Some aspects in the numerical approximation of surfaces evolving by anisotropic mean curvature

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Maurizio Paolini

Catholic University, Brescia

numerical simulations with F. Pasquarelli

Outline

- Anisotropy
- Anisotropic/Crystalline MCF
- Cylindrical anisotropy
- Canonical selection problem
- Prescribed curvature problem
- Capillarity
- Anisotropic Allen-Cahn

Anisotropy (d=2,3)

$\varphi : \mathbb{R}^d \to \mathbb{R}^+$ describes the anisotropy:

- $\varphi(\xi) \geq 0 \quad \forall \xi \in \mathbb{R}^d; \qquad \varphi(\xi) = 0 \iff \xi = 0$
- $\varphi(t\xi) = t\varphi(\xi), \qquad \forall t \geq 0$ (Homogeneity of degree one)
- φ is convex, i.e. $\varphi(\xi + \eta) \leq \varphi(\xi) + \varphi(\eta)$: triangular inequality

That is, φ is a (possibly nonsymmetric) norm.
$W_\varphi = \{\varphi(\xi) \leq 1\}$ (Wulff shape)

φ regular $\iff$ W_φ is smooth and strictly convex
φ crystalline $\iff$ W_φ is a polygon/polyhedron
We shall mainly focus on a cylindrical W_φ

Anisotropy (2)

Dual norm $\varphi^o : \mathbb{R}^d \to \mathbb{R}^+$:

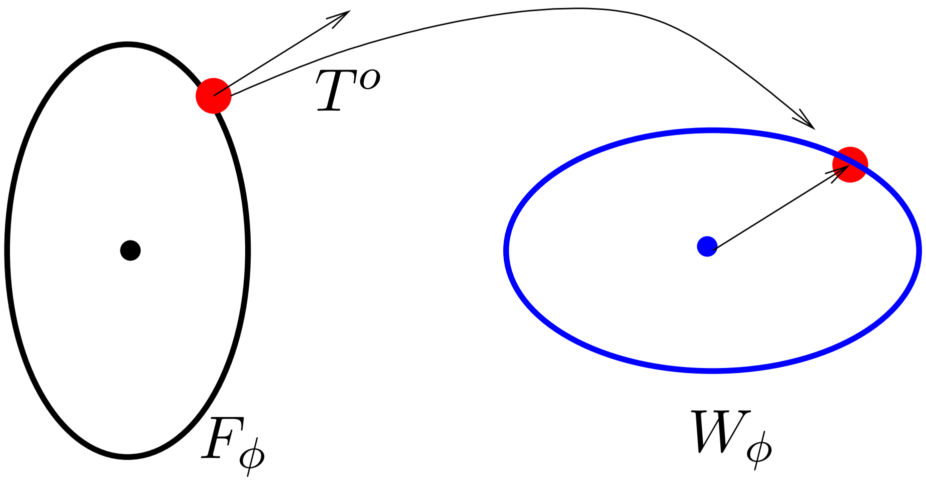
$$\varphi^o(\xi^\star) = \max_{\xi \in W_\varphi} \xi \cdot \xi^\star$$

(φ^o is also a norm, giving the surface energy density)
$F_\varphi = \{\xi : \varphi^o(\xi) \leq 1\}$ (Frank diagram)
$T^o : \mathbb{R}^d \to \mathbb{R}^d$ given by $T^o(\xi) = \varphi^o(\xi)\nabla_\xi \varphi^o(\xi) = \frac{1}{2}\nabla_\xi[\varphi^o(\xi)]^2$

- Duality mapping, nonlinear, monotone, $T^o : F_\varphi \leftrightarrow W_\varphi$, homogeneous of degree one (regular φ)
- Multivalued maximal monotone graph (crystalline φ)

