Modeling Biomembranes

using Cosserat Shell Theory

using Calculus of Variations and the Method of Moving Frames

Andrea Dziubek

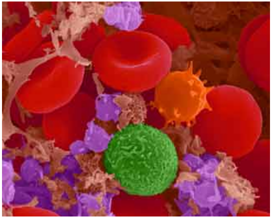
Workshop on Moving Frames in Geometry
June 13-17, 2011

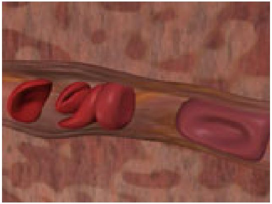
Modeling biomembranes (red blood cells)

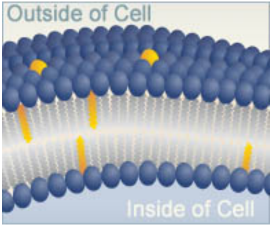
using

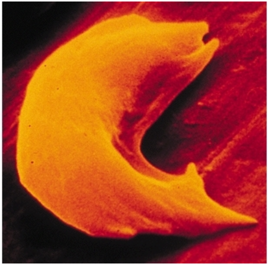
Cosserat Shell Theory

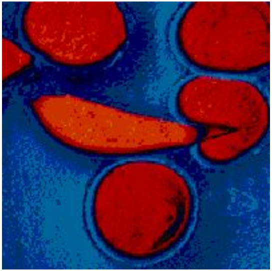
What do we know about human blood?

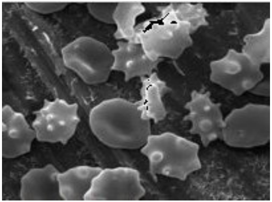












mybloodyourblood.org/hs-biology-red.htm
www.biology.arizona.edu/cell-BIO/problem-sets/membranes/02t.html
www.mybodyindex.com/images/content/bloodvessel-1.gif

bill.srnr.arizona.edu/classes/182/Diploid.htm
www.veeco.com/library/nanotheater.php
www.thechemblog.com

How can we model human blood?

Plasma

- **Incompressible Newtonian fluid**
- Viscosity comparable to water

Fluid inside red blood cell (hemoglobin)

- **Incompressible Newtonian fluid**
- Viscosity higher than plasma

Red Blood Cell Membrane

- **Viscoelastic material**
  Elastic component (amount of deformation = strain) from stretching of cytoskeleton
  Viscous component (rate of change of deformation = fluid friction) from fluid behavior of lipid bilayer
  Membrane is incompressible and not isotropic (bending moments cannot be neglected)

- **Cosserat Shell**
  - Small deformations, small strains (linear stress-strain relation)
  - Small strains but large deformations
  - Finite/large strains and large deformations

- **Navier-Stokes equations** (Eulerian description)   density ρ, viscosity μ_f constant

$$\begin{aligned} \boldsymbol{\nabla} \cdot \boldsymbol{v} &= 0 \\ \rho \underbrace{\left(\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \boldsymbol{\nabla} \boldsymbol{v} \right)}_{\text{inertia}} &= -\underbrace{\boldsymbol{\nabla} p}_{\text{pressure}} + \underbrace{\mu_f \nabla^2 \boldsymbol{v}}_{\text{friction}} + \underbrace{\rho \boldsymbol{g}}_{\text{gravity}} \end{aligned}$$

Stress tensor for incompressible Newtonian fluid $\boldsymbol{\sigma} = -p\boldsymbol{I} + \boldsymbol{T}$, shear stress tensor $\boldsymbol{T} = \mu_f \left[\boldsymbol{\nabla}\, \boldsymbol{v} + (\boldsymbol{\nabla}\, \boldsymbol{v})^T \right]$

- **Navier-Cauchy equations** (Lagrangian description) $\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$, $\mu = \frac{E}{2(1+\nu)}$ constant

$$\rho \ddot{\boldsymbol{u}} = (\lambda + \mu) \boldsymbol{\nabla} (\boldsymbol{\nabla} \cdot \boldsymbol{u}) + \mu \boldsymbol{\nabla}^2 \boldsymbol{u} + \rho \boldsymbol{g}$$

Assuming small displacements $\boldsymbol{u}$, small displacement gradients $\boldsymbol{\nabla u}$, linear stress-strain relation ($\boldsymbol{\sigma} = \boldsymbol{K} : \boldsymbol{\varepsilon}$), isotropic homogeneous material (constant λ, shear modulus μ, Young's modulus E, Poisson ratio ν)

