Curvature flow with nonconvex anisotropy and the bidomain model

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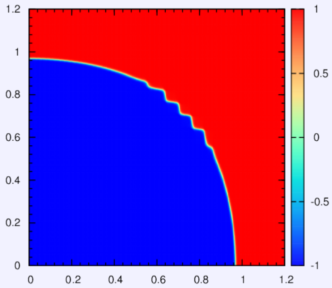
numerical simulations by **Franco Pasquarelli**, based on code by **Meggie Bugatti**, Università Cattolica di Brescia

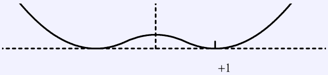
Outline of the talk

- Gradient flow for nonconvex energy (motivation: the graph case)
- Anisotropic mean curvature flow, the nonconvex case
- Allen-Cahn approximation
- **The bidomain model for the cardiac tissue**
- Matched asymptotics and Γ-convergence
- Numerical simulations in 2D



Gradient flows of nonconvex energies

L^2-gradient flow for $\int_\Omega \Psi(u')\,dx$ leads to a forward/backward parabolic problem which we want to "solve" by means of a relaxation technique.



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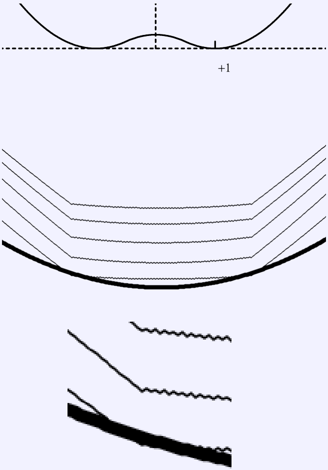
Different approximations can lead in the limit to different notions of "relaxed" solutions. Here e.g. is the result of a numerical relaxation with a finite difference scheme in space, note the formation of wrinkles.
This is $\boxed{\text{not}}$ the evolution by the convexified energy!



[Fierro, Goglione, P. ('98)]

(Nonconvex) anisotropic mean curvature flow

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$$\boxed{V = -\varphi^o(\nu)\kappa_\varphi}$$

where V is the normal velocity and

$$\kappa_\varphi = \mathrm{div}_\Sigma\, n_\varphi, \qquad n_\varphi = T^o(\nu_\varphi), \qquad \nu_\varphi = \frac{\nu}{\varphi^o(\nu)}$$

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Gradient flow for $\int_\Sigma \varphi^o(\nu)\ d\mathcal{H}^{d-1}$.

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Nonconvexity

The evolution law becomes ill-posed when φ^o is nonconvex.

Allen-Cahn approximation and finite elements

Approximation by diffusing the interface:

$$\varepsilon \partial_t u - \varepsilon \,\mathrm{div}\, T^o(\nabla u) + \frac{1}{\varepsilon} f(u) = 0$$

(gradient flow of $\epsilon \int_\Omega [\varphi^o(\nabla u)]^2 \, dx + \frac{1}{\epsilon} \int_\Omega F(u) dx$.) where $\epsilon > 0$ is a small relaxation parameter, u is a "phase" indicator exhibiting a thin transition layer $\mathcal{O}(\varepsilon)$-wide; f is the derivative of a double well potential F (or double-obstacle: deep quench limit [Elliott et al]) with equal minima in ± 1.

[Bellettini, Giga, Elliott, Novaga, P., Schätzle, ...]

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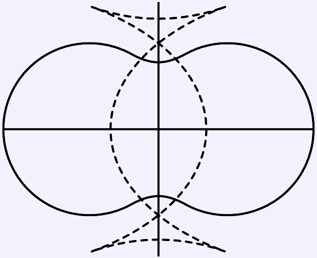
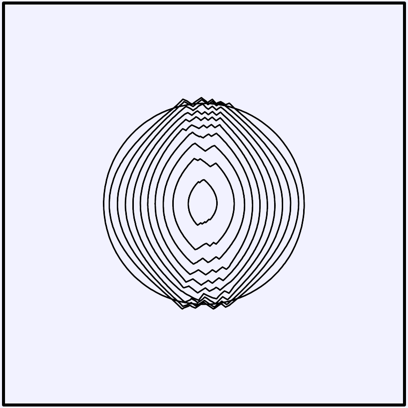
This is again ill-posed for nonconvex φ^o, however spatial discretization such as piecewise linear finite elements does not blow up and could provide a notion of relaxed solution of the limit problem.

