Anisotropic curvature flow as singular limit of the bidomain model

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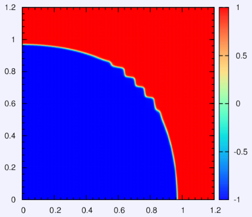
numerical simulations by **Franco Pasquarelli**, based on code by **Meggie Bugatti**, Università Cattolica di Brescia

Outline of the talk

- The Allen-Cahn equation
- Anisotropy and anisotropic Allen-Cahn
- The **bidomain** system
- Historical remarks
- Combined anisotropy and nonconvexity
- Numerical simulations in 2D

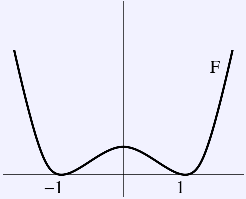


Allen-Cahn equation: brief review

Reaction/diffusion equation arising in the context of **phase transitions** with a diffused interface:

$$\begin{cases} \varepsilon \partial_t u - \varepsilon \Delta u + \frac{1}{\varepsilon} f(u) = 0 & \text{in } \Omega \\ + \text{ initial and boundary conditions} \end{cases}$$

- u: order parameter (phase indicator),
- Ω: domain in $\mathbb{R}^d$, $d = 2, 3$,
- $\varepsilon > 0$: small relaxation parameter,
- $f = F'$: derivative of a double equal well potential F (or double-obstacle: deep quench limit [Elliott et al]).



The solution u exhibits a thin transition layer $\mathcal{O}(\varepsilon)$-wide between the phase $u \approx -1$ and the phase $u \approx +1$.

Gradient flow of $\frac{\varepsilon}{2} \int_\Omega |\nabla u|^2 dx + \frac{1}{\varepsilon} \int_\Omega F(u) dx$.

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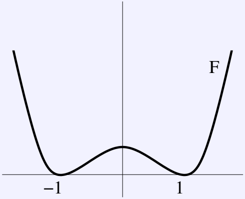

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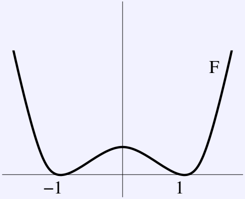

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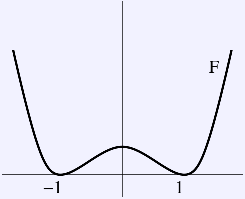

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Singular limit $\varepsilon \to 0$

The transition layer approximates a sharp interface that moves by mean curvature:

$$\boxed{V = -\kappa}$$

[X. Chen, Bronsard-Kohn, Evans-Soner-Souganidis,]
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Optimal $\mathcal{O}(\varepsilon^2)$ or quasi-optimal $\mathcal{O}(\varepsilon^2 |\log \varepsilon|)$ error estimate.
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Anisotropy

Described by a norm $\varphi : \mathbb{R}^d \to \mathbb{R}$:

- $\varphi(\xi) \geq 0 \quad \forall \xi \in \mathbb{R}^d$; $\varphi(\xi) = 0 \iff \xi = 0$;
- $\varphi(t\xi) = t\varphi(\xi) \quad \forall t \geq 0$;
- $\varphi(\xi + \eta) \leq \varphi(\xi) + \varphi(\eta)$.

Dual norm: $\varphi^o(\xi^\star) = \max_{\varphi(\xi)\leq 1} \xi \cdot \xi^\star$.

Duality map (nonlinear, monotone, homogeneous of degree one):

$$\boxed{T(\xi) = \frac{1}{2}\nabla_\xi \left[\varphi^o(\xi)\right]^2}$$

[Wheeler-McFadden, Bellettini-P.]

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Anisotropy (2)

Wulff shape: $W_\varphi = \{\varphi(\xi) \leq 1\}$;
Frank diagram: $F_\varphi = \{\varphi^o(\xi) \leq 1\}$;

$$T : F_\varphi \to W_\varphi$$

Linear anisotropy

$$[\varphi^o(\xi)]^2 = \xi^T A \xi, \qquad A \text{ symmetric positive definite.}$$

So that $[\varphi(\xi)]^2 = \xi^T A^{-1} \xi$ and $T(\xi) = A\xi$.