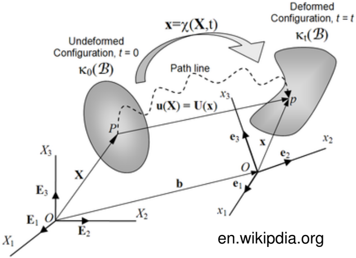
Stress tensor $\boldsymbol{\sigma} = \lambda(\mathrm{tr}\, \boldsymbol{\varepsilon})\boldsymbol{I} + 2\mu\boldsymbol{\varepsilon}$, Green Lagrangian strain tensor $\boldsymbol{\varepsilon} = \frac{1}{2} \left[\boldsymbol{\nabla}\, \boldsymbol{u} + (\boldsymbol{\nabla}\, \boldsymbol{u})^T \right]$, dilatation $\boldsymbol{\nabla} \cdot \boldsymbol{u} = \mathrm{tr}\, \boldsymbol{E}$

- Biomembranes are highly deformable and are described by nonlinear material laws, they are a 3D continuum body where one dimension is small [Holzapfel 2000, 2006]

Finite strains, large deformations, strain energy density

- **Deformation gradient** $\boldsymbol{F} = \frac{\partial x_i}{\partial X_j}$ of a continuum body $\mathcal{B} \in \mathbb{R}^3$ relates current configuration $\boldsymbol{x}(\boldsymbol{X}, t) \in \Omega_t(\mathcal{B})$ and reference configuration $\boldsymbol{X} \in \Omega_0(\mathcal{B})$
  In terms of **displacements**

$$\boldsymbol{u} = \boldsymbol{x} - \boldsymbol{X} \qquad \boldsymbol{F} = \boldsymbol{I} + \boldsymbol{\nabla u}$$



en.wikipdia.org

- **Green Lagrangian strain tensor** is nonlinear

$$\boldsymbol{E} = \tfrac{1}{2}[\boldsymbol{F}^T \cdot \boldsymbol{F} - \boldsymbol{I}]$$
$$= \tfrac{1}{2}\left[\boldsymbol{\nabla u} + (\boldsymbol{\nabla u})^T + (\boldsymbol{\nabla u})^T \cdot \boldsymbol{\nabla u}\right]$$

- From entropy inequality (const. entropy/temp.) follows that Cauchy stress tensor is a function of the **strain energy density function** $W(\boldsymbol{E})$.

$$\boldsymbol{\sigma} = \frac{1}{J}\boldsymbol{F} \cdot \frac{\partial W}{\partial \boldsymbol{E}} \cdot \boldsymbol{F}^T$$

$J = \det \boldsymbol{F} = \frac{\rho_0}{\rho}$, strain energy density is a function of invariants $I_1 = \text{tr}\, \boldsymbol{E}$, $I_2 = \det \boldsymbol{E}$, $I_3 = \frac{1}{2}\left[(\text{tr}\, \boldsymbol{E})^2 - \text{tr}\, \boldsymbol{E}^2\right]$

- **2nd Piola-Kirchhoff tensor** relates forces in reference configuration to areas in reference configuration

$$\boldsymbol{S} = J\boldsymbol{F}^{-1} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{F}^{-T} = \frac{\partial W}{\partial \boldsymbol{E}}$$

For a Saint Venant-Kirchhoff material $\boldsymbol{S} = \lambda(\text{tr}\, \boldsymbol{E})\boldsymbol{I} + 2\mu\boldsymbol{E}$ the strain energy is $W = \frac{\lambda}{2}(\text{tr}\, \boldsymbol{E})^2 + \mu\, \text{tr}\, \boldsymbol{E}^2$

Differential geometry of a thin shell

A **thin shell** can be modeled as a surface consisting of material points with **translational and rotational degrees of freedom**, describing displacement and rotation of an underlying microstructure [Ciarlet, 2000,2005], [Rubin 2000]

- **Point on surface** in reference and present configuration

$$\boldsymbol{X}(\xi^\alpha) \qquad \boldsymbol{x}(\xi^\alpha, t) \qquad \alpha = 1, 2$$

- Covariant surface base vectors and **directors**

$$\boldsymbol{D}_\alpha = \boldsymbol{X}_{,\alpha} \qquad \boldsymbol{D}_3 = \frac{\boldsymbol{D}_1 \times \boldsymbol{D}_2}{|\boldsymbol{D}_1 \times \boldsymbol{D}_2|}$$

$$\boldsymbol{D}_\alpha = \boldsymbol{x}_{,\alpha} \qquad \boldsymbol{d}_3(\xi^\alpha, t) \neq \frac{\boldsymbol{d}_1 \times \boldsymbol{d}_2}{|\boldsymbol{d}_1 \times \boldsymbol{d}_2|}$$

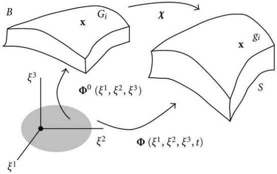
normal extension: $|\boldsymbol{a}| < |\boldsymbol{d}_3|$, shear deformation: angle$(\boldsymbol{a}, \boldsymbol{d}_3) \neq 0$

