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A Stretch-Gradient Model for Membrane Thickness Variations

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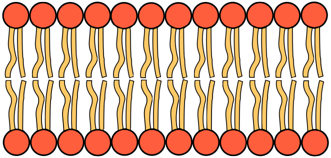
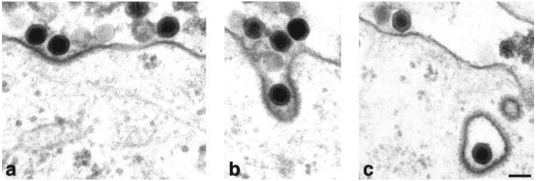
Introduction



Living matter composed of cells enclosed by a membrane - structure is two layers of lipids, with hydrophobic tail groups/hydrophilic head groups.



Endocytosis of an adenovirus
O. Meier et al., JCB, 2002, **158** *(6), 1119.*

Membrane continuously deforms: under cytoskeleton forces, to facilitate cell movement, endocytosis, . . .

Determining the Energy

Membrane energy based on curvature - Helfrich, 1974:

$$W = W(H, K) = kH^2 + \bar{k}K$$

Membrane thickness assumed constant; doesn't model stretch/no area change - include areal stretch J to remedy this.
General form for energy density: Take

$$W = W(H, K, J, Q),$$

$Q = |\nabla J|$ tunable penalty for sudden changes in J - physically, prevents exposure of hydrophobic tail groups.

The Shape Equation

Determine minimizers of the energy

$$E = \int_{\omega} W da = \int_{\Omega} WJ dA$$

by imposing stationarity of the first variation. Equilibrium configurations are then given by $\frac{dE}{d\epsilon} = 0$:

$$\frac{d}{d\epsilon} E = \int_{\omega} (\dot{W} + W\dot{J}/J) da \tag{1}$$

with

$$\dot{W} = W_H \dot{H} + W_K \dot{K} + W_J \dot{J} + W_Q \dot{Q}, \tag{2}$$

Calculation: for position on ω given by $\boldsymbol{r}$, impose variation

$$\dot{\boldsymbol{r}} = \boldsymbol{u} = u^{\alpha} \boldsymbol{a}_{\alpha} + w \boldsymbol{n}, \tag{3}$$

in tangential and normal directions.

For energy without J, Q dependence, tangential variations give trivial equations: just a reparameterisation. Non-trivial when W has J, Q dependence. Set $\boldsymbol{u} = u^\alpha \boldsymbol{a}_\alpha$ and obtain

$$\dot{H} = u^\alpha H_{,\alpha}, \quad \dot{K} = u^\alpha K_{,\alpha}, \quad \dot{J} = J u^\alpha_{;\alpha},$$
$$\dot{Q} = Q^{-1} J_{,\mu} a^{\mu\beta} \left[(J u^\alpha_{;\alpha})_{,\beta} - J_{,\alpha} u^\alpha_{;\beta} \right]$$

Insert in $\dot{E} = \int_\omega \dot{W} + W \dot{J}/J da$; terms factoring u^α give the E-L equations; terms with a divergence go to boundary via Stokes theorem: E-L equations are

$$(J W_J)_{,\alpha} + W_J J_{,\alpha} - 2 J_{,\alpha} (Q^{-1} W_Q J_{,\mu} a^{\mu\beta})_{;\beta} - J (Q^{-1} W_Q J_{,\mu} a^{\mu\beta})_{;\beta\alpha} = 0$$

Boundary terms: later.