Strictly convex anisotropy

Both φ and φ^o strictly convex.

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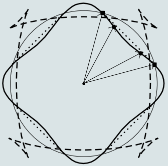
Nonconvex anisotropy

F_φ is not convex: illposedness



[Fierro-Goglione-P.,...]

Anisotropic Allen-Cahn

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Geometric evolution $V \cdot \nu_\varphi = -\kappa_\varphi$; $\kappa_\varphi = \operatorname{div} n_\varphi$;
Cahn-Hoffman vector: $n_\varphi = T(\nu_\varphi)$; $\nu_\varphi = \frac{\nu}{\varphi^o(\nu)}$

[Elliott-Schätzle-P, Bellettini-Colli Franzone-P.]
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The bidomain system

The bidomain model is a singularly perturbed degenerate system of two reaction–diffusion equations in the unknowns u_1 and $u_2 : \Omega \to \mathbb{R}$:

$$\begin{cases} \varepsilon\partial_t(u_1 + u_2) - \varepsilon \operatorname{div} T_1(\nabla u_1) + \frac{1}{\varepsilon} f(u_1 + u_2) = 0 \\ \varepsilon\partial_t(u_1 + u_2) - \varepsilon \operatorname{div} T_2(\nabla u_2) + \frac{1}{\varepsilon} f(u_1 + u_2) = 0 \end{cases}$$

in $\Omega \in \mathbb{R}^d$ with appropriate initial and boundary conditions. $T_{1,2}$ are the duality mappings of two strictly convex anisotropies $\varphi_{1,2}$, $f = F'$ is the derivative of the quartic double-well potential $F(s) = (s^2 - 1)^2$, $\varepsilon > 0$ is a small relaxation parameter.

It can be generalized to more components $u_1, \dots, u_m$.

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Origin: electric model for the myocardium

[Colli Franzone, ...]

- Simulation of a complete heart-beat, but specifically of the depolarization phase;
- starting from a microscopic model of the electrical properties of the (disjoint) intracellular and extracellular media Ω^i and Ω^e in the cardiac tissue
- coupled through the cellular membrane;
- with the addition of a number of "gating variables" (Hodgkin–Huxley model), simplified to a single "recovery variable" (FitzHugh–Nagumo);
- the recovery variable (which we shall neglect) allows to recover the rest state of the cell (repolarization);
- u^i, u^e: intra–cellular and extra–cellular potentials;
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- The bidomain model derives from a **homogeneization** process so that in the end $\Omega^i = \Omega^e = \Omega$ are superposed and the macroscopic potentials u^i and u^e are defined in the same domain.

$$\begin{cases} \partial_t u - \varepsilon \operatorname{div} M^i \nabla u^i + \frac{1}{\varepsilon} f(u) = 0 \\ \partial_t u + \varepsilon \operatorname{div} M^e \nabla u^e + \frac{1}{\varepsilon} f(u) = 0 \end{cases}$$

$$u_1 = u^i; \qquad u_2 = -u^e$$

$$T_{1,2}(\xi) = M^{i,e}\xi$$

- Cells form elongated fibers with orientation that depends strongly on position, and this geometry is the source of the anisotropy;
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Remarks on the bidomain model:

1. the two local minima of F are different;
2. rescaled time: $\partial_t u$ instead of $\varepsilon \partial_t (u_1 + u_2)$;
3. presence of a (pointwise) recovery variable;
4. space dependant anisotropy $M^{i,e} = M^{i,e}(x)$ (Finsler metric).

