

Curvature flow with nonconvex anisotropy relaxed with a well-posed Allen-Cahn system

Nonconvex curvature flow and the bidomain system

Maurizio Paolini

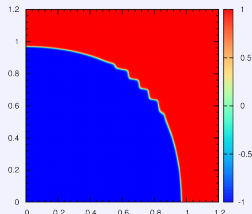
Università Cattolica di Brescia

FBP 2012, 11-15 June 2012

joint work with **Giovanni Bellettini** and **Franco Pasquarelli**

Outline of the talk

- The bidomain system
- Anisotropy
- Anisotropic mean curvature flow
- Combined anisotropy and nonconvexity
- Numerical simulations

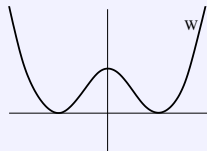


The bidomain system

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

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

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



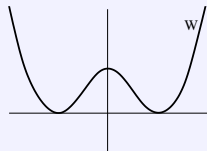
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Origin: propagation of the electric stimulus in the myocardium

The so-called **bidomain model** derives by homogeneization from a microscopic model of the cardiac tissue.

- u^i ($= u_1$): intra-cellular potential,
- u^e ($= -u_2$): extra-cellular potential,

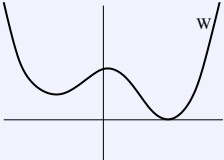
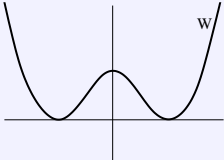
defined in two disjoint domains with different anisotropic structure and a common boundary.

After homogeneization they are defined in the common domain Ω .

Aim: Simulate a complete heart-beat, but specifically the depolarization phase.

[Hodgkin–Huxley, Fitzhugh–Nagumo,...]

Deeply numerically investigated by [Colli Franzone et al]

<p>Bidomain model (electro-cardiology): u^i, u^e</p>	<p>Our bidomain system $u_1 = u^i, u_2 = -u^e$</p>
<p>Unequal wells:</p> 	<p>Equal wells:</p> 
$\partial_t(u^i - u^e)$	$\varepsilon \partial_t(u_1 + u_2)$
<p>Linear anisotropies $M^i \nabla u^i, M^e \nabla u^e$</p>	<p>Nonlinear anisotropies $T_1(\nabla u_1), T_2(\nabla u_2)$</p>
<p>Recovery variable w</p>	

The anisotropy in the bidomain model

Original bidomain model in electro-cardiology (no recovery variable):

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

Matrices M^i and M^e (in general depending on position) are symmetric positive definite with common eigenvectors consistent with fiber orientation. The eigenvalues $\lambda_k^i, \lambda_k^e, k = 1, 2, 3$ come from the homogenization procedure of the microscopic geometry and depend mainly on the shape of the cells.

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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Formal matched asymptotics suggests that $u^i - u^e$ develops a transition region of thickness $\mathcal{O}(\varepsilon)$ moving with normal velocity

$$V = \gamma(\nu)[c_W - \varepsilon\kappa_\gamma + \mathcal{O}(\varepsilon^2)]$$

[Bellettini-Colli Franzone-P.]

where γ describes a suitable **combined** anisotropy,

κ_γ is the corresponding anisotropic curvature,

c_W depends on the potential W and $c_W = 0$ in case of equal wells.

Described by a (possibly nonsymmetric) norm $\gamma : \mathbb{R}^d \rightarrow \mathbb{R}$:

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

Dual norm: $\varphi(\xi^*) = \gamma^\circ(\xi^*) = \max_{\gamma(\xi) \leq 1} \xi \cdot \xi^*$

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

$$T(\xi^*) = \frac{1}{2} \nabla_{\xi^*} [\gamma(\xi^*)]^2$$

[Wheeler-McFadden, Bellettini-P.]