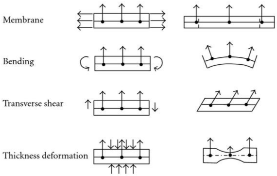
- **Point in 3D shell** in reference configuration

$$\widehat{\boldsymbol{X}}(\xi^i) = \boldsymbol{X}(\xi^\alpha) + \xi^3 \boldsymbol{D}_3$$

- **Covariant base vectors at a point in 3D shell** $\boldsymbol{G}_i = \widehat{\boldsymbol{X}}_{,i}$

$$\boldsymbol{G}_\alpha = \boldsymbol{D}_\alpha + \xi^3 \boldsymbol{D}_{3,\alpha} \qquad \boldsymbol{G}_3 = \boldsymbol{D}_3$$





www.hindawi.com/journals/jnm/2010/402591

Momentum and director momentum balance equations

- **Volume measure at a point in 3D shell**

$$\sqrt{G} = \boldsymbol{G}_1 \times \boldsymbol{G}_2 \cdot \boldsymbol{G}_3 = \sqrt{D}\Big[1 + \xi^3 \underbrace{(\boldsymbol{D}_{3,\alpha} \cdot \boldsymbol{D}^\alpha)}_{\text{mean curvature}} + (\xi^3)^2 \underbrace{\frac{\boldsymbol{D}_{3,1} \times \boldsymbol{D}_{3,2} \cdot \boldsymbol{D}_3}{\sqrt{D}}}_{\text{Gaussian curvature}}\Big]$$

- **Mass per unit area**

constant density ρ_0, shell thickness h

$$m = \int_{-h/2}^{h/2} \rho_0 \sqrt{G} \mathrm{d}\xi^3 = \left(\rho_0 \sqrt{D} h\right) \left[1 + \frac{h^2}{12} \frac{\boldsymbol{D}_{3,1} \times \boldsymbol{D}_{3,2} \cdot \boldsymbol{D}_3}{\sqrt{D}}\right]$$

- **Displacement vector and director displacement vectors**

$$\boldsymbol{u} = \boldsymbol{X} - \boldsymbol{x}$$

$$\boldsymbol{\delta}_i = \boldsymbol{D}_i - \boldsymbol{d}_i$$

For $\alpha = 1, 2$, $\boldsymbol{\delta}_\alpha = \boldsymbol{u}_{,\alpha}$. For small deformations $\boldsymbol{\delta}_3 = -\left(\boldsymbol{D}_3 \cdot \boldsymbol{\delta}_\alpha\right) \boldsymbol{D}^\alpha$

- **Linearized momentum and director momentum equation**

$$m(\ddot{\boldsymbol{u}} + y^3 \ddot{\boldsymbol{\delta}}_3) = \boldsymbol{t}^\alpha{}_{,\alpha} + m\boldsymbol{b}$$

$$m(y^3 \ddot{\boldsymbol{u}} + y^{33} \ddot{\boldsymbol{\delta}}_3) = \boldsymbol{m}^\alpha{}_{,\alpha} - \boldsymbol{t}^3 + m\boldsymbol{b}^3$$

Inertia coefficients $my^3 = \int_{-h/2}^{h/2} \rho_0 \xi^3 \sqrt{G}\, \mathrm{d}\xi^3$, $my^{33} = \int_{-h/2}^{h/2} \rho_0 \xi^3 \xi^3 \sqrt{G}\, \mathrm{d}\xi^3$, in-plane stress vector $\boldsymbol{t}^\alpha$, in-plane couple vector $\boldsymbol{m}^\alpha$, body force vector $m\boldsymbol{b}$, internal $\boldsymbol{t}^3 = \int_{h/2}^{h/2} \boldsymbol{\sigma} \cdot \boldsymbol{n} \mathrm{d}\xi^3$ and external director couple $m\boldsymbol{b}^3$

Displacement, deformation, curvature, strain

- **Couple vector and stress vector** (linear stress-strain relation)

$$\boldsymbol{m}^\alpha = \frac{m}{\rho_0}\left[\left(\boldsymbol{K} : \bar{\boldsymbol{E}}\right)\cdot \boldsymbol{H}^\alpha + \boldsymbol{K}^{\alpha\beta}\cdot \boldsymbol{\beta}_\beta\right]$$

$$\boldsymbol{t}^i = \frac{m}{\rho_0}\left(\boldsymbol{K} : \bar{\boldsymbol{E}}\right)\cdot \boldsymbol{D}^i - \boldsymbol{m}^\alpha\left(\boldsymbol{D}_{3,\alpha}\cdot \boldsymbol{D}^i\right)$$