Normal Variations

Set $\boldsymbol{u} = w\boldsymbol{n}$:

$$\dot{H} = \frac{1}{2}\Delta w + w(2H^2 - K), \quad \dot{K} = 2KHw + (\tilde{b}^{\alpha\beta} w_{,\alpha})_{;\beta},$$
$$\dot{J} = -2HJw,$$
$$\dot{Q} = Q^{-1}\left[J_{,\alpha}J_{,\beta}b^{\alpha\beta}w - a^{\alpha\beta}(HJw)_{,\alpha}J_{,\beta}\right].$$

Substitute to find E-L equation

$$\tfrac{1}{2}\Delta W_H - W_H(2H^2 - K) - 2HKW_K + (W_K)_{;\beta\alpha}\tilde{b}^{\beta\alpha} + 2HJW_J$$
$$- Q^{-1}W_Q J_{,\alpha}J_{,\beta}b^{\alpha\beta} - 2HJ(Q^{-1}W_Q a^{\alpha\beta}J_{,\beta})_{;\alpha} + 2HW = p,$$

p is pressure in liquid bounded by membrane, $b^{\alpha\beta}$ is inverse of curvature tensor, $\tilde{b}^{\alpha\beta} = 2Ha^{\alpha\beta} - b^{\alpha\beta}$, and $\Delta f = \frac{1}{\sqrt{a}}\left(\sqrt{a}a^{\alpha\beta}f_{,\beta}\right)_{,\alpha}$.

Boundary Terms

Terms arising on $\partial\omega$ are

$$B_t = \int_{\partial\omega} u^\alpha [J W_J \nu_\alpha + W \nu_\alpha - J(Q^{-1} W_Q J_{,\mu} a^{\mu\beta})_{;\beta} \nu_\alpha - Q^{-1} W_Q J_{,\mu} J_{,\alpha} \nu^\mu]\, ds.$$

$$T_t = \int_{\partial\omega} Q^{-1} W_Q J J_{,\mu} u^\alpha_{;\alpha} \nu^\mu \, ds.$$

$$B_n = \int_{\partial\omega} [\tfrac{1}{2} W_H w_{,\alpha} \nu^\alpha - \tfrac{1}{2} w (W_H)_{;\alpha} \nu^\alpha + W_K \tilde{b}^{\alpha\beta} w_{,\alpha} \nu_\beta - (W_K)_{;\beta} \tilde{b}^{\alpha\beta} w \nu_\alpha - Q^{-1} W_Q J_{,\beta} J H w \nu^\beta]\, ds$$

These need to be written in vector form to obtain useful relations.

Virtual work statement: work done on boundary is equal to P, the work of applied loads, or

$$\dot{E}^* = P = B_t + T_t + B_n$$

RHS can be put in the form

$$P = \underbrace{\int_{\partial\omega_f} \boldsymbol{F} \cdot \boldsymbol{u}\, ds}_{\text{Force}} + \underbrace{\int_{\partial\omega_t} T \text{div}\, \boldsymbol{u}\, ds}_{\text{Hypertraction}} - \underbrace{\int_{\partial\omega_m} M \boldsymbol{\tau} \cdot \boldsymbol{\omega}\, ds}_{\text{Bending Moment}} + \underbrace{\sum \boldsymbol{f}_i \cdot \boldsymbol{u}_i}_{\text{Force at corner}} \tag{4}$$

where $\boldsymbol{\omega}$ is the variation of the surface orientation,

$$\boldsymbol{F} = F_\nu \boldsymbol{\nu} + F_\tau \boldsymbol{\tau} + F_n \boldsymbol{n}, \quad M = \frac{1}{2} W_H + \kappa_\tau W_K,$$
$$\tau = b^{\alpha\beta} \tau_\alpha \tau_\beta, \quad \kappa_\nu = b^{\alpha\beta} \nu_\alpha \nu_\beta \quad \kappa_\tau = b^{\alpha\beta} \tau_\alpha \tau_\beta$$

are the twist on the $\boldsymbol{\nu}$-$\boldsymbol{\tau}$ axes and the normal $\boldsymbol{\nu}$ and $\boldsymbol{\tau}$ curvatures.

