Small Membrane Deformations on Surfaces

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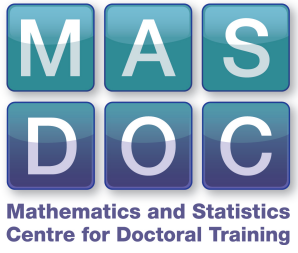
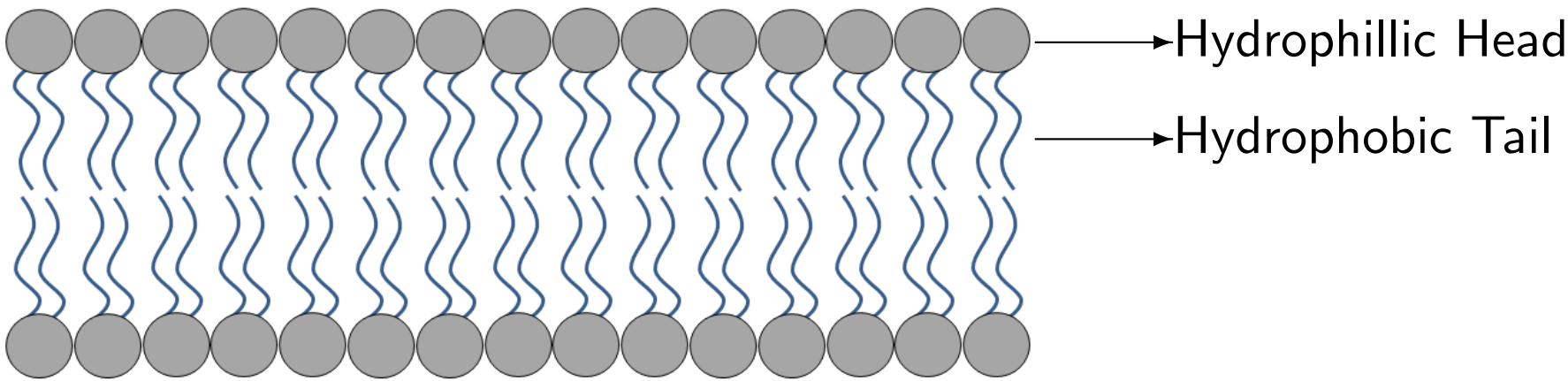


