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

## Nonconvex curvature flow and the bidomain system

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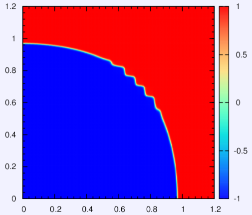
joint work with **Giovanni Bellettini** and **Franco Pasquarelli**

# Outline of the talk

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

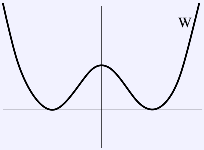


# The bidomain system

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

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

in $\Omega \in \mathbb{R}^d$ with appropriate initial and boundary conditions. $T_{1,2}$ are the duality mappings of two strictly convex anisotropies $\gamma_{1,2}$, $f = W'$ 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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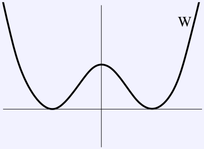


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# Origin: propagation of the electric stimulus in the myocardium

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

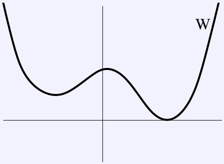
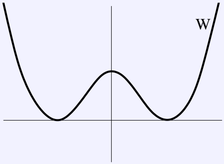
- $u^i$ $(= u_1)$: intra-cellular potential,
- $u^e$ $(= -u_2)$: extra-cellular potential,

defined in two disjoint domains with different anisotropic structure and a common boundary.
After homogeneization they are defined in the common domain $\Omega$.
**Aim:** Simulate a complete heart-beat, but specifically the depolarization phase.

[Hodgkin–Huxley, Fitzhugh–Nagumo,...]

Deeply numerically investigated by [Colli Franzone et al]

# Differences

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

# The anisotropy in the bidomain model

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

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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 homogeneization procedure of the microscopic geometry and depend mainly on the shape of the cells.

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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 $u = u^i - u^e$

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

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 $\gamma$ describes a suitable **combined** anisotropy,
$\kappa_\gamma$ is the corresponding anisotropic curvature,
$c_W$ depends on the potential $W$ and $c_W = 0$ in case of equal wells.

# Anisotropy

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

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

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

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

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

[Wheeler-McFadden, Bellettini-P.]

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# Anisotropy (2)

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

$$T : F_\gamma \to W_\gamma$$

**Linear anisotropy**

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

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

**Strictly convex anisotropy**

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$W_\gamma$ is a convex polygon/polyhedron (and so is $F_\gamma$.)
$T$ is multivalued maximal monotone.

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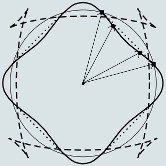
## Nonconvex anisotropy

$F_\gamma$ is not convex: illposedness of a.m.c.f.



$\gamma$ is **not** a norm

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

# Anisotropic mean curvature flow

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

**Anisotropic mean curvature flow**

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

**Allen-Cahn relaxation**

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

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

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# The bidomain system: combined anisotropy

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The *combined anisotropy* $\gamma$ 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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$$V_\gamma = -\kappa_\gamma + \mathcal{O}(\varepsilon)$$

**Anisotropic mean curvature flow**

$\gamma$ 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 the combined anisotropy) as $\epsilon \to 0$.

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# 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. $\Gamma$-convergence result for the stationary bidomain system, consistent with the formal asymptotics, but without a complete identification of the $\Gamma$-limit [Ambrosio-Colli Franzone-Savaré]
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# Inverted anisotropic ratio, $d = 2$

We make a linear choice for the anisotropies

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

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.

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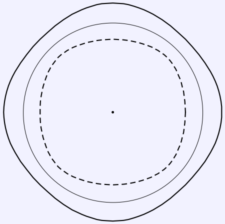
$\rho = 2$ (convex combined anisotropy)



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

# Numerical simulations. Two choices for $\rho$

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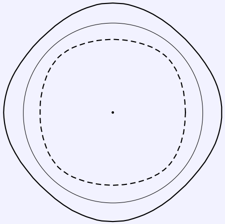
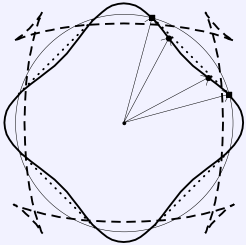


**Strong inverted ratio**

$\rho = 5$ (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 $\epsilon$ 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.

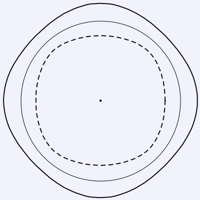
# Discretization

- 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



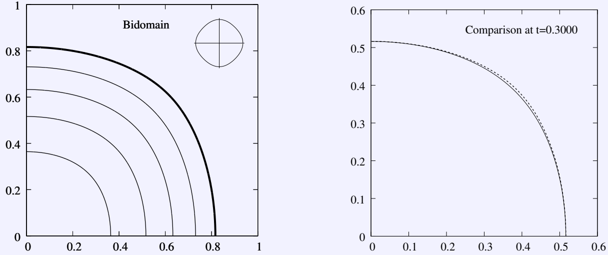
**Evolving the Wulff shape**

The Wulff shape evolves selfsimilarly by anisotropic mean curvature

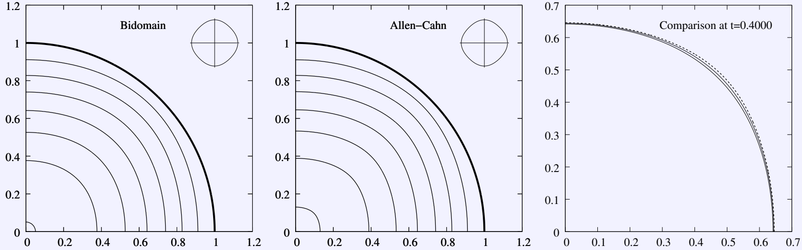
In all pictures we plot the zero-level curve of $u_1 + u_2$ at different time steps.