Allen-Cahn with nonconvex anisotropy





Numerical simulation with piecewise linear finite elements for a smooth nonconvex choice of φ^o.
Dashed line is the so-called Wulff shape (with swallowtails!).

The bidomain model for the cardiac tissue

[Colli Franzone, ...]

The bidomain model is a singularly perturbed system of two reaction–diffusion equations in the unknowns u^i and $u^e : \Omega \to \mathbb{R}$:

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

in $\Omega \in \mathbb{R}^d$ with appropriate initial and boundary conditions.

- u^i, u^e: intra–cellular and extra–cellular potentials;
- M^i, M^e: symmetric positive definite matrices modelling the anisotropy induced by the cell orientations;
- $u = u^i - u^e$: transmembrane potential
- $f(\cdot) = F'(\cdot)$: cubic–like function, derivative of a *double well* potential.
- $\varepsilon > 0$: small perturbation parameter

Remarks on the bidomain model (cardiac tissue)

- It originates from a microscopic model of the electrical properties of the (disjoint) intracellular and extracellular media Ω^i and Ω^e, 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 w (which we shall neglect) allows to recover the rest state of the cell.

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- Cells form elongated fibers with orientation that depends strongly on position, and this geometry is the source of the anisotropy.

The anisotropy in the bidomain model

Recall:

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

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^i_k, λ^e_k, $k = 1, 2, 3$ come from the homogeneization procedure of the microscopic geometry and depend on properties of the intra and extra–cellular media.

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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.

Differences w/r to the standard bidomain model

In contrast to the actual bidomain model we assume:

- F has two equal minima $F(-1) = F(1) = 0$;
- rescaled time ($\epsilon\partial_t u$ instead of $\partial_t u$);
- no recovery variable;
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Remark

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

$$\operatorname{div}(M^i \nabla u^i + M^e \nabla u^e) = 0 \qquad \text{in } \Omega.$$

The bidomain model is a degenerate parabolic system.

Vectorial formulation and Wellposedness

[P. Colli Franzone, G. Savaré ('96)]

$$\mathbf{u} = [u^i, u^e]^T, \quad \mathbf{q} = [M^i \nabla u^i, -M^e \nabla u^e]^T$$

$$\boxed{\varepsilon \partial_t (B\mathbf{u}) - \varepsilon \,\mathrm{div}\, \mathbf{q} + \frac{1}{\varepsilon} \mathcal{F}(\mathbf{u}) = 0}$$

where

- $B = \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}$;
- div acts componentwise
- $\mathcal{F}([u^i, u^e]^T) = [f(u^i - u^e), f(u^i - u^e)]^T$

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Although matrix B is singular the problem is well-posed for any choice of the two symmetric positive–definite matrices M^i, M^e.

Formal asymptotics and singular limit

[Bellettini, Colli Franzone, P. ('97)]

Matched asymptotics suggests that the transmembrane potential u develops a thin $\mathcal{O}(\varepsilon)$–wide transition region that moves with normal velocity

$$\boxed{V_\varepsilon = -\varphi^o(\nu)\kappa_\varphi + \mathcal{O}(\varepsilon)}$$

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where ν is normal to the limit interface,

$$\varphi^o(\xi) = \sqrt{\frac{\alpha^i \alpha^e}{\alpha^i + \alpha^e}}$$

with $\alpha^i = \xi^T M^i \xi$, $\alpha^e = \xi^T M^e \xi$ and

$$\kappa_\varphi = \mathrm{div}\, n_\varphi, \qquad n_\varphi = T^o(\nu_\varphi), \qquad \nu_\varphi = \frac{\nu}{\varphi^o(\nu)}$$

$$T^o(\xi) = \varphi^o(\xi)\nabla_\xi \varphi^o(\xi)$$

Formal asymptotics and singular limit (2)

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Asymptotic Allen-Cahn approximation