Modified stress tensor $\boldsymbol{K} : \bar{\boldsymbol{E}} = \lambda(\text{tr}\, \bar{\boldsymbol{E}})\boldsymbol{I} + 2\mu\bar{\boldsymbol{E}}$, Bending tensors $\boldsymbol{K}^{\alpha\beta}$ (two parameter) [Rubin 2000]

General geometry in reference configuragion $\boldsymbol{H}^\alpha = \frac{1}{m}\int_{-h/2}^{h/2}\rho_0\,\xi^3\sqrt{G}\boldsymbol{G}^\alpha\,\mathrm{d}\xi^3$ (flat: $\boldsymbol{H}^\alpha = \boldsymbol{0}$)

- **Deformation gradient and Green Lagrangian strain tensor in curvilinear coordinates**

$$\boldsymbol{F} = \boldsymbol{d}_i \otimes \boldsymbol{D}^i \qquad\qquad \boldsymbol{E} = \frac{1}{2}(\boldsymbol{F}^T\cdot \boldsymbol{F} - \boldsymbol{I})$$

For small deformations $\boldsymbol{E} = \frac{1}{2}\left(\boldsymbol{\delta}_i \otimes \boldsymbol{D}^i + \boldsymbol{D}^i \otimes \boldsymbol{\delta}_i\right)$

- **Curvature vector**

curvature tensor $\boldsymbol{\kappa} = (\boldsymbol{F}^{-1}\cdot \boldsymbol{d}_{3,\alpha} - \boldsymbol{D}_{3,\alpha})\otimes \boldsymbol{D}^\alpha$

$$\boldsymbol{\beta}_\alpha = \boldsymbol{F}^{-1}\cdot \boldsymbol{d}_{3,\alpha} - \boldsymbol{D}_{3,\alpha}$$

For small deformations $\boldsymbol{\beta}_\alpha = \boldsymbol{\delta}_{3,\alpha} - \left(\boldsymbol{D}^i\cdot \boldsymbol{D}_{3,\alpha}\right)\boldsymbol{\delta}_i$

- **Modified deformation gradient and Green Lagrangian strain tensor** (not symmetric)

$$\bar{\boldsymbol{F}} = \boldsymbol{F}\cdot(\boldsymbol{I} + \boldsymbol{\beta}_\alpha \otimes \boldsymbol{H}^\alpha) \qquad\qquad \bar{\boldsymbol{E}} = \boldsymbol{E} + \frac{1}{2}\left(\boldsymbol{\beta}_\alpha \otimes \boldsymbol{H}^\alpha + \boldsymbol{H}^\alpha \otimes \boldsymbol{\beta}_\alpha\right)$$

Modeling biomembranes (red blood cells)

using

Calculus of Variations and the Method of Moving Frames

Helfrich and BCM energy functionals

- **Potential energy** of a thin (no tension along any normal) biomembrane, assuming small deformations and isotropic homogeneous material (see e.g. [Hemmen, Leibold 2007])

$$\Delta E_{pot} = \left(\frac{k_c}{2} H^2 + \frac{k_g}{2} K \right) \mathrm{d}A$$

bending rigidities $k_c = \frac{E}{1-\nu^2} \frac{h^3}{12}$, $k_g = -\frac{E}{1+\nu} \frac{h^3}{6}$, Young's modulus E, Poisson ratio ν

- **Helfrich energy functional** includes **spontaneous curvature** [Helfrich 1973]

$$\mathcal{F} = \int \left(\frac{k_c}{2} \left[H - k_0 \right]^2 + \frac{k_g}{2} K \right) \mathrm{d}A$$

- Areas of the inner leaf and the outer leaf of the lipid bilayer may differ [Evans 1974] **Integrated mean curvature** $M = \int H \mathrm{d}A$ should be constant ($\Delta A = hM$)

- Adding **area and volume constraints** gives the **bilayer coupling model (BCM)**

$$\mathcal{F} = \frac{1}{2} \int \left(k_c H^2 + k_g K \right) \mathrm{d}A + \gamma A - PV + QM$$

surface tension γ, pressure P, volume V, Lagrange multiplyer Q

Integrated Gaussian curvature does not change (topological invariant) and can be dropped

- Assume a **moving** point $\boldsymbol{x}$ of a surface M embedded in $\mathbb{R}^3$ with a **frame** $\boldsymbol{e}_i$ attached to it which moves to another position at time $s + \Delta s$

$$\begin{aligned} \mathsf{d}\boldsymbol{x} &= \lim_{\Delta s \to 0} \left[\boldsymbol{x} - \boldsymbol{x}'\right] \\ \mathsf{d}\boldsymbol{e}_i &= \lim_{\Delta s \to 0} \left[\boldsymbol{e}_i - \boldsymbol{e}_i'\right] \end{aligned}$$