# Simulations with $\rho = 2$

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



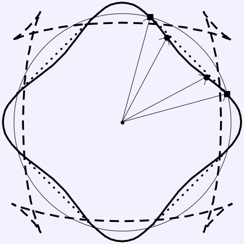

Starting from the unit circle, $\varepsilon = 0.08$, $h = 0.01$, bidomain vs Allen-Cahn:



# Strong inverted anisotropic ratio

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

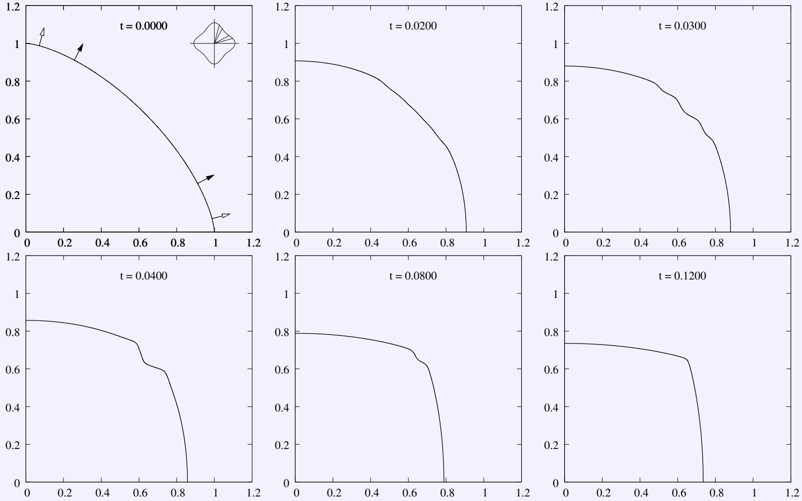
Solid line: Frank diagram
Dashed line: Wulff shape



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

# Simulation with $\rho = 5$

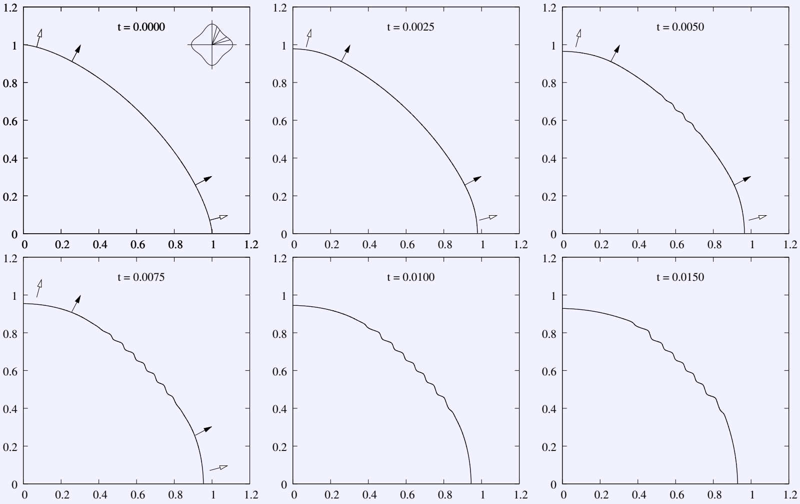
Starting from $p = 1.5$ unit ball, $\varepsilon = 0.008$, $h = 0.002$:




[see animation.avi]

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

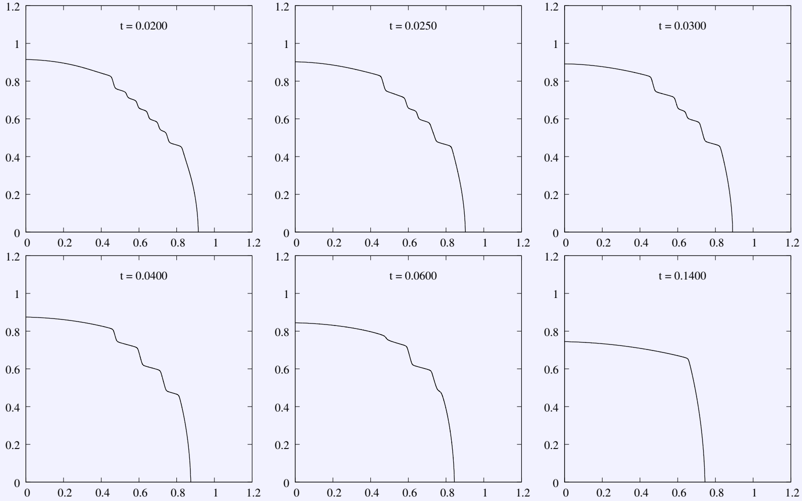
$\varepsilon = 0.004$, $h = 0.002$:




[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 an 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 $\varepsilon \to 0$ (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 $\varepsilon$.

# 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

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

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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 $A_1$, $A_2$.

[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 ($\alpha_i$ 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 $\phi$

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 $\phi$ 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)

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