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Anisotropy (2)

Wulff shape: $W_\gamma = \{\varphi(\xi) \leq 1\}$

Frank diagram: $F_\gamma = \{\gamma(\xi) \leq 1\}$

$$T : F_\gamma \rightarrow W_\gamma$$

Linear anisotropy

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

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

Smooth anisotropy

Both W_γ and F_γ have smooth boundary (hence φ and γ strictly convex).

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Strictly convex anisotropy

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Anisotropy (3)

Cristalline anisotropy

W_γ is a convex polygon/polyhedron (and so is F_γ .)

T is multivalued maximal monotone.

[Taylor, Giga, Rybka, Bellettini-Novaga-P.,....]

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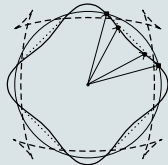
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[Taylor, Giga, Rybka, Bellettini-Novaga-P.,....]

Nonconvex anisotropy

F_γ is not convex: illposedness of a.m.c.f.



γ is **not** a norm

[Fierro-Gogliione-P.,....]

Anisotropic mean curvature flow

- $\nu_\gamma = \frac{\nu}{\gamma(\nu)}$
- Cahn-Hoffman vector: $n_\gamma = T(\nu_\gamma)$
- Anisotropic mean curvature: $\kappa_\gamma = \operatorname{div} n_\gamma$

Allen-Cahn equation

$$V_\gamma = \mathbf{V} \cdot \nu_\gamma = -\kappa_\gamma \quad \iff \quad V_\nu = -\gamma(\nu)\kappa_\gamma$$

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$$\begin{cases} \varepsilon \partial_t u - \varepsilon \operatorname{div} [T](\nabla u) + \frac{1}{\varepsilon} f(u) = 0 & \text{in } \Omega \times (0, T) \\ + \text{initial and boundary conditions} \end{cases}$$

Singular limit $\varepsilon \rightarrow 0$: anisotropic m.c.f. $V_\gamma = -\kappa_\gamma$

[Elliott-Schätzle-P., Bellettini-P.]

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The bidomain system: combined anisotropy

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where $T_{1,2}(\xi) = \frac{1}{2} \nabla_{\xi} [\gamma_{1,2}(\xi)]^2$

The *combined anisotropy* γ is defined by

$$\gamma^{-2} = \gamma_1^{-2} + \gamma_2^{-2}$$

Remarks

- 1 Linear anisotropies generally produce a **nonlinear** combined anisotropy;
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The singular limit $\varepsilon \rightarrow 0$

Formal matched asymptotics suggests that the sum $u_1 + u_2$ develops a thin $\mathcal{O}(\varepsilon)$ -wide transition region that moves approximately by γ -anisotropic mean curvature flow:

$$V_\gamma = -\kappa_\gamma + \mathcal{O}(\varepsilon)$$

A γ is not guaranteed to be convex. If it is, then it is a norm and we have anisotropic curvature flow.

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Asymptotic Allen-Cahn approximation

The bidomain system behaves (formally) like the anisotropic Allen-Cahn equation (with the combined anisotropy) as $\varepsilon \rightarrow 0$.

Some known results

- 1 Wellposedness of the bidomain model by [Colli Franzone-Savaré] in case of linear anisotropies
- 2 Formal matched asymptotics up to second order shows that we should expect an optimal error $\mathcal{O}(\varepsilon)$ between the zero-level of $u_1 + u_2$ and anisotropic mean curvature flow
[Bellettini-Colli Franzone-P.]
- 3 Γ -convergence result for the stationary bidomain system, consistent with the formal asymptotics, but without a complete identification of the Γ -limit
[Ambrosio-Colli Franzone-Savaré]
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Inverted anisotropic ratio, $d = 2$

We make a linear choice for the anisotropies

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

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

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

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.

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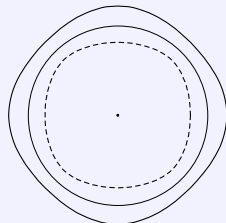
Numerical simulations. Two choices for ρ

Weak inverted ratio

$\rho = 2$ (convex combined anisotropy)

Solid line: Frank diagram $\{\gamma(\xi) = 1\}$.

