What I do

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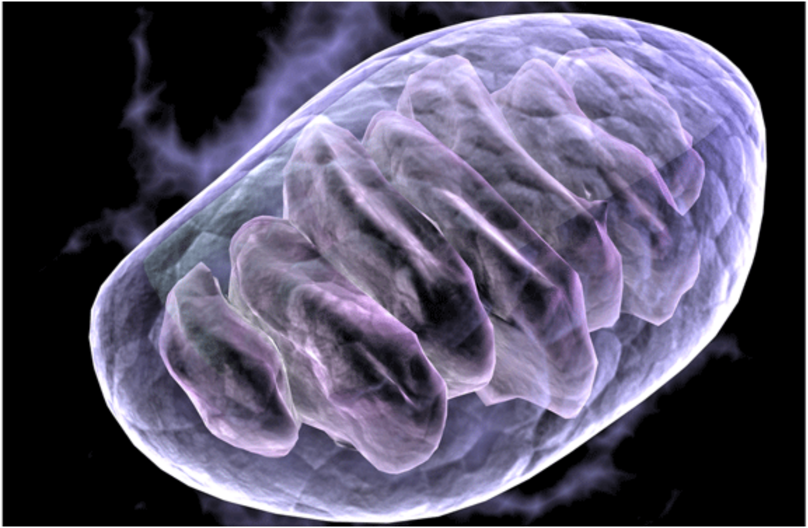
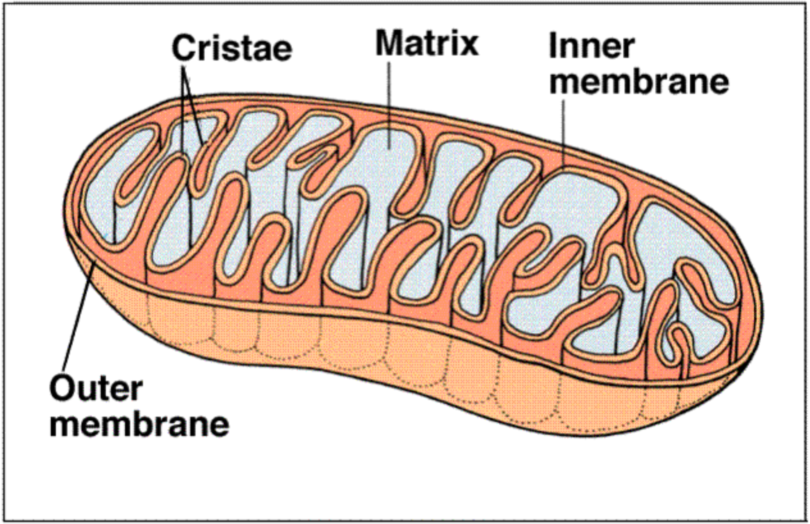


Mitochondrion



How do we model Mitochondria Cells?

So essentially, it is our topic to find out how elastic membranes inside a fixed container behave, e.g. the inner membrane of a Mitochondrion.

Naive idea: $n = 2, 3$. We have

1. $\Omega \subset\subset \mathbb{R}^n$ and
2. a subset $E \subset \Omega$ such that it is smooth in the sense that $M \equiv \partial E \in C^2$ and its one/two-dimensional volume is fixed to $\mathscr{H}^{n-1}(M) \equiv S \in \mathbb{R}$.

In physics we can safely assume that the realized membranes minimize some sort of energy - but which one?

Some Differential Geometry

Let $M \in C^2$ be a submanifold of $\mathbb{R}^3$. The **metric** g on M (or the first fundamental form) is the restriction of the scalar product of $\mathbb{R}^3$ to the tangent spaces of M. The **second fundamental form** II is defined by

$$II(x, y) = \langle D_x \nu, y \rangle$$

for a unit normal ν of M and two tangent vectors x, y to M. Geometrically it measures how fast the submanifold bends with respect to the surrounding space or how quickly the normal vectors change as seen by the submanifold. The **mean curvature** H is the trace of II with respect to g:

$$H = g^{ij} II_{ij} \, .$$

The Willmore Functional

The Willmore Functional is a widely accepted simple model for a suitable bending energy:

$$\mathscr{W}(M) = \int_M H^2 \, d\mathscr{H}^{n-1} \, .$$

So we are looking for minimizers of $\mathscr{W}$ in the class of connected orientable compact C^2-manifolds embedded into Ω with Hausdorff volume $\mathscr{H}^{n-1}(M) \equiv S$. **Big question:** Do these exist?!?

n=2

We have to enlarge the class by a bit. The class defined before are just C^2-closed curves parametrized by arclength:

$$M \equiv \gamma : [0, S] \to \mathbb{R}^2, \qquad \mathscr{W}(M) = \int_0^S |\ddot{\gamma}(t)|^2 \, dt \, .$$

Clearly, we find a minimizer in $W^{2,2}(S^1_S)$, so by Sobolev embeddings in $C^1(S^1_S)$ by the direct method of the calculus of variations: Take a minimizing sequence and show that it

1. is bounded, hence has a weakly convergent subsequence and
2. that the functional is lower semi-continuous with respect to weak convergence.

