DISMA Dipartimento di Scienze Matematiche G. L. Lagrange
ECCELLENZA 2018 · 2022

The Helfrich model for the elasticity of biomembranes as a limit of mesoscopic energies

Luca Lussardi
luca.lussardi@polito.it

XXI Geometry, Integrability and Quantization
Varna (Bulgaria) - June 7, 2019

POLITECNICO DI TORINO

POLITECNICO DI TORINO

Outline

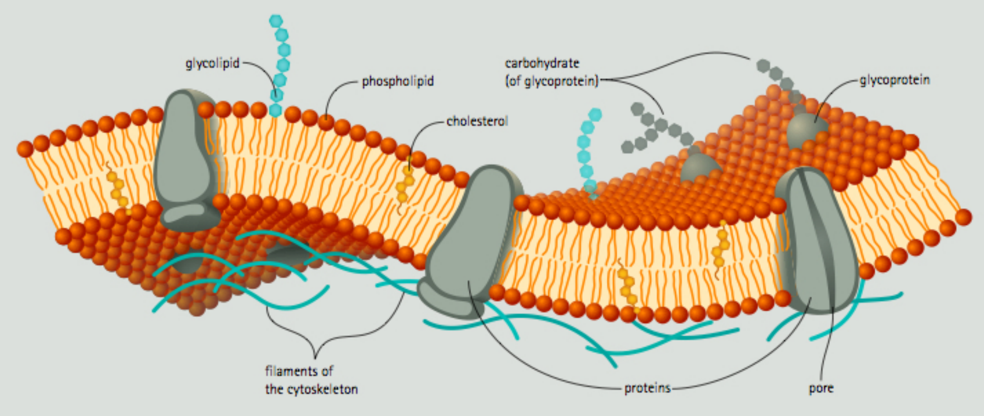
- Cell membranes
- Models for cell membranes
- Qualitative description of the Peletier-Röger mesoscopic model
- How to pass to the limit in a rigorous way: Γ-convergence
- Main tools for the 3D-analysis

References:

- L. Lussardi, M.A. Peletier and M. Röger, *Variational analysis of a mesoscale model for bilayer membranes*, J. Fixed Point Theory Appl. 15 (2014), no. 1, 217-240
- L. Lussardi and M. Röger, *Gamma convergence of a family of surface-director bending energies with small tilt*, Arch. Rational Mech. Anal. 219 (2016), no. 3, 985-1016

DISMA Dipartimento di Scienze Matematiche G. L. Lagrange ECCELLENZA 2018 · 2022

The cell membrane



The Helfrich energy functional (1973)

For a smooth surface S in the space we let

$$E(S) = \int_S \kappa_b (\mathrm{H}_S - \mathrm{H}_0)^2 - \kappa_G \mathrm{K}_S \, d\sigma$$

- H_S is the mean curvature of S and K_S is the Gauss curvature of S
- $\kappa_b > \kappa_G > 0$ (Mathematics & Physics)
- H_0 is the spontaneous curvature

The shape of the cell membrane minimizes E

We notice that if S is a closed surface and $\mathrm{H}_0 = 0$ then E reduces (up to constants) to the Willmore energy functional

$$W(S) = \int_S \mathrm{H}_S^2 \, d\sigma$$

A microscopic model (Peletier-Röger, ARMA 2009)

Probabilistic model:

- In $\Omega \subset \mathbb{R}^d$: positions of heads X_h^i, tails X_t^i and water particles X_w^j, with $i = 1, \dots, N_\ell$ and $j = 1 \dots, N_w$. Set $\mathcal{X} := \Omega^{2N_\ell + N_w}$ and

$$\mathcal{X} \ni X = (X_t^1, \dots, X_t^{N_\ell}, X_h^1, \dots, X_h^{N_\ell}, X_w^1, \dots, X_w^{N_w})$$