- Complex 3D geometry
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The anisotropy in the bidomain model

Recall:

$$\begin{cases} \partial_t(u^i - u^e) - \varepsilon \,\mathrm{div}\, M^i \nabla u^i + \frac{1}{\varepsilon} f(u^i - u^e) = 0 \\ \partial_t(u^i - u^e) + \varepsilon \,\mathrm{div}\, M^e \nabla u^e + \frac{1}{\varepsilon} f(u^i - u^e) = 0 \end{cases}$$

Matrices M^i and M^e (in general depending on position) are symmetric positive definite with common eigenvectors consistent with fiber orientation. The eigenvalues λ_k^i, λ_k^e, $k = 1, 2, 3$ come from the homogeneization procedure of the microscopic geometry and depend on properties of the intra and extra–cellular media.

Special case $M^e = \rho M^i$ (equal anisotropic ratio) the system reduces to a single reaction–diffusion Allen-Cahn equation for $u = u^i - u^e$

However **equal anisotropic ratio** is not physiologically feasible.

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Bidomain system: elliptic/parabolic formulation

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Remark

We can substitute one of the two parabolic equations with the elliptic combination

$$\operatorname{div} T_1(\nabla u_1) = \operatorname{div} T_2(\nabla u_2) \qquad \text{in } \Omega.$$

The bidomain model is a degenerate parabolic system.

Vectorial formulation and Wellposedness

$$\mathbf{u} = [u_1, u_2]^T, \quad \mathbf{q} = [T_1(\nabla u_1), T_2(\nabla u_2)]^T$$

$$\boxed{\varepsilon \partial_t (B\mathbf{u}) - \varepsilon \operatorname{div} \mathbf{q} + \frac{1}{\varepsilon}\mathbf{f}(\mathbf{u}) = 0}$$

where

- $B = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ (singular!);
- div acts componentwise
- $\mathbf{f}(\mathbf{u}) = [f(u_1 + u_2), f(u_1 + u_2)]^T$

Although matrix B is singular the problem is well-posed, at least for linear anisotropies $T_i(\xi) = A_i \xi$ and any choice of two symmetric positive–definite matrices A_1, A_2.

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The combined anisotropy

For convenience we introduce $\alpha_i(\xi) = [\varphi_i^o(\xi)]^2, \;\; i = 1, 2$.
(For the bidomain model they are $\alpha^{i,e} = \xi^T M^{i,e} \xi$.)

The *combined* value α is their **harmonic mean**:

$$\alpha = \frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2}$$

The **combined anisotropy** is defined as

$$\varphi^o(\xi) = \sqrt{\alpha} = \sqrt{\frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2}}$$

Remarks

1. Linear anisotropies generally produce a **nonlinear** combined anisotropy;
2. Strictly convex anisotropies (even linear) can produce a **nonconvex** combined anisotropy (using φ^o is an abuse of notation in this case).

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The singular limit $\varepsilon \to 0$

Formal matched asymptotics suggest that (for a **convex** combined anisotropy) the sum $u_1 + u_2$ (the transmembrane potential) develops a thin $\mathcal{O}(\varepsilon)$–wide transition region that moves by φ-anisotropic mean curvature flow with velocity

$$\boxed{V \cdot \nu_\varphi = -\kappa_\varphi + \mathcal{O}(\varepsilon)}$$

where φ denotes the (dual of the) combined anisotropy.

Anisotropic mean curvature flow

φ^o is not guaranteed to be convex. If it is, then it is a norm and we have anisotropic curvature flow.

Asymptotic Allen-Cahn approximation

The bidomain system behaves (formally) like the anisotropic Allen-Cahn equation (with this particular choice of the anisotropy) as $\epsilon \to 0$.

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Convergence results

Very few...

