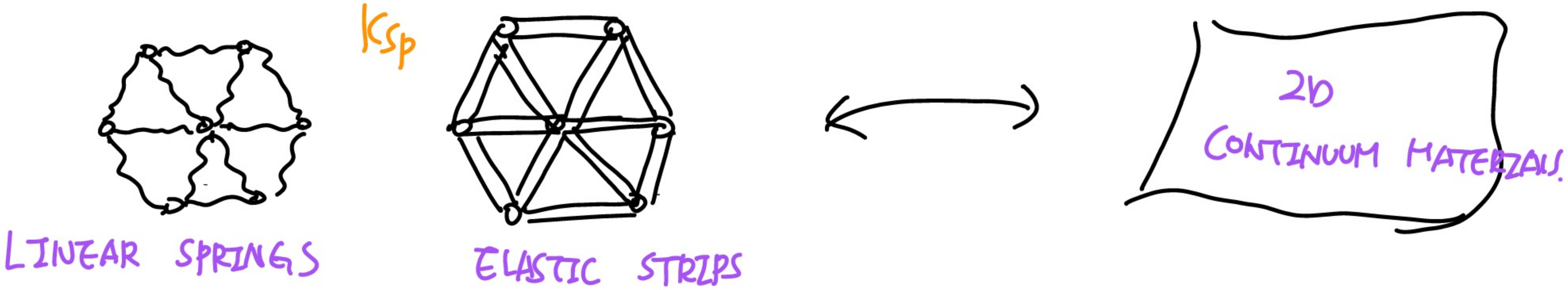
(uniaxial stretching)

$$\boxed{\sigma_{xx} = \frac{F_x}{A} = \frac{N}{AL_{0,x}} k_B T\left(\lambda - \frac{2}{\lambda^2}\right) = \rho_c k_B T\left(\lambda - \frac{2}{\lambda^2}\right)}$$

Chain volume density

$$\Rightarrow \quad \boxed{E = 3\rho_c k_B T}$$

Part 2: 2D network

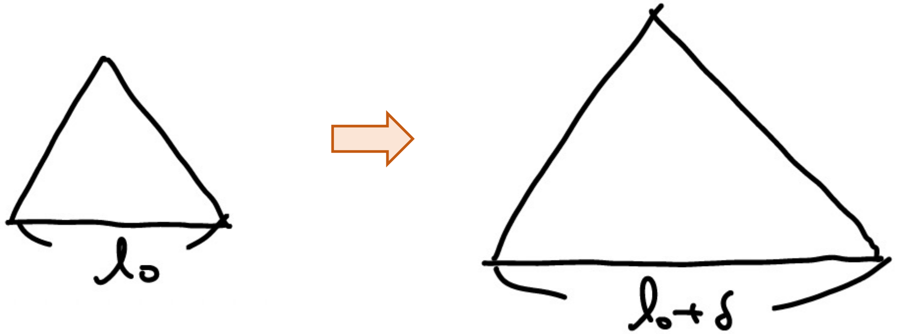


Constitutive relation (2D linear elastic): $\tau_{ij} = C_{ijkl}\varepsilon_{kl} \qquad i, j, k, l \in \{x, y\}$

- Symmetry and thermodynamics reduces coefficients from 16 to 6
- 6-fold symmetry only leaves 2 independent coefficients
- Regular triangular spring network as 2D isotropic homogeneous elastic materials!