Extension of Circular Disc

Disc of uniform reference thickness, mid-surface occupying

$$\Omega = \{\boldsymbol{X} = R\boldsymbol{e}_R(\theta) \,|\, 0 \leq R \leq R_0, 0 \leq \theta \leq 2\pi\}$$

Stretch in radial direction: current configuration is

$$\omega = \{\boldsymbol{x}(\boldsymbol{X}) = r(R)\boldsymbol{e}_R(\theta) \,|\, 0 \leq R \leq R_0, 0 \leq \theta \leq 2\pi\}$$

Deformation is $\boldsymbol{f} : \mathbb{R}^2 \rightarrow \mathbb{R}^2, (R, \theta) \rightarrow (r(R), \theta)$ gradient $\nabla \boldsymbol{f} = \text{diag}(r', r/R)$, tangent/normal vectors

$$\boldsymbol{a}_1 = r'\boldsymbol{e}_R, \quad \boldsymbol{a}_2 = \frac{r}{R}\boldsymbol{e}_\theta, \quad \boldsymbol{n} = \hat{\boldsymbol{k}}, \tag{5}$$

metric is $a_{\alpha\beta} = \text{diag}(r'^2, r^2/R^2)$, giving area element

$$\sqrt{g} = \sqrt{\det(a_{\alpha\beta})} = rr'/R$$

.

Extension of Circular Disc

For Q, the spatial gradient of J: taking $Q = |\nabla_\omega J| = |J_{,\alpha}\boldsymbol{a}^\alpha| = \frac{J'}{r'}$, which coincides with J_ν, normal derivative, in this symmetry.
Identify boundary normal and tangent vectors as

$$\boldsymbol{\nu} = \boldsymbol{e}_R, \quad \boldsymbol{\tau} = \boldsymbol{e}_\theta, \tag{6}$$

respectively.
Interested in **thickness profile**: impose bulk incompressibility, $\phi J = 1$, for thickness field ϕ, gives access to a measure of thickness,

$$\phi = \frac{1}{J}. \tag{7}$$

Other authors define ϕ as a a field on the mid-surface and include in energy - uncoupled/can be solved independently of shape equations, which seems unrealistic.

Extension of Circular Disc

Since the mean and Gaussian curvatures are both zero (no bending terms), the energy is of the form

$$W = W(J, Q),$$

for $Q = \nabla J$; thus we take a density quadratic in J and Q,

$$W = a_1(J-1)^2 + a_2 Q^2,$$

for constants a_1, a_2 (which in general should depend on J). Normal equation and one tangential equation are trivial. Remaining tangential equation gives:

$$a_1\left[\left(JJ'(J-1)\right)' + J'(J-1)\right] - a_2\left[\frac{2J'}{J}\left(\frac{JJ'}{r'^2}\right)' + \left(\frac{JJ'}{r'^2}\right)''\right] = 0,$$

third order in $J \implies$ fourth order in R.

Boundary Terms

F_τ, F_n are also zero: remaining components are F_ν and T.
Appropriate boundary conditions:

1. Fixed at origin: $r(R=0)=0$;
2. Specify extension/stretch: $r(R=R_0)=\lambda R_0$;
3. Fixed reference thickness at boundary:
   $\phi(R=R_0)=1 \implies r'(R=R_0)=\lambda^{-1}$;
4. Zero hypertraction at boundary:
   $T|R=R_0=0 \implies r''(R=R_0)=\frac{1}{\lambda R_0}(1-\lambda^{-2})$.

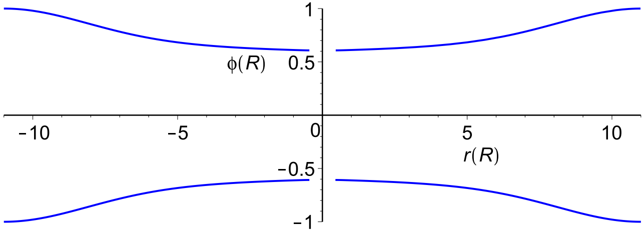


Figure: Plot of solution for $\phi = 1/J = R/rr'$, with $\lambda = 1.1$