1. Formal matched asymptotics up to second order shows that an optimal error $\mathcal{O}(\varepsilon)$ between the zero-level of $u_1 + u_2$ and anisotropic mean curvature flow should be expected.
   [Bellettini-Colli Franzone-P.]
2. Γ-convergence result for the stationary bidomain system, consistent with the formal asymptotics, but without a complete identification of the Γ-limit.
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Gamma-limit of the stationary problem

[L. Ambrosio, P. Colli Franzone, G. Savaré ('00)]

In the linear case (α_i are quadratic forms), the functional

$$\mathcal{F}_\varepsilon(\mathbf{u}) = \varepsilon \int_\Omega [\alpha_1(\nabla u_1) + \alpha_2(\nabla u_2)]\, dx + \frac{1}{\varepsilon} \int_\Omega F(u_1 + u_2)\ dx$$

where $\mathbf{u} = [u_1, u_2]^T$, Γ-converges (in the L^2 topology) to a limit functional

$$\mathcal{F}(\mathbf{u}) = \int_{S_u^*} \phi(\nu(x))\ d\mathcal{H}^{d-1}(x)$$

that depends only in the sum $u = u_1 + u_2$ which is a BV function taking values in $\{-1, 1\}$ with S_u^* as its jump set and $\nu(x)$ the corresponding unit normal.

Identification of ϕ

Although the formal asymptotics suggests that

$$\phi(\xi) = c_0 \varphi^o(\xi) = c_0 \sqrt{\frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2}}$$

with c_0 depending on the specific shape of F, the actual value on ϕ is not known yet. [Ambrosio et al] proved the following estimates

$$\underline{\phi}(\xi) \leq \phi(\xi) \leq c_0 \varphi^o(\xi)$$

with (setting $\alpha_i(\xi) = \xi^T A_i \xi$, A_i symmetric positive definite)

$$\underline{\phi}(\xi) = \sqrt{\xi^T A_1 (A_1 + A_2)^{-1} A_2 \xi}$$

We make a linear choice for the anisotropy:

$$[\varphi_i^o(\xi)]^2 = \xi^T A_i \xi, \quad T_i(\xi) = A_i \xi, \qquad i = 1, 2.$$

For $\rho \geq 1$ we choose diagonal matrices A_1, A_2 as (inverted anisotropic ratio):

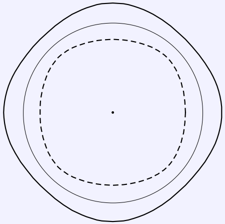
$$A_1 = \begin{bmatrix} 1 & 0 \\ 0 & \rho \end{bmatrix}, \qquad A_2 := \begin{bmatrix} \rho & 0 \\ 0 & 1 \end{bmatrix}.$$

This choice is not physiologically feasible for the bidomain model of the heart tissue, however it leads to a nonconvex combined anisotropy if $\rho > 3$.
Might correspond to a pathological situation.

Weak inverted ratio

$\rho = 2$ (convex anisotropy)

Solid line: Frank diagram $\{\varphi^o(\xi) = 1\}$.
Dashed line: Wulff shape (dual shape).



Numerical simulations. Two choices for ρ

Weak inverted ratio

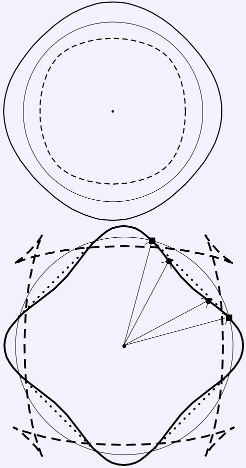
$\rho = 2$ (convex anisotropy)

Solid line: Frank diagram $\{\varphi^o(\xi) = 1\}$.
Dashed line: Wulff shape (dual shape).

Strong inverted ratio

$\rho = 5$ (nonconvex anisotropy)

Convexification of Frank diagram corresponds to cutting off the swallowtails in the Wulff shape.



Numerical simulations

In all simulations we chose a square domain $\Omega = (0, 1.2) \times (0, 1.2)$.
The initial condition is such that $u_1 + u_2 = \tanh \frac{\tilde{\varphi}(x)}{\epsilon}$ for some appropriate choice of a norm $\tilde{\varphi}$.
The relaxation parameter ϵ related to space discretization h through $h = C\epsilon$ (C small enough to resolve the transition layer).
Reflection conditions along the axes and Dirichet condition on the other two sides.
Matrices A_1, A_2 are fixed according to the choice of weak or strong inverted ratio.