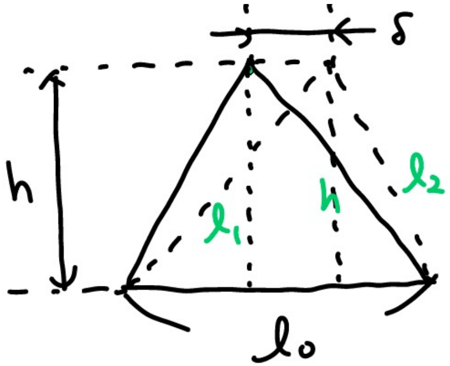
Part 2: 2D network

Bulk modulus



$$\boxed{K_A = \frac{\sqrt{3}}{2} k_{sp}}$$

Shear modulus

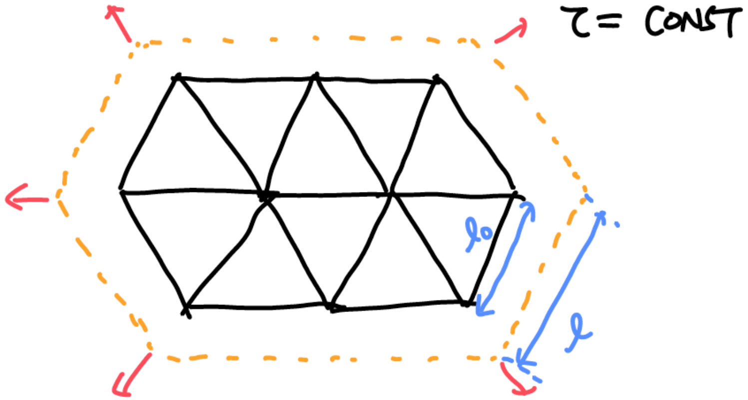


$$\boxed{\mu_A = \frac{\sqrt{3}}{4} k_{sp}}$$

Part 2: 2D network

Network under external stress

extension



$$\boxed{l = \frac{l_0}{1 - \tau/\tau_b}}$$

$$\tau_b = \sqrt{3}k_{sp}$$

Compression

Mode1: uniform contraction

Mode2: collapse

$\tau_c < \tau < 0$ Uniform contraction

$\tau < \tau_c$ Collapse

$$\tau_c = \frac{1}{8}\tau_b$$

Part 2: 2D network

Prestressed network

$$\boxed{K_A = \frac{\sqrt{3}}{2} k_{sp} \left(1 - \frac{\tau}{\sqrt{3} k_{sp}} \right)}$$

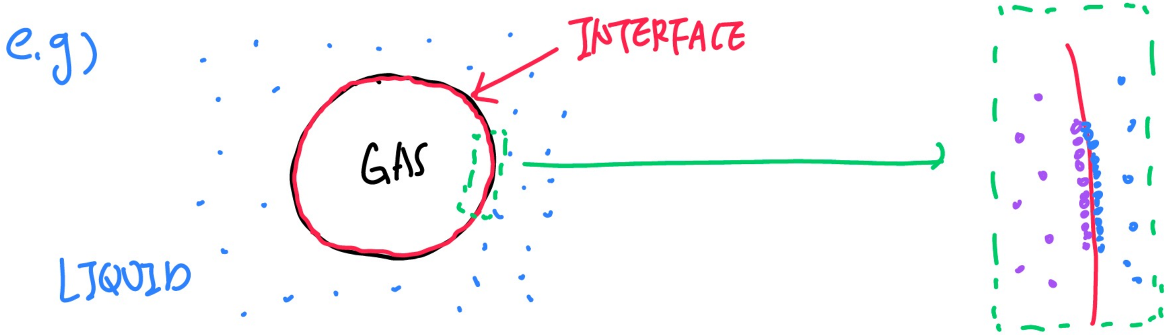
$$\boxed{\mu_A = \frac{\sqrt{3}}{4} k_{sp} \left(1 + \frac{\sqrt{3}\tau}{k_{sp}} \right)}$$

Numerical simulation of 2D network

- Rigidity percolation transition
- Entropic effects (finite temperature)
- Disordered network structure (diluted triangular lattice, Mikado network, packing inspired network)

Part 3: Membrane

Simple interface: surface tension



Young-Laplace law

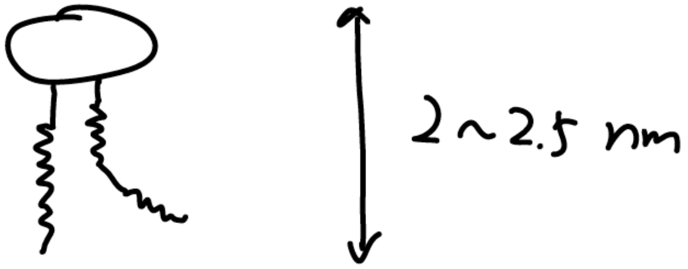
$$\boxed{\Delta P = P_g - P_l = \gamma \frac{dA}{dV}}$$

Surfactants: makes interface become elastic

Phospholipids (e.g. DOPC)