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

Gamma-limit of the stationary problem

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

The functional

$$\mathcal{F}_\varepsilon(\mathbf{u}) = \varepsilon \int_\Omega \left[M^i \nabla u^i \cdot \nabla u^i + M^e \nabla u^e \cdot \nabla u^e \right] dx + \frac{1}{\varepsilon} \int_\Omega F(u)\, dx$$

where $\mathbf{u} = [u^i, u^e]^T$ and $u = u^i - u^e$, 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 difference $u = u^i - u^e$ 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

$$\phi(\xi) = c_0 \varphi^o(\xi) = c_0 \sqrt{\frac{\alpha^i \alpha^e}{\alpha^i + \alpha^e}}$$

with c_0 depending on the actual 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

$$\underline{\phi}(\xi) = \sqrt{\xi^T M^i (M^i + M^e)^{-1} M^e \xi}$$

Remark

φ^o is not always convex (depending on the eigenvalues of M^i and M^e) whereas ϕ must be convex.

Inverted anisotropic ratio, $d = 2$

Suppose that the fibers are oriented in the x_1 direction, then M^i and M^e are diagonal. Let

$$\rho^i = \frac{\lambda_1^i}{\lambda_2^i}, \qquad \rho^e = \frac{\lambda_1^e}{\lambda_2^e}$$

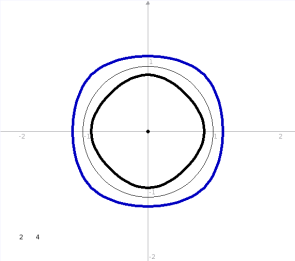
We chose $\boxed{\rho^e = 1/\rho^i}$. This is to some extent the opposite of "equal anisotropic ratio" ($\rho^i = \rho^e$). This choice is not physiologically feasible, however it leads to a noncovex combined anisotropy if $\rho^i > 3$.

Numerical simulations. Two choices for ρ

Weak inverted ratio

$\rho = 2$ (convex anisotropy):
$\lambda^i_{1,2} = 2, 4$, $\lambda^e_{1,2} = 4, 2$

Black: Frank diagram $\{\varphi^o(\xi) = 1\}$
Blue: Wulff shape (dual shape).



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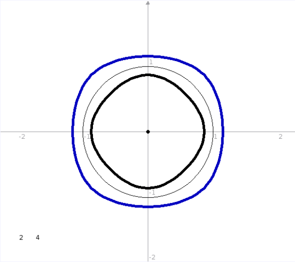
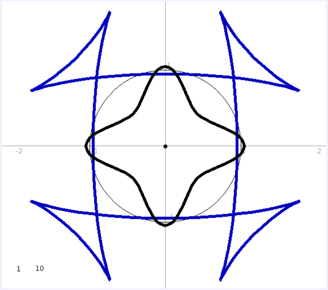


Strong inverted ratio

$\rho = 10$ (nonconvex anisotropy):
$\lambda^i_{1,2} = 1, 10$, $\lambda^e_{1,2} = 10, 1$

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 $u = \tanh \frac{|x|}{\epsilon}$ (unit circle).
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 $M^{i,e}$ are selected according to the choice of weak or strong inverted ratio.

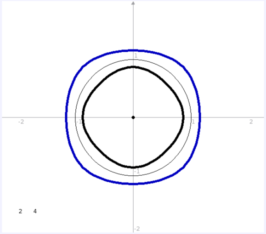
Discretization

We use P_1 finite elements in space.
One parabolic equations is discretized with explicit Euler in time to get the difference $u_{n+1} = u^i_{n+1} - u^e_{n+1}$ at the next time step.
Then we recover u^i_{n+1} and u^e_{n+1} by solving an elliptic problem with a preconditioned conjugate gradient.