So far, there is no regularity theory for this constrained minimization. Note that if the length of the curves is not sufficiently large with respect to Ω, they will always just converge to a circle.

n=3. Varifolds

A few problems in three dimensions:

1. The only compact 1-manifold is the circle. In two dimension, there is a countable set of admissible surfaces.
2. Even when restricting to one topological type, due to (Gaussian) curvature, there is no analogue of the arclength parametrization. (Like there is no isometric atlas of the earth...)
3. Even if there were, the Sobolev embeddings get significantly weaker in this dimension.

$\Rightarrow$ We need a different approach over the generalized surfaces of geometric measure theory, so called varifolds. Here we basically take measure theoretic $W^{1,1}$-limits of smooth manifolds.

Remark

At this point, generalized surfaces (Varifolds and Currents) enter the stage. They are sort of like Lipschitz surfaces that admit singularities. It is the analogue of looking at abstract submanifolds and moving away from a particular parametrization, just in a measure theoretic setting. I am thinking about giving a presentation about this at some point. For example, the C^1-limit curve of a minimizing sequence might have points where it tangentially touches itself (just immersed, not embedded). This is not problematic due to our relying on the parametrization, but it poses major problems in higher dimensions.

First Field of Problems. Sharp Interface Limit

We look at a sequence of sets $E_k \subset\subset \Omega$ such that $\mathscr{W}(\partial E_k) \to \inf \mathscr{W}(M)$ where M is admissible. We can show the existence of a limit set E of E_k and a varifold limit L of ∂E_k such that $\partial E \subset L$ and $\mathscr{W}(L) \leq \liminf_{k\to\infty} \mathscr{W}(\partial E_k)$. Questions:

1. Is it true that the multiplicity of L is odd if and only if we are on the boundary ∂E? Explanation: The curve can touch itself tangentially again. When it touches itself an even number of times, the different orientations delete each other in a sense - but to avoid a loss of mass in the limit, we count it multiple number of times in the varifold setting in $n = 3$.
2. For all L that can be obtained this way, can we always find a sequence E_k such that $\mathscr{W}(\partial E_k) \to \mathscr{W}(L)$? (Where mean curvature is extended to varifolds through the variation of the area functional)

Towards Computation

In our proofs, we look at sequences $E_k, \partial E_k$ and their characteristic functions $\chi_{E_k} \in BV(\Omega)$ (functions with vector valued measures as derivatives which can live on sets of Hausdorff dimension s with $n-1 \leq s \leq n$). Two problems occur:

1. A conceptual theoretic problem: $BV(\Omega)$ is not separable and fairly horrible to work with,
2. a practical problem: In computer programming we are restricted to working with meshes (of a fairly high resolution, but still)... It is quite hard to allow for boundaries lying in arbitrary locations and - at least with linear meshes - it is not easy to incorporate a curvature quantity of those systems.

$\Rightarrow$ regularization of the problem and an approach over diffuse interfaces.

Γ-convergence and diffuse interfaces

Instead of working with $2\chi_E - 1$ and the minimization of $\mathscr{W}(\partial E)$ under the condition $\mathscr{H}^{n-1}(\partial E) = S$ we work with $u_\epsilon \in W^{2,2}(\Omega)$ such that $u_\epsilon \to 2\chi_E - 1$ in $L^1(\Omega)$ as $\epsilon \to 0$ and $u_\epsilon = -1$ on $\partial\Omega$ (Thus E is embedded in Ω). We then think of $\{u = 0\}$ as the membrane and try to minimize a functional

$$\mathscr{E}_\epsilon(v) = \mathscr{W}_\epsilon(v) + \epsilon^{\sigma-1}(\mathscr{S}_\epsilon(v) - S)^2$$

where $\sigma \in (0, 1)$ and $\mathscr{W}_\epsilon$ is an approximation of the Willmore energy $\mathscr{W}$, $\mathscr{S}_\epsilon$ is an approximation of the area functional.

Γ-convergence and diffuse interfaces

In practice one picks

$$\mathscr{W}_\epsilon(v) = \frac{1}{c_0\epsilon}\int_\Omega \left(\epsilon\Delta v - \frac{W'(v)}{\epsilon}\right)^2\,dx$$

$$\mathscr{S}_\epsilon(v) = \frac{1}{c_0}\int_\Omega \frac{\epsilon}{2}|\nabla v|^2 + \frac{1}{\epsilon}W(v)\,dx$$

where $W(z) = (1-z^2)^2$ and $c_0 = \frac{2\sqrt{2}}{3}$.

Question: In what sense to $\mathscr{W}_\epsilon$ and $\mathscr{S}_\epsilon$ converge? And in what sense do the corresponding minmization problems converge?

The minimization of $\mathscr{S}_\epsilon$ means to have a function being almost everywhere close to ± 1 (the W term) and having as short a transit area as possible (the gradient term), so far the heuristics. We then think of $\{u = 0\}$ as the approximate interface.