Hydrophilic head

Hydrophobic tail



- Critical concentration n_{agg}, where interface gets preferentially populated!
- Monolayer: $K_A = (k+1)$

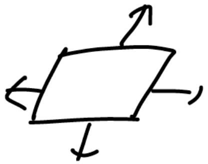
EPFL

Part 3: Membrane

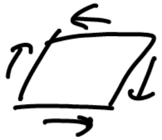
Bilayer

Membrane as 2D continuum materials

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



(2) shear: liquid in plane



(3) bending

- Plate bending in one direction: $k_b = \frac{1}{12} h^2 K_A$
- 3D thin plate: $U_{b,plate} = \frac{1}{2}\left(\frac{Eh^3}{12(1-\nu^2)}\right) \iint \left[(\varsigma_{xx} + \varsigma_{yy})^2 + 2(1-\nu)(\varsigma_{xy}^2 - \varsigma_{xx}\varsigma_{yy})\right]\ dxdy$

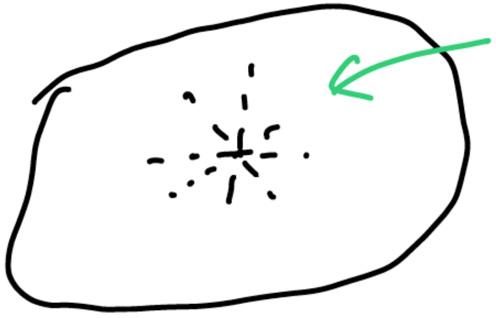
$$\boxed{U = \frac{1}{2} k_b \iint (2H)^2 dA + k_G \iint K_G\, dA}$$

Helfrich free energy

Part 3: Membrane

Differential geometry

More general definition of mean and Gaussian curvature:



∞LY MANY CURVATURES AT EVERY POINT

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

Gauss-Bonnet Theorem: for closed surface

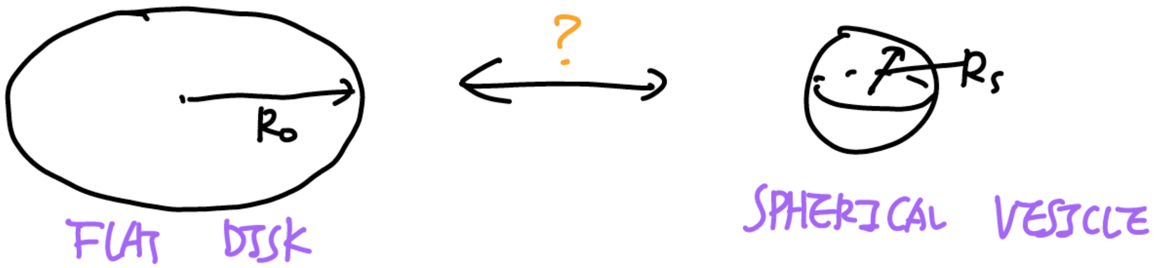
$$\iint K_G dA = \oint K_G dA = 4\pi(1 - g)$$

General differential geometric formalism to compute H and K_G:

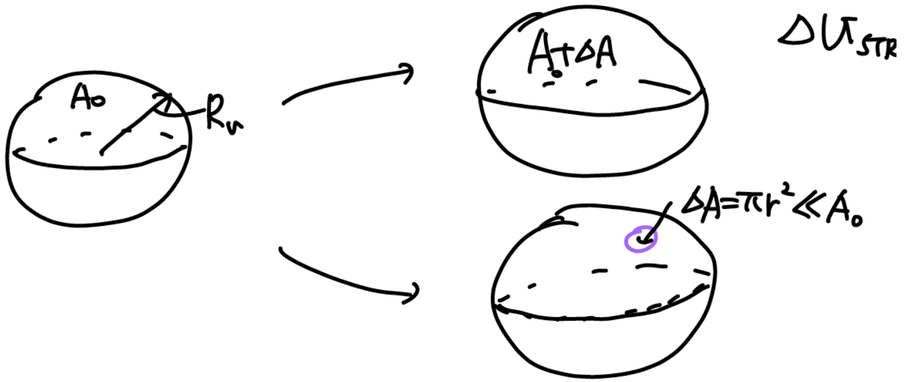
$$\boxed{\begin{aligned} H &= \frac{eG - 2fF + gE}{2(EG - F^2)} \\ K_G &= \frac{eg - f^2}{EG - F^2} \end{aligned}}$$