Contents

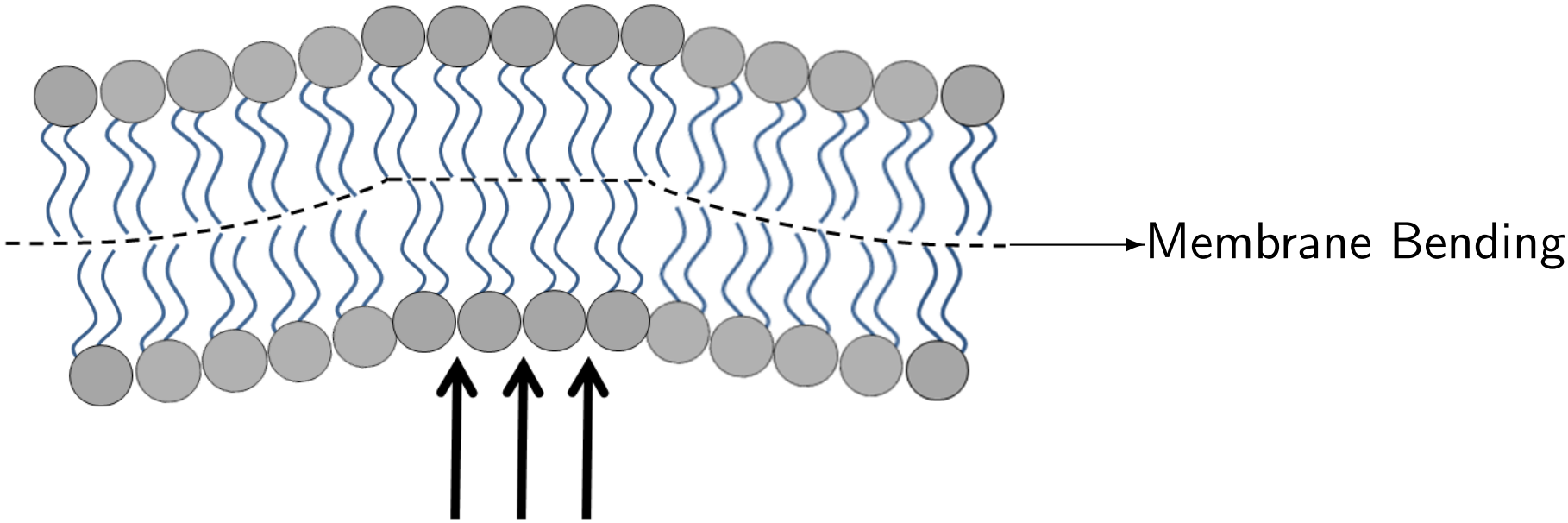
Biomembranes

Biomembranes are composed of phospholipid molcules, built from a hydrophilic phosphate 'head' and a hydrophobic lipid 'tail'. When immersed in water they form structures in which the heads point towards the water and the tails away. Biomembranes are composed of one such structure, the bilayer sheet.



Biomembrane Deformation - Actin Filaments

Biomembrane deformation can be caused by the action of exterior proteins. Actin filaments push against the membrane and cause it to bend.



Modelling Assumptions

- The membrane is a single elastic sheet and may be represented by a small deformation of a given surface $\Gamma \subset \mathbb{R}^3$.
- Actin filaments are modelled as single points.
- Filaments may apply a point constraint to h or apply a point force to the membrane.
- The energy due to the curvature of the membrane is given by the Willmore energy functional.

Willmore Energy Functional

We consider the Willmore energy functional with surface tension given by

$$\mathcal{W}(\Gamma) := \frac{1}{2}\int_{\Gamma} \kappa H^2 + \sigma \, do.$$

- $\kappa > 0$ is the bending modulus.
- $\sigma > 0$ accounts for the surface tension.

We wish to minimise this energy over some appropriate set of surfaces Γ under volume and centre of mass constraints. The constraints will be introduced via Lagrange multipliers.

Volume and Centre of Mass

Assuming $\Gamma = \partial\Omega$, where $\Omega \subset \mathbb{R}^3$ is a bounded domain, the volume and centre of mass are given by

$$V(\Gamma) := \frac{1}{3}\int_\Gamma X \cdot \nu \; do \quad \textit{and} \quad C(\Gamma) := \int_\Gamma X \; do.$$

Introducing Lagrange multipliers yields the energy functional

$$\mathcal{J}(\Gamma, \lambda, v) = \mathcal{W}(\Gamma) + \lambda(V(\Gamma) - V_0) + v \cdot (C(\Gamma) - C_0).$$

The multipliers $\lambda \in \mathbb{R}, v \in \mathbb{R}^3$ will be fixed later.

Possible Deformed Surfaces

We assume that the deformed surfaces are small deformations of a given surface $\Gamma \subset \mathbb{R}^3$ of the form

$$\Gamma_{\varepsilon,h} = \{X + \varepsilon h(X)\nu(X) \mid X \in \Gamma\}$$

where $0 < \varepsilon \ll 1$ and $h : \Gamma \to \mathbb{R}$ is sufficiently smooth.

Performing $O(\varepsilon)$ variations around the Lagrange multipliers also we obtain the functional

$$\mathcal{J}(\varepsilon; h, \mu, w) := \mathcal{J}(\Gamma_{\varepsilon,h}, \lambda + \varepsilon\mu, v + \varepsilon w).$$

Minimising this energy over $(h, \mu, w) \in V \times \mathbb{R} \times \mathbb{R}^3$ is equivalent to minimising $\mathcal{W}$ over $\{\Gamma_{\varepsilon,h} \mid h \in V, V(\Gamma_{\varepsilon,h}) = V_0, C(\Gamma_{\varepsilon,h}) = C_0\}$.