- Write $\mathsf{d}\boldsymbol{x} = \mathsf{d}x\boldsymbol{i} + \mathsf{d}y\boldsymbol{j} + \mathsf{d}z\boldsymbol{k}$ and $\mathsf{d}\boldsymbol{e}_i$ in terms of $\boldsymbol{e}_i$ and get **structure equations**

$$\begin{aligned} \mathsf{d}\boldsymbol{x} &= \sigma_1\boldsymbol{e}_1 + \sigma_2\boldsymbol{e}_2 \\ \mathsf{d}\boldsymbol{e}_i &= \omega_{ij}\boldsymbol{e}_j \end{aligned}$$

where σ_i and ω_{ij} are 1-forms. From $\boldsymbol{e}_i \cdot \boldsymbol{e}_j = \delta_{ij}$ follows that $\omega_{ij} = -\omega_{ji}$, i.e. antisymmetric

- From $\mathsf{d}\left(\mathsf{d}\boldsymbol{x}\right) = 0$ and $\mathsf{d}\left(\mathsf{d}\boldsymbol{e}_i\right) = 0$ obtain **integrability conditions** for a surface ($\sigma_3 = 0$)

$$\begin{aligned} \mathsf{d}\sigma_1 &= \omega_{12} \wedge \sigma_2 \\ \mathsf{d}\sigma_2 &= \omega_{21} \wedge \sigma_1 \\ 0 &= \omega_{31} \wedge \sigma_1 + \omega_{32} \wedge \sigma_2 \\ \mathsf{d}\omega_{ij} &= \omega_{ik} \wedge \omega_{ki} \end{aligned}$$

Mean and Gaussian curvature, vector calculus

- Define **Gaussian curvature** by one and only linearly independent 2-form on $\mathbb{R}^2$

$$\omega_{31} \wedge \omega_{32} = K \sigma_1 \wedge \sigma_2$$

- Define **mean curvature** by another 2-form

$$\omega_{31} \wedge \sigma_2 - \omega_{32} \wedge \sigma_1 = 2H \sigma_1 \wedge \sigma_2$$

- ω_{31}, ω_{32} are linear combinations of σ_1, σ_2. With $0 = \omega_{31} \wedge \sigma_1 + \omega_{32} \wedge \sigma_2$, $\begin{bmatrix} \omega_{31} \\ \omega_{32} \end{bmatrix} = \underbrace{\begin{bmatrix} a & b \\ b & c \end{bmatrix}}_{\boldsymbol{R}} \begin{bmatrix} \sigma_1 \\ \sigma_2 \end{bmatrix}$

$$\begin{aligned} H &= \operatorname{tr} \boldsymbol{R} = a + c \\ K &= \det \boldsymbol{R} = a\,c - b^2 \end{aligned}$$

- The **Hodge star operator** applied to a differential k-form in $\mathbb{R}^2$ gives the complement to $\mathrm{d}A = \sigma_1 \wedge \sigma_2$, i.e. $*\sigma_1 = \sigma_2$ and $*\sigma_2 = -\sigma_1$. Using integrability conditions obtain

$$\begin{aligned} \boldsymbol{\nabla} \cdot \boldsymbol{u}\,\mathrm{d}A &= \mathrm{d} * (\boldsymbol{u} \cdot \mathrm{d}\boldsymbol{x}) \\ &= \mathrm{d} * (u_i \boldsymbol{e}_i \cdot \sigma_j \boldsymbol{e}_j) = \mathrm{d} * (u_1 \sigma_1 + u_2 \sigma_2) = \mathrm{d}\,(u_1 \sigma_2 - u_2 \sigma_1) \\ &= (\mathrm{d}u_1) \wedge \sigma_2 + u_1 (\omega_{21} \wedge \sigma_1) - (\mathrm{d}u_1) \wedge \sigma_2 - u_2 (\omega_{12} \wedge \sigma_2) \\ \Delta f\,\mathrm{d}A &= \mathrm{d} * \mathrm{d}f \end{aligned}$$

First variations of point in surface and frame

- Describe an **infinitesimal deformation of a surface** by a displacement vector at each point of the surface

$$\delta \boldsymbol{x} = \boldsymbol{u} = \Sigma_1 \boldsymbol{e}_1 + \Sigma_2 \boldsymbol{e}_2 + \Sigma_3 \boldsymbol{e}_3$$