Part 3: Membrane

Vesicle formation: competition between line tension and bending energy



Rupture: competition between line tension and stretching energy



$$\boxed{U = \frac{1}{2} k_b \iint (2H)^2 dA + k_G \iint K_G \, dA + \int_{\partial A} \lambda \, ds + \frac{1}{2} K_A \iint \varepsilon_{ll}^2 \, dA}$$

Bending | Bending | Line tension | stretching

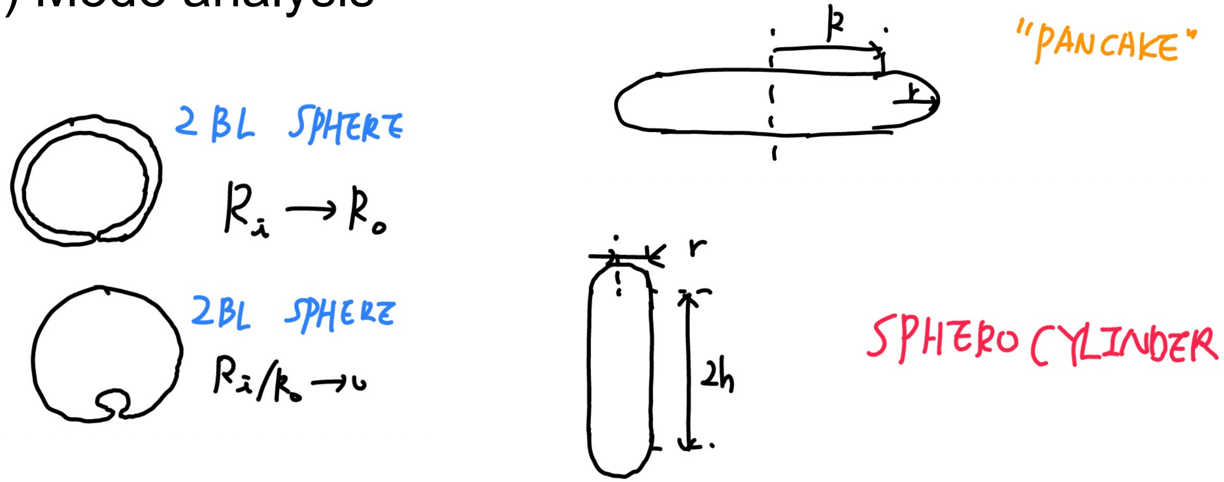
Refined membrane bending model

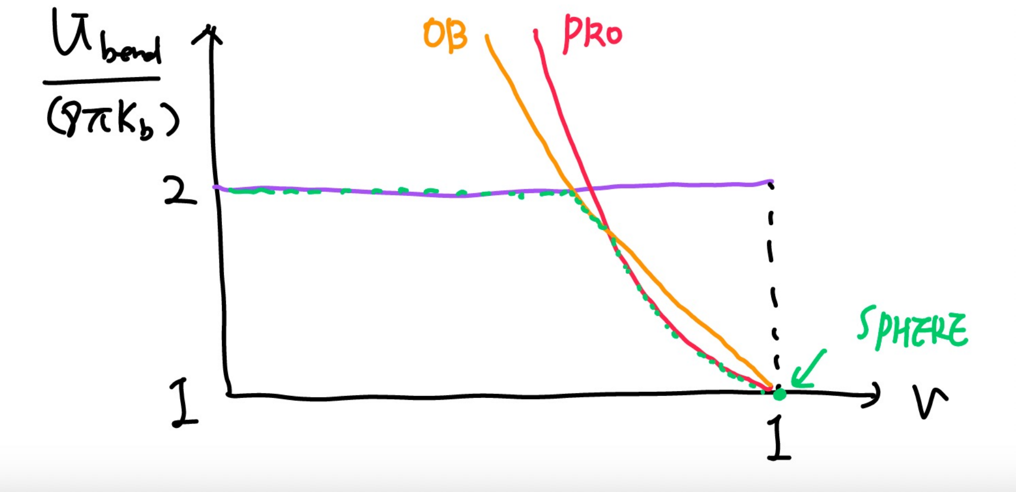
- Spontaneous curvature
- Area – difference elasticity model (ADE model)