Dashed line: Wulff shape (dual shape).

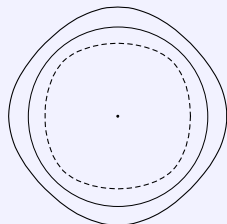


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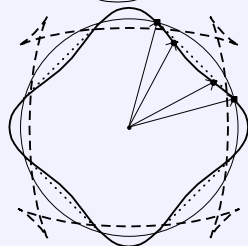
Solid line: Frank diagram $\{\gamma(\xi) = 1\}$.
Dashed line: Wulff shape (dual shape).



Strong inverted ratio

$\rho = 5$ (nonconvex combined 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.

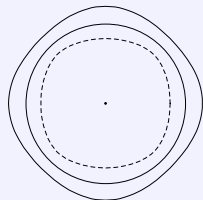
- We use P_1 finite elements in space.
- The first parabolic equations is discretized with explicit Euler in time to get the sum $u_1^{(n+1)} + u_2^{(n+1)}$ at the next time step.
- Then we recover $u_1^{(n+1)}$ and $u_2^{(n+1)}$ by solving an elliptic problem with a preconditioned conjugate gradient.

Weak inverted anisotropic ratio

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

Solid line: Frank diagram

Dashed line: Wulff shape



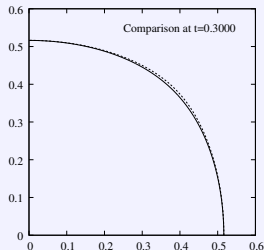
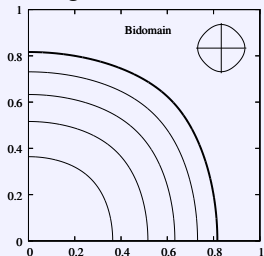
Evolving the Wulff shape

The Wulff shape evolves selfsimilarly by anisotropic mean curvature

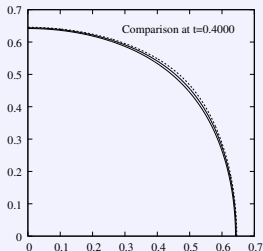
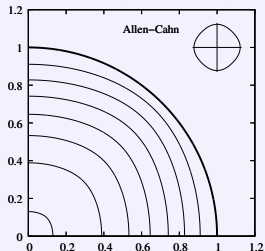
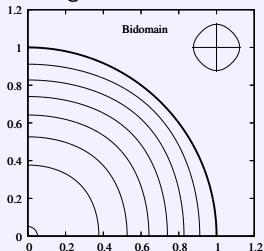
In all pictures we plot the zero-level curve of $u_1 + u_2$ at different time steps.

Simulations with $\rho = 2$

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



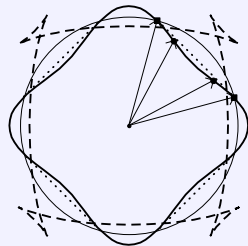
Starting from the unit circle, $\varepsilon = 0.08$, $h = 0.01$, bidomain vs Allen-Cahn:



Strong inverted anisotropic ratio

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

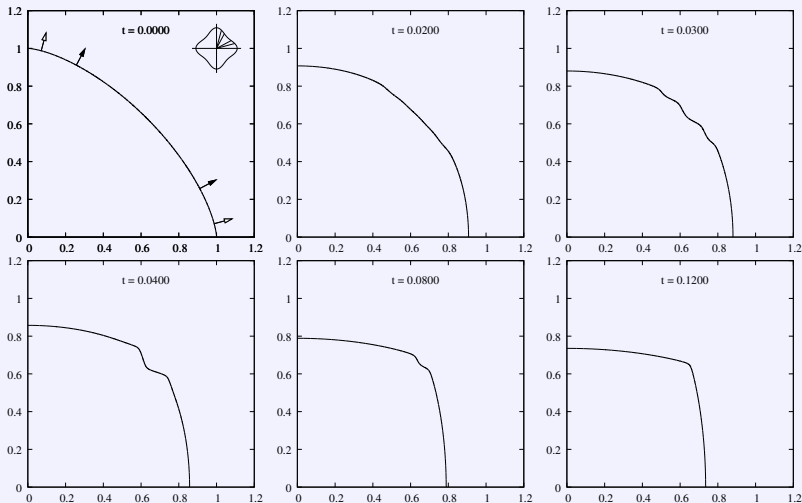
Solid line: Frank diagram
Dashed line: Wulff shape