Weak inverted anisotropic ratio

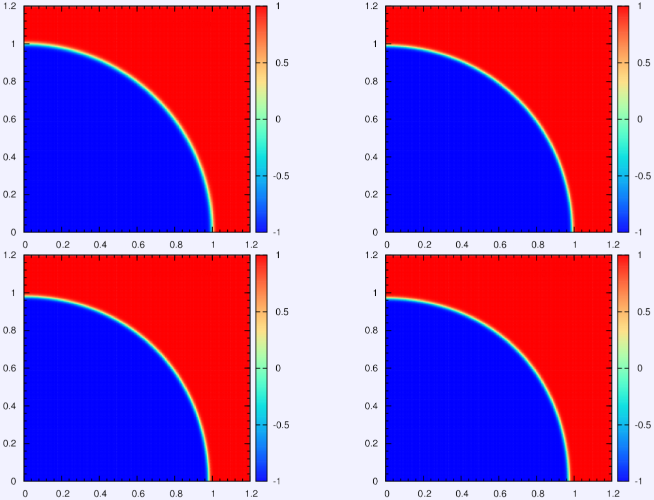
By chosing the eigenvalues $2, 4, 4, 2$ we obtain a convex combined anisotropy.

Black: Frank diagram
Blue: Wulff shape



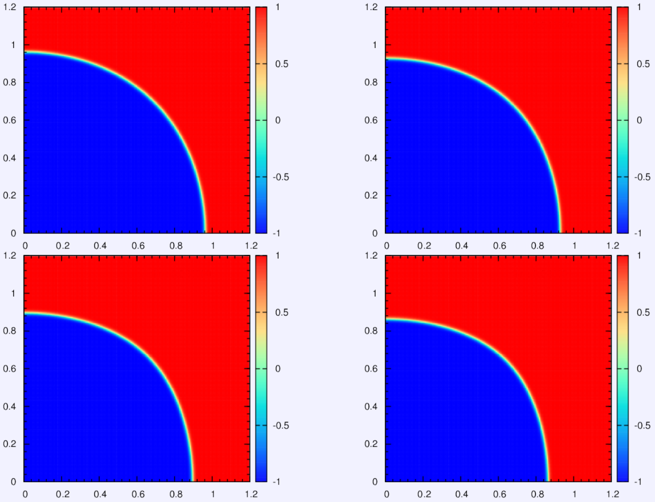
Simulation with $\rho = 2$ ($h = 0.006$)

Time increments of 0.005.



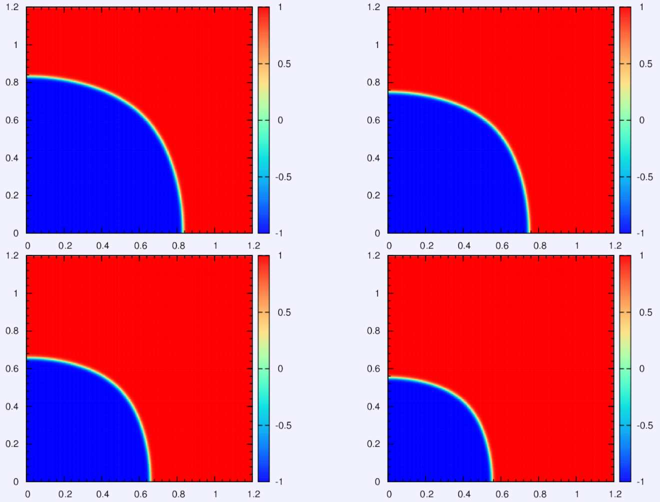
Simulation with $\rho = 2$

Times 0.02, 0.04, 0.06, 0.08.



Simulation with $\rho = 2$

Times 0.10, 0.15, 0.20, 0.25.



Strong inverted anisotropic ratio

By chosing $\rho = 10$ we obtain a nonconvex combined anisotropy.

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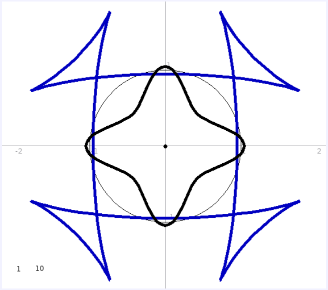
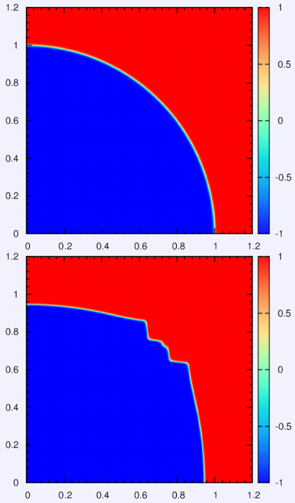
Blue: Wulff shape