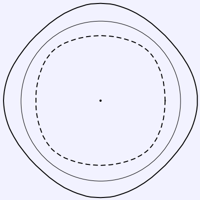
Discretization

- We use P_1 finite elements in space.
- The first parabolic equations is discretized with explicit Euler in time to get the sum $u_1^{(n+1)} + u_2^{(n+1)}$ at the next time step.
- Then we recover $u_1^{(n+1)}$ and $u_2^{(n+1)}$ by solving an elliptic problem with a preconditioned conjugate gradient.

Weak inverted anisotropic ratio

By chosing $\rho = 2$ we obtain a convex combined anisotropy.

Solid line: Frank diagram
Dashed line: Wulff shape



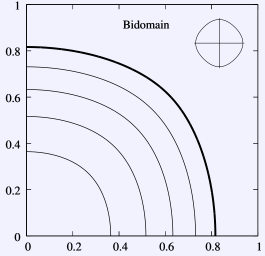
Evolving the Wulff shape

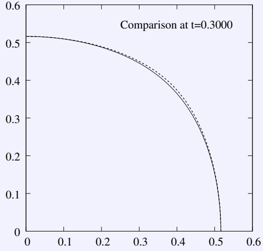
The Wulff shape evolves selfsimilarly by anisotropic mean curvature

In all pictures we plot the zero-level curve of $u_1 + u_2$ at different time steps.

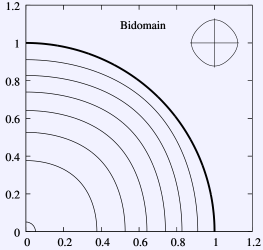
Simulations with $\rho = 2$

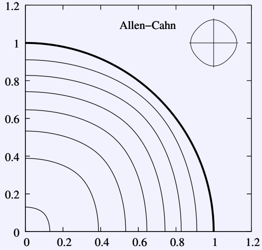
Starting from the Wulff shape, $\varepsilon = 0.04$, $h = 0.005$, time intervals of 0.1:

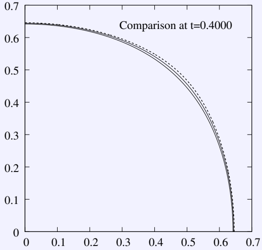




Starting from the unit circle, $\varepsilon = 0.08$, $h = 0.01$, bidomain vs Allen-Cahn:



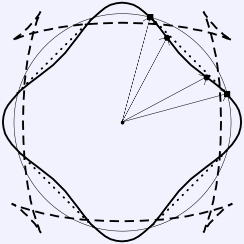




Strong inverted anisotropic ratio

By chosing $\rho = 5$ we obtain a nonconvex combined anisotropy.

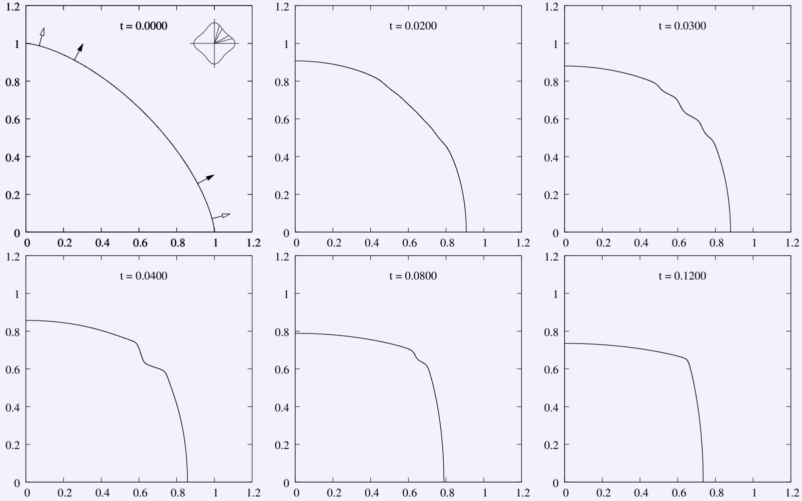
Solid line: Frank diagram
Dashed line: Wulff shape



Interest in the evolution of those portions of the evolving front where the normal points in the nonconvex parts of the Frank diagram.