- Probability density ψ on $\mathcal{X}$:

$$\psi \colon \mathcal{X} \to [0,1], \qquad \int \psi = 1$$

- Volume fractions of heads/tails/water:

$$r_t(\psi)(x), \quad r_h(\psi)(x), \quad r_w(\psi)(x)$$

A microscopic model (Peletier-Röger, ARMA 2009)

Energy contributions:

- Penalize the proximity of hydrophilic and hydrophobic grains:

$$\int\int (r_w(\psi)(x) + r_h(\psi)(x))r_t(\psi)(y)\rho(x-y)dxdy$$

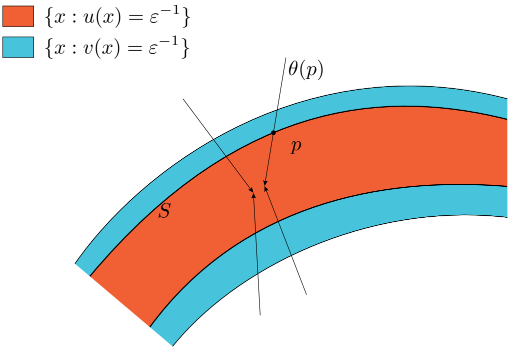
- Incompressibility:

$$r_t(\psi)(x) + r_h(\psi)(x) + r_w(\psi)(x) = 1$$

- Interaction between head and tail:

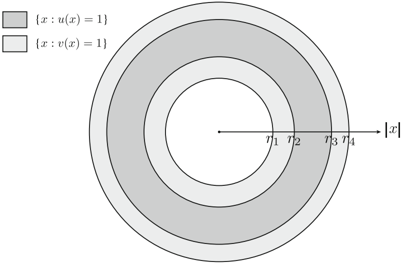
$$\int_{\mathcal{X}} \sum_{i=1}^{N_\ell} |X_h^i - X_t^i| \psi(X)\, dX$$

The mesoscopic model formally derived (Peletier-Röger, ARMA 2009)



- Energy arising from hydrophilic/hydrophobic behavior: area of the boundary of the region occupied by u_ε
- Energy arising from the covalent bond between heads and tails: Monge-Kantorovich distance between u_ε and v_ε

The behavior of the energy on ring structures



$$\text{Energy} \sim 2M + \underbrace{\frac{M}{4}\left(\frac{r_4 - r_1}{2\varepsilon} - 2\right)^2}_{\textit{partial localization}} + \underbrace{\frac{M\varepsilon^2}{(r_4 + r_1)^2}}_{\textit{bending energy}}$$

We thus study $G_\varepsilon(u_\varepsilon, v_\varepsilon) := (\text{Energy} - 2M)/\varepsilon^2$

What happens as $\varepsilon \to 0$? A review on Γ-convergence

Approximate energies by means of simpler functionals with a stability property of the minimum problems during the limit process. General framework: Γ-convergence (De Giorgi, 1975). If (X, d) is a metric space, $F_\varepsilon \colon (X, d) \to [-\infty, +\infty]$, $F_\varepsilon \xrightarrow{\Gamma} F$ as $\varepsilon \to 0$ if

- $\forall u \in X$, $\forall u_\varepsilon \to u$:
$$F(u) \le \liminf_{\varepsilon\to 0} F_\varepsilon(u_\varepsilon)$$
- $\forall u \in X$, $\exists u_\varepsilon \to u$:
$$\limsup_{\varepsilon\to 0} F_\varepsilon(u_\varepsilon) \le F(u)$$

Why does Γ-convergence work?

$$\left.\begin{array}{r} F_\varepsilon \xrightarrow{\Gamma} F \\ F_\varepsilon(u_\varepsilon) = \min\limits_X F_\varepsilon \\ u_\varepsilon \to u_0 \end{array}\right\} \Rightarrow \left\{\begin{array}{l} F(u_0) = \min\limits_X F \\ \min\limits_X F_\varepsilon \to \min\limits_X F \end{array}\right.$$