Part 4: Cell & Tissues

Vesicle shapes using the minimal model:

(1) Mode analysis





(2) Numerical computation: discretizing vesicle shape into triangulation

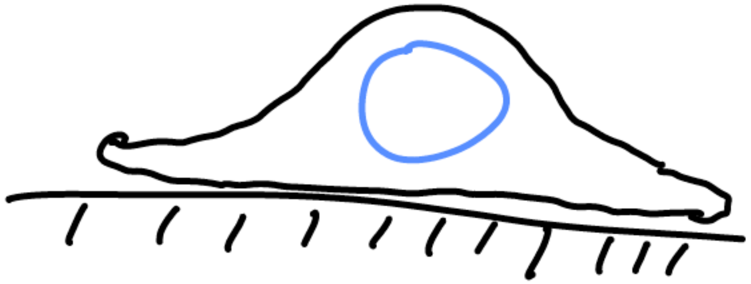
(3) Variational calculus: analytic approach to minimize a functional

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

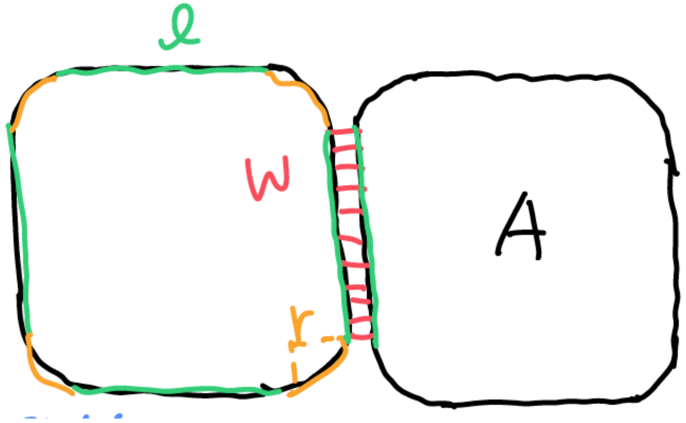
Plate equation!