Simulation with $\rho = 5$

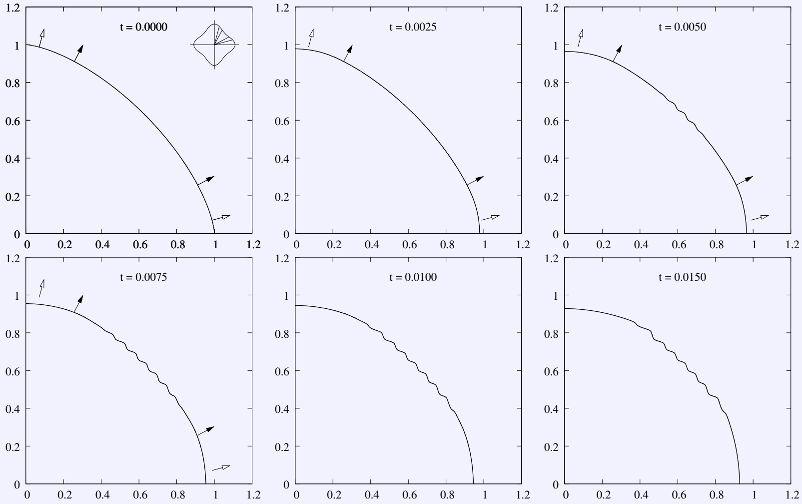
Starting from $p = 1.5$ unit ball, $\varepsilon = 0.008$, $h = 0.002$:



[see animation.avi]

Simulation with $\rho = 5$ $\varepsilon = 0.004$

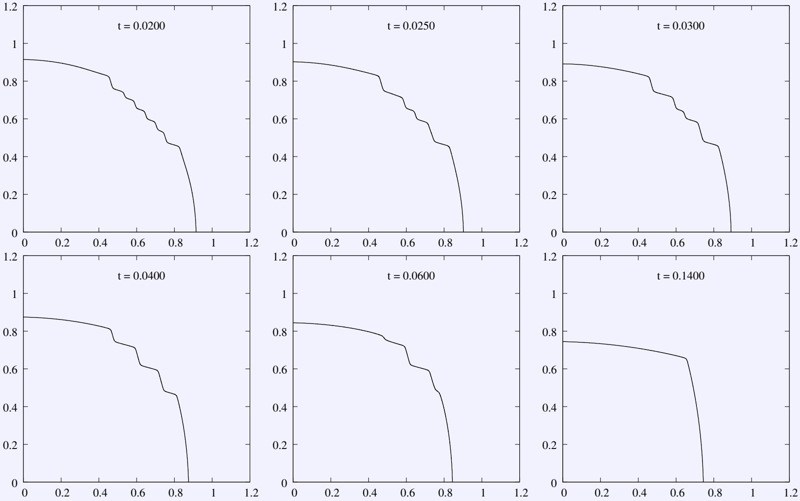
$\varepsilon = 0.004$, $h = 0.002$:



[see animation2.avi]

Simulation with $\rho = 5$ $\varepsilon = 0.004$ (2)

Subsequent times...



[see animation2.avi]

The wrinkling phenomenon and conclusions

- What we observe numerically (formation of wrinkles) is somewhat typical of an illposed evolution problem formally arising as gradient flow for an energy that is not convex when relaxed with the addition of a small higher order perturbation, or due to the discretization.
- The question is whether or not there is a “natural” way to describe the evolution in the singular limit $\varepsilon \to 0$ (or $h \to 0$).
- Surprisingly it seems that in most cases the limit **is not** the gradient flow by the **convexified energy**.
- This is not easily seen for the bidomain system due to the large wrinkles that arise even for quite small values of ε.