The main estimate (L-Peletier-Röger, JFPTA 2014)

$S_\varepsilon :=$ interface between u_ε and v_ε (smooth enough), then

$$G_\varepsilon(u_\varepsilon, v_\varepsilon) \gtrsim \frac{1}{\varepsilon^2} \int_{S_\varepsilon} \left(\frac{1}{\theta_\varepsilon \cdot \nu_\varepsilon} - 1 \right)^2 d\sigma + \int_{S_\varepsilon} \frac{1}{4(\theta_\varepsilon \cdot \nu_\varepsilon)^3} (\lambda_\varepsilon^{(1)} + \lambda_\varepsilon^{(2)})^2 - \frac{1}{6} \lambda_\varepsilon^{(1)} \lambda_\varepsilon^{(2)} \, d\sigma$$

where:

- ν_ε is an orientation on S_ε and $\theta_\varepsilon \cdot \nu_\varepsilon > 0$ on S_ε
- $\lambda_\varepsilon^{(1)}, \lambda_\varepsilon^{(2)}$ are the eigenvalues of the covariant derivative of θ_ε

This estimate suggests that the limit energy should take the form

$$\int_S \frac{1}{4} \mathrm{H}_S^2 - \frac{1}{6} \mathrm{K}_S \, d\sigma$$

Generalized surfaces (Geometric Measure Theory)

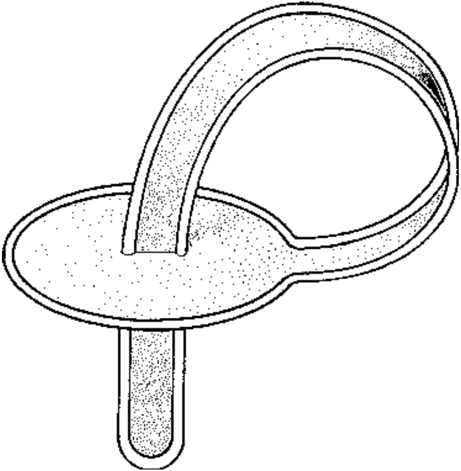
- PDEs/Classical variational problem $\longrightarrow$ weak notion of function
- Geometric variational problem $\longrightarrow$ weak notion of surface

smooth objects	weak objects
functions	distributions
surfaces	currents, varifolds, ...

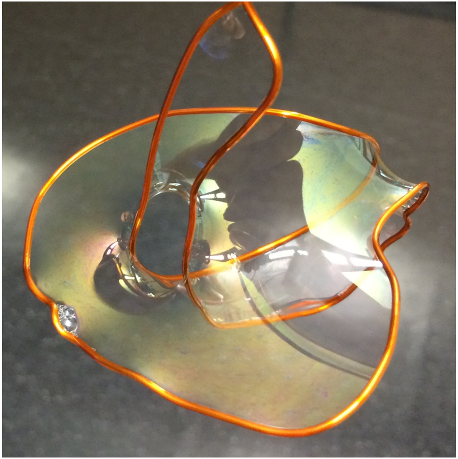
By definition:

- Currents: dual of the space of test differential forms (work fine with oriented-area problems)
- Varifolds: Radon measures on $\mathbb{R}^d \times$Grassmann manifold of all unoriented hyperplanes (work fine with curvature problems)

Intermezzo: are generalized surfaces really necessary?



Intermezzo: are generalized surfaces really necessary?