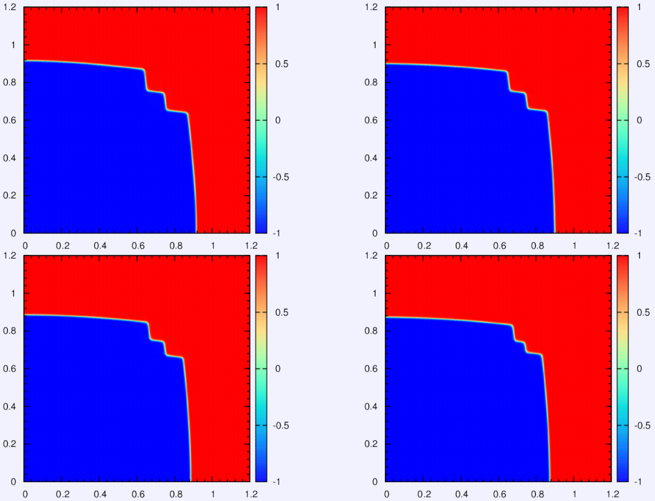
Simulation with $\rho = 10$ ($h = 0.003$)

Time increments of 0.005.



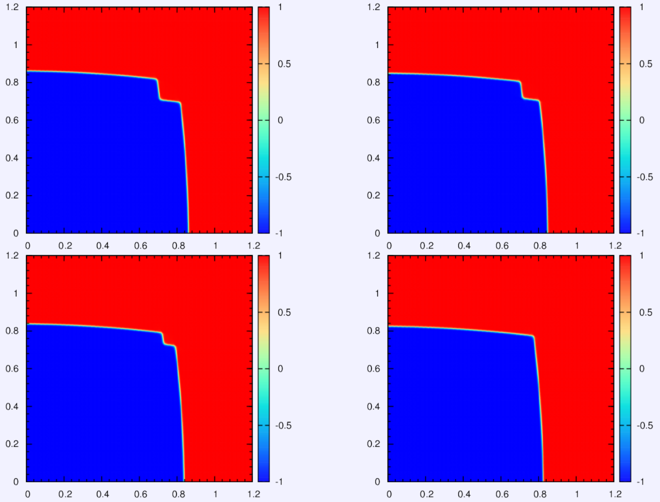
Simulation with $\rho = 10$

Times 0.02, 0.03, 0.04, 0.05.



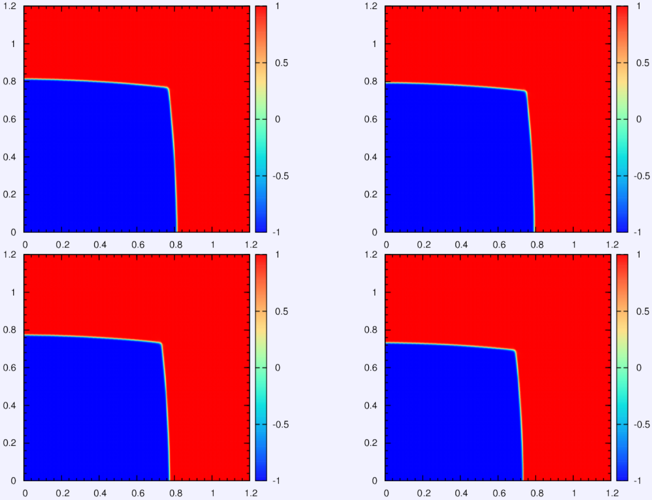
Simulation with $\rho = 10$

Times 0.06, 0.07, 0.08, 0.09.



Simulation with $\rho = 10$

Times 0.10, 0.12, 0.14, 0.18.



Future work and Open problems

- Numerical simulatations of nonconvex Allen-Cahn with the combined anisotropy (convex and nonconvex)
- Dependence on position for φ^o
- Nonequal wells: $F(-1) \neq F(1)$, and original time scaling
- Prove convergence of the bidomain model to the sharp limit as $\epsilon \to 0$, in the convex case.
- Identify the surface energy of the Γ-limit (for the stationary problem), which is conjectured to be the convex hull of φ^o
- Sensitivity to the boundary conditions

Thank you for your attention