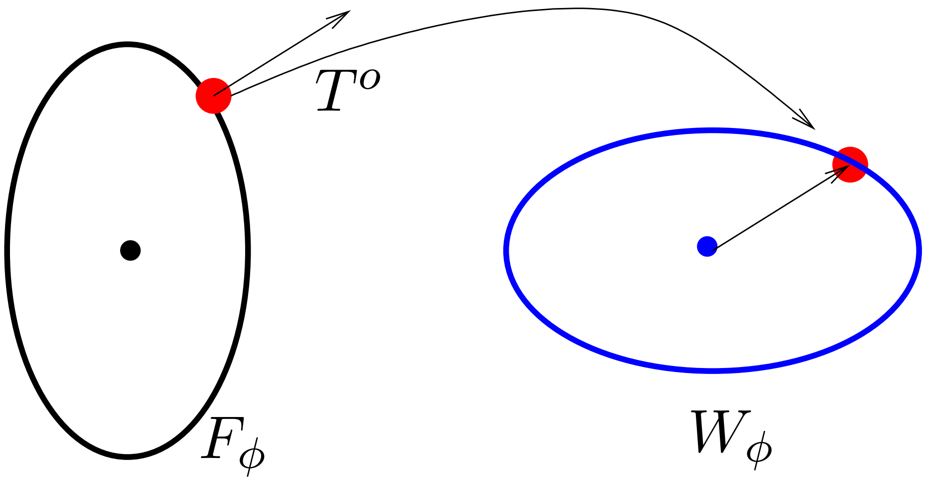
$$T^o(\xi) = \frac{1}{2}\partial_\xi[\varphi^o(\xi)]^2$$

Some examples: 2D

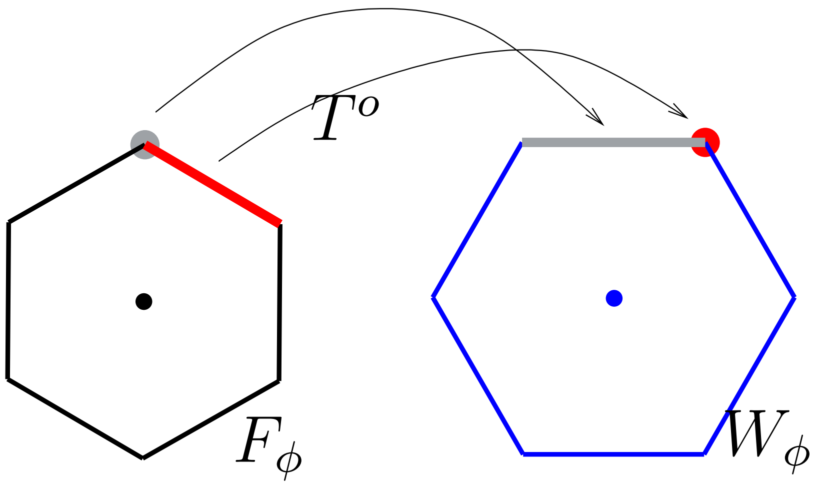


Regular anisotropy

Some examples: 2D

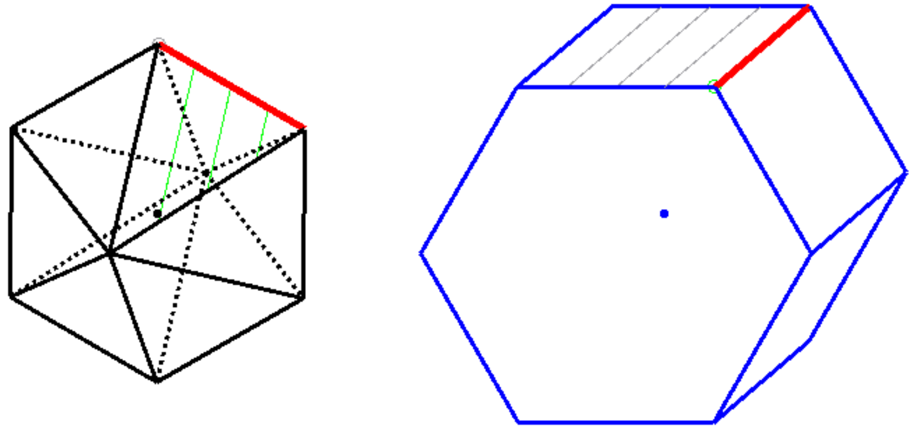


Regular anisotropy



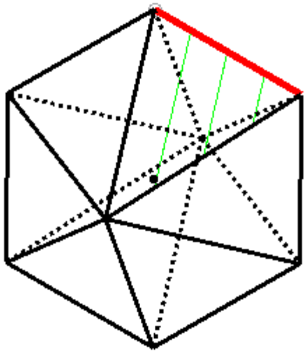
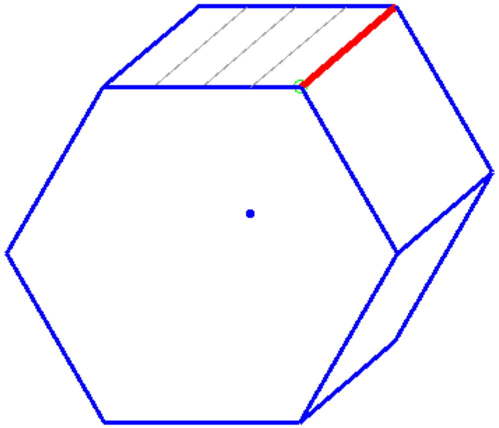
Crystalline anisotropy