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

Simulation with $\rho = 5$

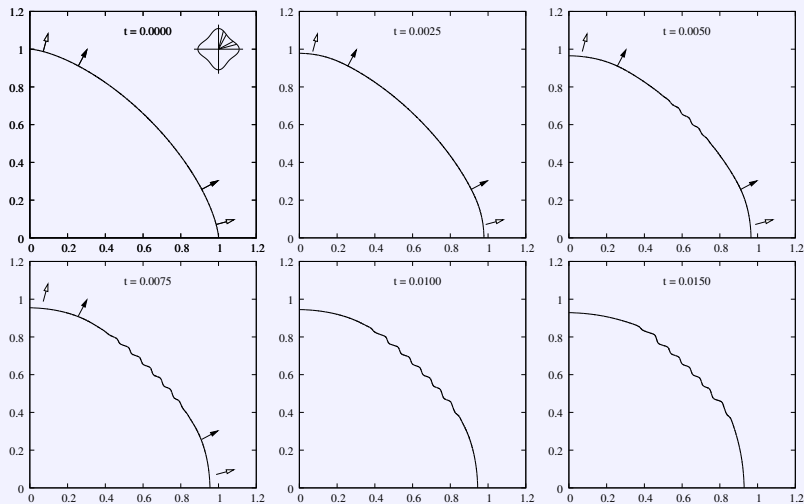
Starting from $p = 1.5$ unit ball, $\varepsilon = 0.008$, $h = 0.002$:



[see animation.avi]

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

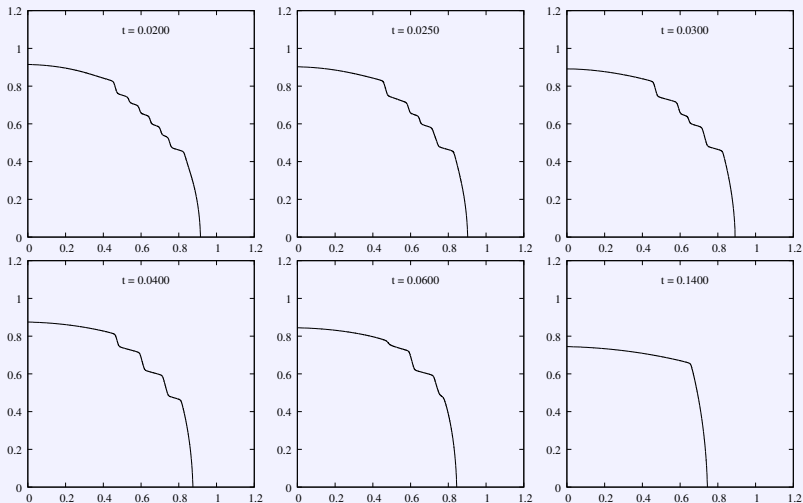
$\varepsilon = 0.004$, $h = 0.002$:



[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 a nonconvex energy when relaxed with 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 $\varepsilon \rightarrow 0$ (or $h \rightarrow 0$).
- 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 .

Thank you!

THANK YOU!

Recall:

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

Remark

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

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

The bidomain model is a degenerate parabolic system.

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

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

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 .

[Colli Franzone-Savaré]

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[Colli Franzone-Savaré]

Gamma-limit of the stationary problem

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

In the linear case (α_j 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)

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