Linearisation

For each h, μ, w consider the Taylor expansion

$$\begin{aligned}\mathcal{J}(\varepsilon; h, \mu, w) =& \mathcal{J}(0; h, \mu, w) + \varepsilon \frac{\mathrm{d}\mathcal{J}(\varepsilon; h, \mu, w)}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon=0} \\ &+ \frac{\varepsilon^2}{2} \frac{\mathrm{d}^2\mathcal{J}(\varepsilon; h, \mu, w)}{\mathrm{d}\varepsilon^2}\bigg|_{\varepsilon=0} + O(\varepsilon^3).\end{aligned}$$

- $\mathcal{J}(0; h, \mu, w) = \mathcal{W}(\Gamma)$ is a constant.
- We may choose λ, v such that the first variation vanishes.
- As ε is small we discard the $O(\varepsilon^3)$ term.

Linearisation

We are left with the second variation term.

$$\begin{aligned} J(h,\mu,w) =& \frac{\mathrm{d}^2 \mathcal{J}(\varepsilon; h,\mu,w)}{\mathrm{d}\varepsilon^2}\bigg|_{\varepsilon=0} \\ =& \mathcal{W}''(\Gamma)[h\nu, h\nu] + \lambda V''(\Gamma)[h\nu, h\nu] + v \cdot C''(\Gamma)[h\nu, h\nu] \\ &+ 2\mu V'(\Gamma)[h\nu] + 2w \cdot C'(\Gamma)[h\nu] \end{aligned}$$

We seek to minimise this over $(h,\mu,w) \in K \times \mathbb{R} \times \mathbb{R}^3$, where $K \subset H^2(\Gamma)$ is a suitably chosen subset.

Application to a Sphere

Now take $\Gamma = \left\{x \in \mathbb{R}^3 \mid |x| = R\right\}$ and fix the Lagrange multipliers $\lambda = -2\sigma/R, v = 0$. The linearised energy functional becomes

$$J(h, \mu, w) = \int_\Gamma \kappa(\Delta_\Gamma h)^2 + \left(\sigma - \frac{2\kappa}{R^2}\right)|\nabla_\Gamma h|^2 - \frac{2\sigma}{R^2}h^2 + (\mu + 3w \cdot \nu)h \, do.$$

At a minimum we must have

$$0 = \frac{\partial J}{\partial \mu}(h, \mu, w) = \int_\Gamma h \, do,$$

$$0 = \nabla_w J(h, \mu, w) = \int_\Gamma h\nu \, do.$$

Thus it is equivalent to minimise $J(h, 0, 0)$ over

$$\tilde{K} := \left\{ h \in K \;\middle|\; 0 = \int_\Gamma h \, do = \int_\Gamma h\nu_i \, do, \; i = 1, 2, 3 \right\}.$$

Fixed Heights Problem

We first consider filaments applying a point constraint to the displacement h.

This corresponds to the action of actin filaments anchored to the cytoskeleton.

Let $N \in \mathbb{N}$ and take $X \in \Gamma^N$ to be the inclusion locations. The inclusions apply the point constraints

$$h(X_i) = \alpha_i \; \forall 1 \leq i \leq N$$

for some $\alpha \in \mathbb{R}^N$.

We look to minimise $J(h, 0, 0)$ over a subset of $H^2(\Gamma)$ subject to these constraints.

Fixed Heights Problem

We put this minimisation problem into a general framework developed previously.