Γ-convergence and diffuse interfaces

A sequence of functions $F_\epsilon : X \to \mathbb{R}$ on a topological space X is said to be Γ-convergent to $F : X \to \mathbb{R}$ if

1. $\liminf_{\epsilon \to 0} F_\epsilon(u_\epsilon) \leq F(u)$ whenever $u_\epsilon \to u$ and
2. there is a sequence $u_\epsilon \to u$ such that $F(u) \geq \limsup_{\epsilon \to 0} F_\epsilon(u_\epsilon)$.

Interesting Properties of Γ-convergence:

1. If $F_\epsilon(u_\epsilon) \leq \inf F_\epsilon + \epsilon$ and $u_\epsilon \to u$, then $F(u) = \inf F$.
2. Γ-limits are always lower semi-continuous.
3. $\Gamma - \lim_{\epsilon \to 0} F = \overline{F}$.
4. Pointwise limits and Γ-limits can disagree.
5. $-(\Gamma - \lim F_\epsilon) \neq \Gamma - \lim(-F_\epsilon)$, i.e. Γ-limits do not necessarily behave linearly.

Remark

This obviously causes problems... $\mathscr{W}_\epsilon$ is Γ-convergent to $\mathscr{W}$ and $\mathscr{S}_\epsilon$ is Γ-convergent to the $n-1$-dimensional Hausdorff measure of the discontinuity set, but what does that mean for $\mathscr{E}_\epsilon = \mathscr{W}_\epsilon + (S_\epsilon - S)^2$? This is problematic due to the non-linearity of Γ-convergence... Also the gradient flow approach is helpful for finding local minimizers only, while Γ-convergence only works for global minimizers - and the gradient flow seemed to be the most reasonable approach to finding minimizers, since it actually helps preserve a starting topology.

On the other hand, it seems to work pretty well. Also, in this model it would be relatively easy to incorporate volume forces (e.g. the tendency of the interior of the membrane to keep to a certain volume etc.)

And to be fair, membranes do have volume, so probably the sharp interface model should even be approximated by a Γ-limit in a philosophical sense.

Practical Implementation

We hand our program a starting interface, e.g. (a slightly smoothed version of)

$$u = \begin{cases} 1 & r < 4.5 \cdot sin(8\phi) + 5 \\ -1 & \text{else} \end{cases}$$

and let it relaxate under the influence of a gradient flow.
Heuristically, if we vary u then an energy

$$\mathscr{E}(u) = \int_\Omega f(x, u, Du, \Delta u)\, dx$$

evolves by $\delta \mathscr{E}_u(\dot{u})$ i.e.

$$\begin{aligned} \frac{d}{dt}\bigg|_{t=0} \mathscr{E}(u + t\phi) &= \int_\Omega f_u \phi + f_{D_i u} D_i \phi + f_{\Delta u} \Delta \phi\, dx \\ &= \int_\Omega (f_u - \mathrm{div}(f_{D_i} u) + \Delta f_{\Delta u})\, \phi\, dx \end{aligned}$$

Practical Implementation

This means that the steepest descent is in direction

$$\phi = -(f_u - \mathrm{div}(f_{D_i u}) + \Delta f_{\Delta u})$$

so we would want to solve the PDE

$$u_t(x,t) = -(f_u - \mathrm{div}(f_{D_i u}) + \Delta f_{\Delta u}) \,.$$

In our case, we get

$$\begin{aligned} u_t(x,t) = -\frac{1}{c_0} \Bigg(& \frac{2\,W'(u)\,W''(u)}{\epsilon^3} - \frac{2\,W''(u)\Delta u}{\epsilon} + 2\epsilon\,\Delta\Delta u \\ & - \frac{2\,W''(u)\,\Delta u + W'''(u)\,|\nabla u|^2}{\epsilon} \Bigg) \\ & - \frac{2}{c_0\,\epsilon^{1-\sigma}} \left(\int_\Omega \frac{\epsilon}{2} |\nabla u|^2 + \frac{W(u)}{\epsilon}\,dx - S \right) \left\{ \frac{W'(u)}{\epsilon} - \epsilon \Delta u \right\} \end{aligned}$$

Second Field of Problems. Implementation

Written out like this, it is probably the most horrible PDE I have ever seen :-) Fourth order non-linear and including a global term of u via the integral... Still, it is quasi-linear so we can solve it with a Galerkin Space Finite Elements Scheme :-)

1. Implementation of a Topological Energy Term which will allow for topological transitions (e.g. sphere to torus) but prevent splitting into multiple connected components.
2. Parallelization of the Computations.
3. Finding a better Γ-approximation of the connectedness condition and/or Γ-approximations in other problems (e.g. minimizing magnetic fields with known topology).

What I actually do

To be honest - at the moment, mostly read and think about stuff. The approximation of S_ϵ and $\mathscr{W}_\epsilon$ is relatively well known (although the rigorous proof for $\mathscr{W}_\epsilon$ is fairly recent). A major focus of my supervisor's research is the phase field implementation of topological conditions. The computer implementation is to a large degree his, and I am now involved in the adjustments and improvement of it. There are also many open questions about the sharp interface that we wish to address, as well as the issue of convergence of the gradient flow of $\mathscr{E}_\epsilon$ to that of $\mathscr{W}$ under an area condition.