POLITECNICO DI TORINO
DISMA Dipartimento di Scienze Matematiche G. L. Lagrange
ECCELLENZA 2018 · 2022

Working with currents: compactness but no curvature

Given a smooth surface S the canonical current associated to S is given by

$$\langle S, \omega \rangle := \int_S \langle \omega, \eta \rangle \, d\sigma, \quad \eta \text{ orientation on } S$$

- Compactness holds true if we have a bound on the area

For our problem we have compactness of the currents S_ε, but we do not have a good notion of curvature of a current

Working with varifolds: curvature but no compactness

Given a smooth surface S the canonical varifold associated to S is given by

$$\langle V_S, \psi \rangle := \int_S \psi(x, T_x S)\, d\sigma, \quad \psi \in C_c^0(\mathbb{R}^3 \times G(2,3))$$

- We have a good notion of a second fundamental form of a varifold (hence good notions of mean curvature and gaussian curvature)
- Compactness holds true if we have a bound on the second fundamental form

For our problem the bound

$$G_\varepsilon(u_\varepsilon, v_\varepsilon) \leq c$$

does not provide a bound on the second fundamental form of the varifold V_{S_ε} since θ_ε is not orthogonal to S_ε

Working with Gauss graphs

Exploiting the estimate

$$c \geq G_\varepsilon(u_\varepsilon, v_\varepsilon) \geq \int_{S_\varepsilon} \frac{1}{4}(\lambda_\varepsilon^{(1)} + \lambda_\varepsilon^{(2)})^2 - \frac{1}{6}\lambda_\varepsilon^{(1)}\lambda_\varepsilon^{(2)} \, d\sigma$$

it is relatively easy to realize that the area of

$$G_\varepsilon := \{(p, \theta_\varepsilon(p)) : p \in S_\varepsilon\}$$

remains bounded. When $\varepsilon \sim 0$ the area of G_ε should be the area of the graph of the Gauss map on S. In the area of the graph of the Gauss map are encoded informations on the curvature of S: the idea is therefore to consider the currents

$$G_\varepsilon$$

Generalized Gauss graphs (Anzellotti-Serapioni-Tamanini, Indiana 1990)

If T is a Generalized Gauss graph, that is a limit, as a current, of Gauss graphs of smooth surfaces, then:

- T is an integer rectifiable current, i.e.

$$\langle T, \omega \rangle = \int_R \langle \omega, \eta \rangle \beta \, d\sigma, \quad R \text{ rectifiable, } \eta \text{ orientation on } R,$$

$$\beta \colon R \to \mathbb{Z}$$

- Up to $\mathcal{H}^2$-negligible sets, R is a countable union of Gauss graphs of smooth and orientable surfaces
- There exists a stable notion of principal curvatures of T

Back to compactness and liminf

- The estimate

$$G_\varepsilon(u_\varepsilon, v_\varepsilon) \gtrsim \int_{S_\varepsilon} \frac{1}{4}(\lambda_\varepsilon^{(1)} + \lambda_\varepsilon^{(2)})^2 - \frac{1}{6}\lambda_\varepsilon^{(1)}\lambda_\varepsilon^{(2)}\, d\sigma$$

  says that the area of G_ε is bounded
- When $\varepsilon \to 0$ the transport rays θ_ε tend to be normal, therefore

$$T_{G_\varepsilon} \rightharpoonup \text{Generalized Gauss graph}$$

- Thanks to the stability of principal curvatures it is possible to pass to the limit in

$$\int_{S_\varepsilon} \frac{1}{4}(\lambda_\varepsilon^{(1)} + \lambda_\varepsilon^{(2)})^2 - \frac{1}{6}\lambda_\varepsilon^{(1)}\lambda_\varepsilon^{(2)}\, d\sigma$$

DISMA Dipartimento di Scienze Matematiche G. L. Lagrange ECCELLENZA 2018 · 2022

POLITECNICO DI TORINO

Further investigations

- Complete the Γ-$\liminf$ inequality
- Biological structure of limits currents/varifolds
- Higher codimension
- Local minimizers of F_ε (recent papers by Buttazzo et al.)
- Try to minimize directly the Helfrich functional on generalized Gauss graphs (with M. Morandotti)
- Local minimizers/critical points of Helfrich?
- ......

DISMA Dipartimento di Scienze Matematiche G. L. Lagrange ECCELLENZA 2018 · 2022

Thank you!