- **Frame is changed (rotated)** by deformation of the surface

$$\delta \boldsymbol{e}_i = \Omega_{ij} \boldsymbol{e}_j$$

- From $\delta \mathrm{d}\boldsymbol{x} = \mathrm{d}\delta\boldsymbol{x}$, $\delta \mathrm{d}\boldsymbol{e}_i = \mathrm{d}\delta\boldsymbol{e}_i$, structure equations, integrability conditions, and mean and Gaussian curvatures compute **first variations** of σ_i, ω_{ij} and Ω_{13}, Ω_{23}

$$\begin{aligned}
\delta\sigma_1 &= \mathrm{d}\boldsymbol{u} \cdot \boldsymbol{e}_1 - \sigma_2 \Omega_{21} \\
\delta\sigma_2 &= \mathrm{d}\boldsymbol{u} \cdot \boldsymbol{e}_2 - \sigma_1 \Omega_{12} \\
\delta\omega_{ij} &= \mathrm{d}\Omega_{ij} + \Omega_{ik}\omega_{kj} - \omega_{ik}\Omega_{kj} \\
\Omega_{13} &= \Omega_{3,1} + a\Sigma_1 + b\Sigma_2 \\
\Omega_{23} &= \Omega_{3,2} + b\Sigma_1 + c\Sigma_2
\end{aligned}$$

First variation of energy functional

- From $\sigma_i \wedge \sigma_i = 0$, mean curvature H, and $\boldsymbol{\nabla} \cdot \boldsymbol{u}\,\mathsf{d}A = \mathsf{d} * \boldsymbol{u} \cdot \mathsf{d}\boldsymbol{x}$ compute **first variation of surface area element and of mean curvature**

$$\delta\,\mathsf{d}\,A = (\boldsymbol{\nabla} \cdot \boldsymbol{u} - 2H\Sigma_3)\,\mathsf{d}A$$

$$\delta H = \left[\nabla^2 + H^2 - 2K\right]\Sigma_3 + \nabla H \cdot \boldsymbol{v}$$

Change in area is due curvature or due change in the boundary curve ($\boldsymbol{\nabla} \cdot \boldsymbol{u} = \boldsymbol{\nabla} \cdot \delta\boldsymbol{x}$)

- **Energy functional of a fluid membrane** (only bending, no in-plane shear strain) was

$$\mathcal{F} = \frac{1}{2}\int \left(k_c H^2 + k_g K\right)\mathsf{d}A + \gamma A - PV + Q\int H\,\mathsf{d}A$$

- **First variation** of $\mathcal{F} = \int H^2\,\mathsf{d}A$

$$\delta\mathcal{F} = \int (2H\delta H)\;\mathsf{d}A + H^2\,(\delta\mathsf{d}A) = \int \left(2H\left[\boldsymbol{\nabla}^2 + H^2 - 2K\right] - H^3\right)\Sigma_3\,\mathsf{d}A$$

- Integrating by parts (no boundary integrals) and adding other terms gives ($\delta\int\mathsf{d}V = \int\Sigma_3\mathsf{d}A$) **Euler-Lagrange equation (shape equation) for a closed lipid bilayer**

$$\frac{k_c}{2}\left[2\boldsymbol{\nabla}^2 H + H\left(H^2 - 4K\right)\right] - 2\gamma H + P = 0$$

Bending and shear stress and open biomembranes

- For **open biomembranes** the first variation has boundary integrals. The resulting equations are shape equation, force and momentum equations.
- Assume 2D isotropic homogeneous material. For **small in-plane strains** energy functional is additionally a function of the **strain invariants**

$$\boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} \\ \varepsilon_{21} & \varepsilon_{22} \end{bmatrix} \qquad J = \tfrac{1}{2}\mathrm{tr}\,\boldsymbol{\varepsilon} = \varepsilon_{11} + \varepsilon_{22} \qquad Q = \det \boldsymbol{\varepsilon} = \varepsilon_{11}\varepsilon_{22} - \varepsilon_{12}^2$$

- Free energy of a cell membrane [Tu, Ou-Yang 2004, 2008]

$$\mathcal{F}(H, K; J, Q) = \int \Big(W_H[H, K] + W_J[J, Q]\Big)\mathrm{d}A + \gamma A - PV + QM$$

where $W_H = \frac{1}{2}\left(k_c H^2 + k_g K\right)$ and $W_J = \frac{1}{2}\left(k_d J^2 + k_s Q\right)$ $\qquad k_d = \frac{Eh}{1-\nu^2}, k_s = -\frac{2Eh}{1+\nu}$

- Take **first variations** and get three equilibrium (Euler Lagrange) equations, **one for shape and two for in-plane stresses**

Modeling biomembranes

using

Discrete Exterior Calculus

DEC and FEEC

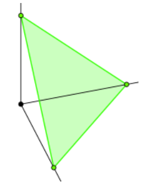
- **Discrete Exterior Calculus** (DEC)
  Reformulate operators from exterior calculus in such a way that the discretized operator preserves the essential mathematical features of the continuous operator
  [Hirani 2006], [Desbrun, Kanso, Tong 2006] (Caltech)
  Stable numerical methods (Laplace equations, Darcy flow, time integrators, fluids)
  New results on discretization of Euler fluids. How to discretize stress tensor?