Part 4: Cell & Tissues

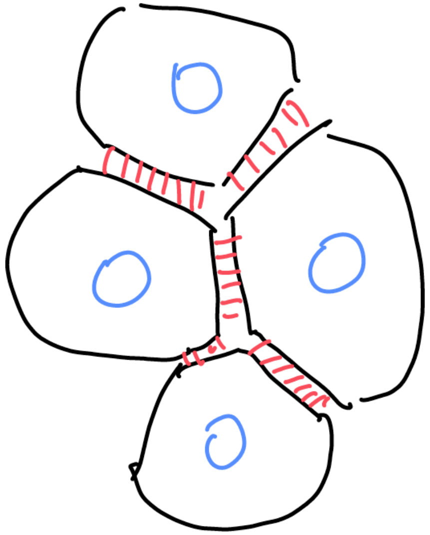
Cell-substrate adhesion



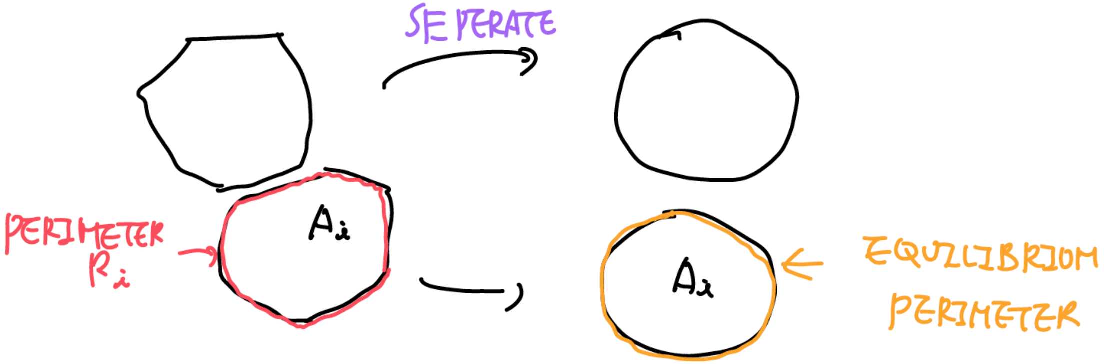
Competition between adhesion & bending



Cell-substrate adhesion

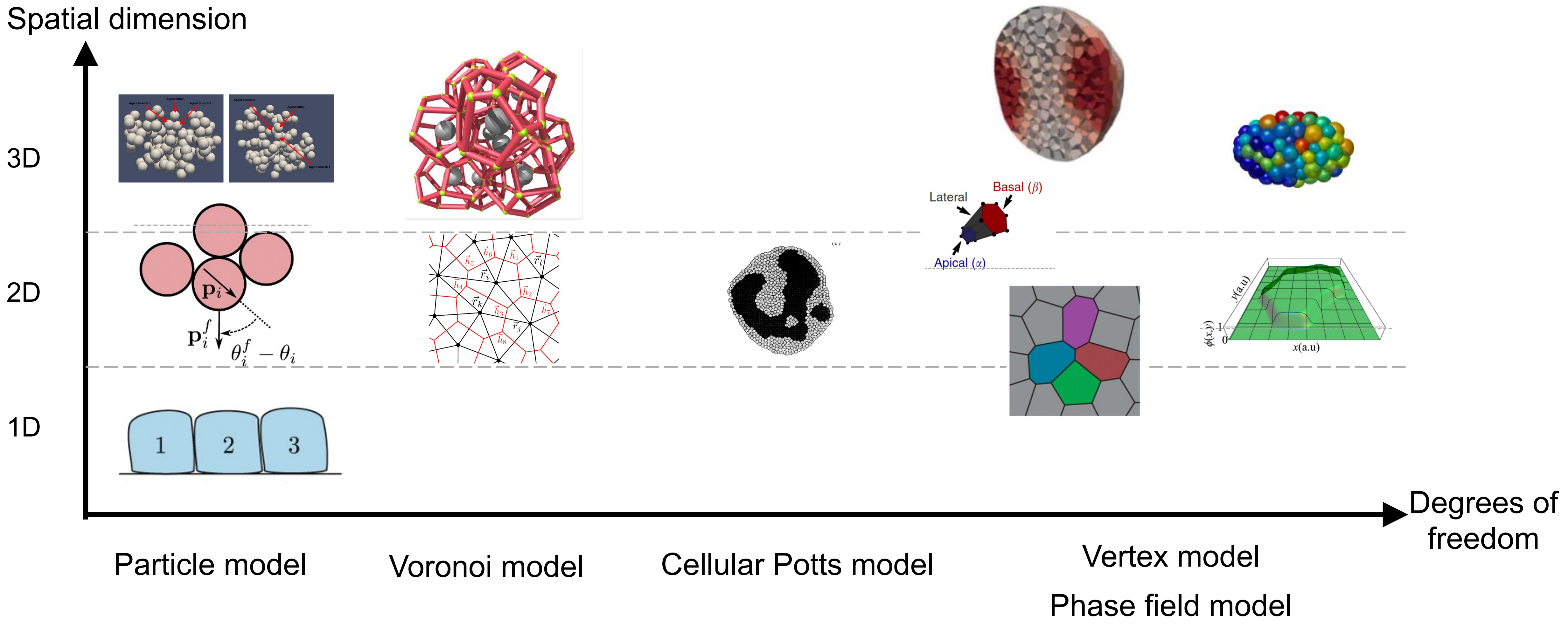


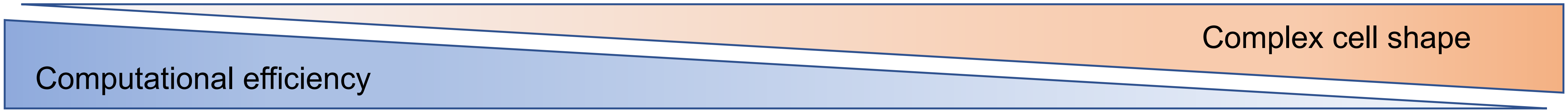
Competition between adhesion & stretching



Part 4: Cell & Tissues

Cell-based discrete model





Final exam

- 2:15pm – 5:15pm (3hours), December 19th, 2024, CE15
- You must bring your **STUDENT ID** and **CALCULATOR**
- A formula sheet and scratch papers will be provided.
- Format
  - 10 short questions
  - 3 quantitative analysis questions