Define $V \subset H^2(\Gamma)$ by

$$V := \left\{ h \in H^2(\Gamma) \,\middle|\, 0 = \int_\Gamma h \, do = \int_\Gamma h\nu_i \, do, \; i = 1, 2, 3 \right\}.$$

Define $a : V \times V \to \mathbb{R}$ by

$$a(g, h) = \int_\Gamma \kappa \Delta_\Gamma g \Delta_\Gamma h + \left(\sigma - \frac{2\kappa}{R^2} \right) \nabla_\Gamma g \cdot \nabla_\Gamma h - \frac{2\sigma}{R^2} gh \, do.$$

Define a convex subset of V:

$$K_\alpha^X := \{ v \in V \mid v(X_i) = \alpha_i \; \forall 1 \leq i \leq N \}.$$

Abstract Quadratic Programming Problem

Theorem (Quadratic programming problem (QPP))

Let V be a Hilbert Space, fix $N \in \mathbb{N}$, $\alpha \in \mathbb{R}^N$ and a set of linearly independent functionals $\{F_1, ..., F_N\} \subset V^*$. We thus define a convex subset $K_\alpha^F \subset V$ by:

$$K_\alpha^F := \{v \in V \mid F_j(v) = \alpha_j \; \forall \, 1 \leq j \leq N\}.$$

Let $a : V \times V \to \mathbb{R}$ be bilinear, symmetric, bounded and coercive.
Let $l : V \to \mathbb{R}$ be a bounded linear functional.
Define $J : V \to \mathbb{R}$ by $J(v) := \frac{1}{2}a(v, v) - l(v)$.
Then $\exists! u \in K_\alpha^F$ such that

$$J(u) \leq J(v) \; \forall \, v \in K_\alpha^F.$$

Checking assumptions

The assumptions we need to check are for the bilinear form

$$a(g,h) = \int_\Gamma \kappa \left(\Delta_\Gamma g \Delta_\Gamma h - \frac{2}{R^2} \nabla_\Gamma g \cdot \nabla_\Gamma h \right) + \sigma \left(\nabla_\Gamma g \cdot \nabla_\Gamma h - \frac{2}{R^2} gh \right) \, do.$$

- Bilinearity, boundedness and symmetry are clear.
- We would like coercivity for any $\kappa > 0, \sigma \geq 0$, this is not so clear.

Poincaré to the Rescue?

As $\int_\Gamma h = 0$ for each $h \in V$ we may apply the Poincaré inequality and integration by parts to obtain the inequalities

$$\int_\Gamma (\Delta_\Gamma h)^2 \, do \geq C \|h\|^2_{H^2(\Gamma)}$$

$$a(h,h) \geq \int_\Gamma \kappa \left(1 - \frac{2C_P^2(\Gamma)}{R^2}\right)(\Delta_\Gamma h)^2 + \sigma \left(1 - \frac{2C_P^2(\Gamma)}{R^2}\right)|\nabla_\Gamma h|^2$$

- So we have the required coercivity provided $C_P^2(\Gamma) < R^2/2$.
- For a sphere radius R, $C_P^2(\Gamma) = R^2/2$.

Optimal Poincaré Constant

In fact we may replace the Poincaré constant used above by the optimal Poincaré constant over V, satisfying:

$$C_V^{-2} = \inf_{v \in V} \frac{\int_\Gamma |\nabla_\Gamma v|^2 \, do}{\int_\Gamma v^2 \, do} \geq \inf_{v \in X} \frac{\int_\Gamma |\nabla_\Gamma v|^2 \, do}{\int_\Gamma v^2 \, do} = \lambda_2$$

where $X := \left\{ h \in H^1(\Gamma) \mid 0 = \int_\Gamma h \, do = \int_\Gamma h \nu_i \, do, \; i = 1, 2, 3 \right\}$ and λ_2 is the second non-zero eigenvalue for the Laplace-Beltrami operator.

- $\lambda_2 = 6/R^2$ thus $C_V^2 = R^2/6 < R^2/2$ and a is coercive over V.

Further Work

- We can also show existence of global minimisers for the fixed heights problem.
- We can model point forces by studying the energy

$$v \mapsto \frac{1}{2}a(v,v) - \sum_{i=1}^{N} \beta_i h(X_i)$$

- We can apply similar techniques to model inclusions applying point curvature constraints.