- **Finite Element Exterior Calculus** (FEEC)
  Theory of constructing stable finite element spaces in the framework of exterior calculus, de Rham cohomology, and Hodge theory
  [Arnold (UMN), Falk, Winther 2010]
  Constructing stable finite element spaces for shells, elasticity complex

- In electromagnetism exterior calculus and **Whitney forms** (FEs) was used earlier
  [Bossavit 1988, 1998]

- Computations are independent of geometry, operate on simplices (vertices, triangles)
  Defined on general manifolds, suitable for problems with moving interfaces and shells
  Workshop: Discrete Differential Geometry for Multiphase Flow Problems (4/2010)

Simplices, boundary operator, chains



- A **k-simplex** σ^k is the non degenerate convex hull of $(k+1)$ (oriented) vertices $\sigma^k = (v_0, v_1, v_2, ..., v_k)$

0-simplex	point	$\sigma^0 = (v_0)$
1-simplex	directed line	$\sigma^1 = (v_0, v_1)$
2-simplex	oriented triangle	$\sigma^2 = (v_0, v_1, v_2)$

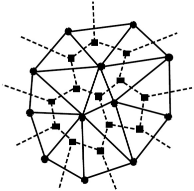
- The **boundary of a k-simplex** is a sum of $(k-1)$-simplices $\partial_k(v_0, v_1, v_2, ..., v_k) = \sum_{i=0}^{k}(-1)^i(v_0, v_1, ..., v_{i-1}, v_{i+1}, v_k)$

boundary of a point	$\partial_0(v_0) = \emptyset$
boundary of an edge	$\partial_1(v_0, v_1) = (v_1) - (v_0)$
boundary of a triangle	$\partial_2(v_0, v_1, v_2) = (v_1, v_2) - (v_0, v_2) + (v_0, v_1)$

- Let $T(\Omega)$ be a triangulation of a manifold. The primal mesh (black) is a **simplicial complex.** We denote all k-simplices of T by T_k

- A **k-chain** is a linear combination of simplices $\sum_{\sigma^k \in T_k} c(\sigma^k)\sigma^k$

  The set of all this vectors form the **space of k-chains $\mathcal{C}^k$**
  The dual space to $\mathcal{C}^k$ is the **space of k-cochains $\mathcal{C}_*^k$**



nice simplicial complex

www.sagemath.org/doc/reference/sage/homology/simplicial_complex.html
www-sop.inria.fr/members/Herve.Delingette/simplex

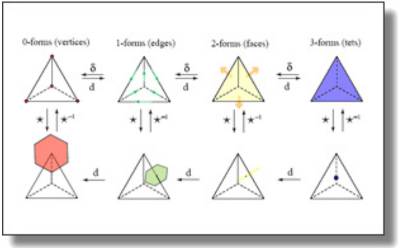
Discrete: diff. forms, exterior derivative, Hodge star

- A **discrete differential k-form** is the linear map $\omega^k : \mathcal{C}^k \to \mathbb{R}$, associated with a **$k$-cochain**

  Integrating a diff. form over a simplex gives a number

  $$\int_{\sigma^k} \omega^k = \int_{\sigma^k} \omega^k \qquad \langle \sigma^k, \omega^k \rangle$$

0-forms	values at points
1-forms	circulation along edges
2-forms	flux through faces
3-forms	integrated densities



- The **discrete exterior derivative** is defined by Stokes theorem

  $$\int_{\sigma^k} \mathrm{d}_{k-1}\omega^{k-1} = \int_{\partial_k \sigma^k} \omega^{k-1} \qquad \langle \sigma^k, \mathrm{d}\omega^{k-1} \rangle = \langle \partial\sigma^k, \omega^{k-1} \rangle$$

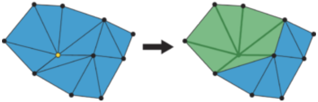
  $$\mathbb{D}_0 = \begin{array}{c} \\ e_0 \\ e_1 \\ e_2 \end{array} \begin{array}{ccc} v_0 & v_1 & v_2 \\ \hline -1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{array}$$

  Discrete exterior derivative is the **transpose of the boundary operator**

- **Discrete Hodge star** brings forms to dual simplices

  Cotangent formula and circumcenters leads to diagonal matrix

  Whitney forms are generalized barycentric coordinates



www.geometry.caltech.edu/pubs.html
en.wikipedia.org/wiki/Simplicial_complex

Vector calculus, exterior derivative and Hodge star

- The coefficients of the 1-form $*\mathbf{d}\alpha$ are the components of the vector curl $\langle A, B, C\rangle$

$$\underset{1\,2\,1}{\overset{\uparrow\uparrow\uparrow}{*\mathbf{d}\alpha}} = *\mathbf{d}\,(A\mathrm{d}x + B\mathrm{d}y + C\mathrm{d}z)$$

$$= *\left[\left(\frac{\partial C}{\partial y} - \frac{\partial B}{\partial z}\right)\mathrm{d}y\wedge\mathrm{d}z - \left(\frac{\partial A}{\partial z} - \frac{\partial C}{\partial x}\right)\mathrm{d}x\wedge\mathrm{d}z + \left(\frac{\partial B}{\partial x} - \frac{\partial A}{\partial y}\right)\mathrm{d}x\wedge\mathrm{d}y\right]$$

$$= \left(\frac{\partial C}{\partial y} - \frac{\partial B}{\partial z}\right)\mathrm{d}x + \left(\frac{\partial A}{\partial z} - \frac{\partial C}{\partial x}\right)\mathrm{d}y + \left(\frac{\partial B}{\partial x} - \frac{\partial A}{\partial y}\right)\mathrm{d}z$$

- The 0-form $*\mathbf{d}*\alpha$ is div $\langle A, B, C\rangle$

$$*\alpha = A\,\mathrm{d}y\wedge\mathrm{d}z - B\,\mathrm{d}x\wedge\mathrm{d}z + C\,\mathrm{d}x\wedge\mathrm{d}y$$

$$\underset{3\,2\,1}{\overset{\uparrow\uparrow\uparrow}{\mathbf{d}*\alpha}} = \left(\frac{\partial A}{\partial x} + \frac{\partial B}{\partial y} + \frac{\partial C}{\partial z}\right)\mathrm{d}x\wedge\mathrm{d}y\wedge\mathrm{d}z$$

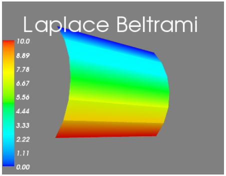
- The Laplace operator $\Delta f =$ div grad f is the 0-form $*\mathbf{d}*\mathbf{d}f$

$$\underset{0\,3\,2\,1}{\overset{\uparrow\uparrow\uparrow\uparrow}{*\mathbf{d}*\mathbf{d}f}} = \frac{\partial^2 f}{\partial x^2} + \frac{\partial f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

Where is the pressure defined?

Primal and dual cochain complex

$$\begin{array}{ccccccc}
\mathcal{C}^0 & \xrightarrow{\mathbb{D}_0} & \mathcal{C}^1 & \xrightarrow{\mathbb{D}_1} & \mathcal{C}^2 & \xrightarrow{\mathbb{D}_2} & \mathcal{C}^3 \\
\downarrow \mathbb{M}_0 & & \downarrow \mathbb{M}_1 \ \mathbb{M}_1 & & \downarrow \mathbb{M}_2 & & \downarrow \mathbb{M}_3 \\
\mathcal{C}^3_* & \xleftarrow[\mathbb{D}_0^T]{} & \mathcal{C}^2_* & \xleftarrow[\mathbb{D}_1^T]{} & \mathcal{C}^1_* & \xleftarrow[\mathbb{D}_2^T]{} & \mathcal{C}^0_*
\end{array}$$



Laplace Beltrami on $\Omega \subset \mathbb{R}^3$

$$\begin{aligned} \Delta u &= 0 \quad \text{in} \quad \Omega \\ \frac{\partial u}{\partial n} &= 0 \quad \text{on} \quad \partial\Omega \end{aligned}$$

$$\mathbb{D}_0^T \mathbb{M}_1 \mathbb{D}_0 u = f$$

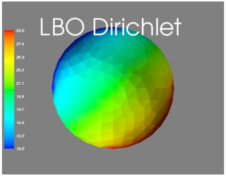
$u \in \mathcal{C}^0$, [Bell 2008], [Gillette 2010]

Darcy flow on $\Omega \subset \mathbb{R}^3$
(mixed LBO for $\phi = 0$)

$$\begin{aligned} \boldsymbol{v} + \frac{k}{\mu}\boldsymbol{\nabla} p &= 0 \quad \text{in} \quad \Omega \\ \boldsymbol{\nabla} \cdot \boldsymbol{v} &= \phi \quad \text{in} \quad \Omega \\ \boldsymbol{v} \cdot \boldsymbol{n} &= \psi \quad \text{on} \quad \partial\Omega \end{aligned}$$

$$\begin{bmatrix} -\frac{k}{\mu}\mathbb{M}_1 & \mathbb{D}_1^T \\ \mathbb{D}_1 & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{v} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \psi \end{bmatrix}$$

$\boldsymbol{v} \in \mathcal{C}^2$, $p \in \mathcal{C}^0_*$, [Hirani 2011]



END

THANK YOU