Some examples: 3D

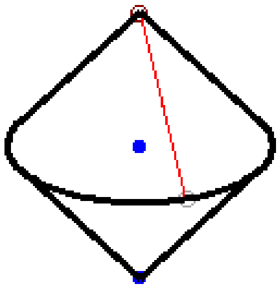
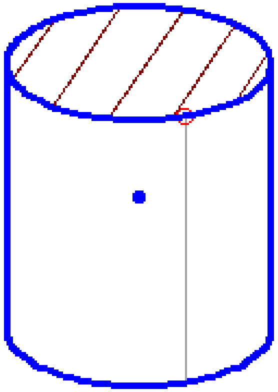


Crystalline anysotropy in 3D (hexagonal prism)

Some examples: 3D

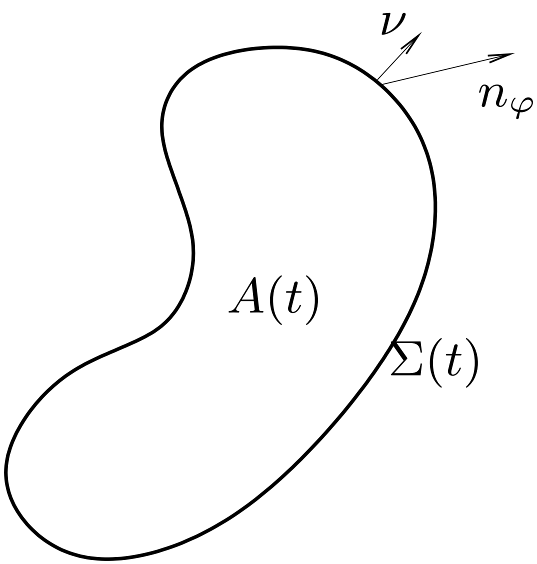



Crystalline anysotropy in 3D (hexagonal prism)

Mixed-type anisotropy in 3D (cylinder)

Anisotropic MCF



Cahn-Hoffmann vector field:

$$n_\varphi = T^o(\nu_\varphi) \qquad \text{where} \quad \nu_\varphi = \frac{\nu}{\varphi^o(\nu)}$$

Anisotropic curvature:

$$\kappa_\varphi = \operatorname{div}\, n_\varphi \qquad \text{note that} \quad \kappa = \operatorname{div}\, \nu$$

Anisotropic MCF (2)

Evolution law:

$$\mathbf{V} = -\kappa_\varphi n_\varphi$$

[“Gradient flow” of $\mathcal{P}_\varphi = \int_\Sigma \varphi^o(\nu)$]
Also equivalent to $V_\nu = -\varphi^o(\nu)\kappa_\varphi$

Known exact evolution: The Wulff shape shrinks selfsimilarly

$$\Sigma(t) = \sqrt{1 - 2(d-1)t}\;\partial W_\varphi$$

Crystalline evolution

[Bellettini,Novaga,P.]

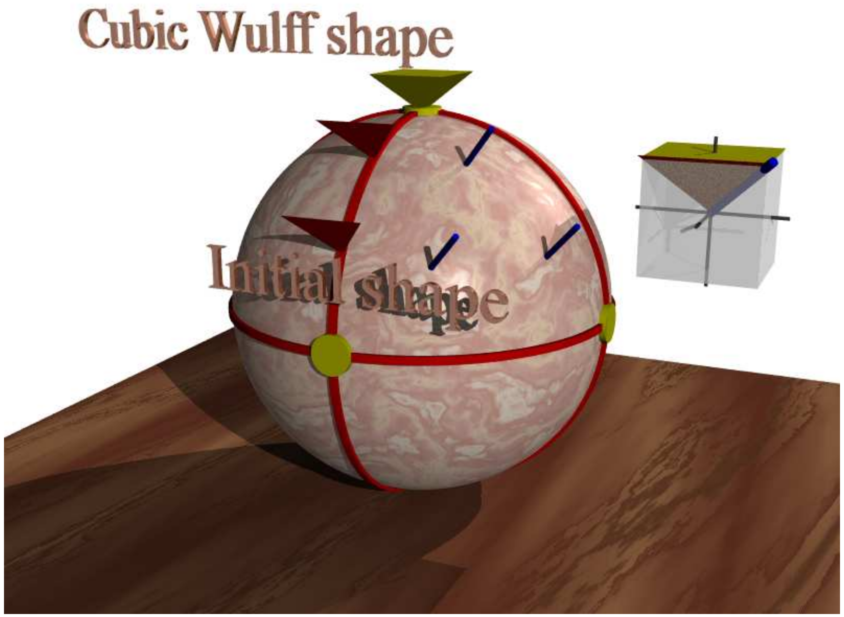
What if φ is crystalline?
n_φ is **not** determined by ν:

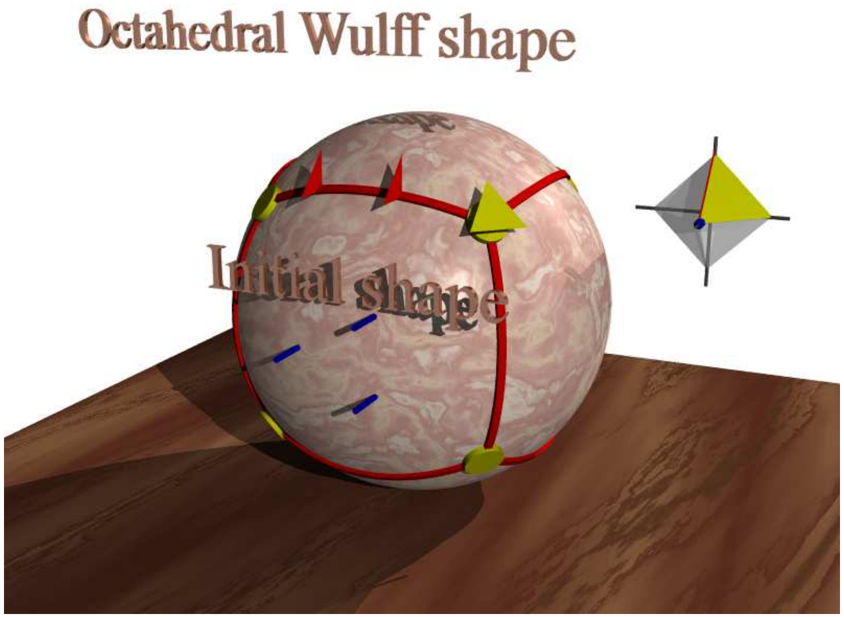
$$n_\varphi \in T^o(\nu_\varphi)$$

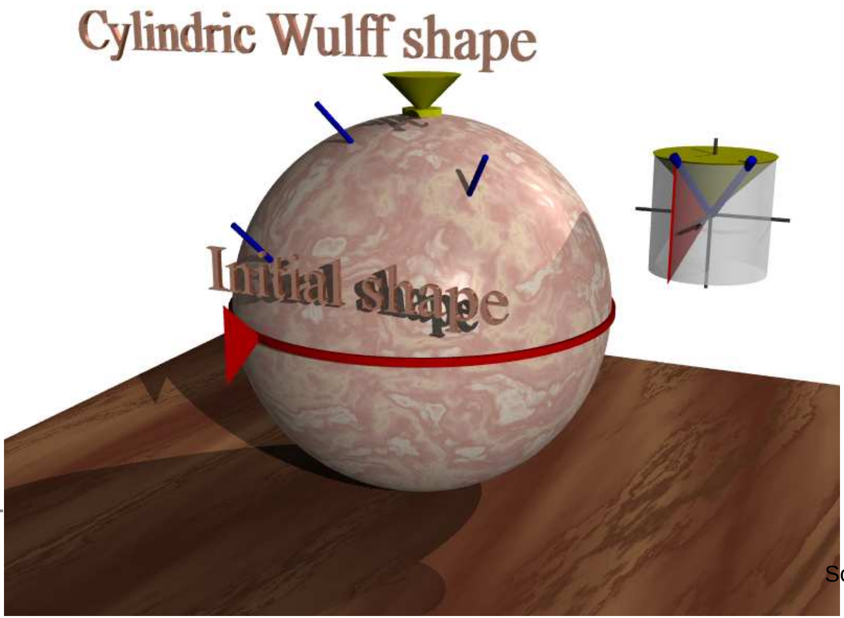
Consequently the curvature $\kappa_\varphi = \mathrm{div}\, n_\varphi$ cannot be derived pointwise from the shape of $\Sigma(t)$. n_φ must be treated as an unknown itself.
Selfsimilar evolution starting from the Wulff shape still gives an explicit solution by choosing

$$n_\varphi(x) = x/\varphi(x), \qquad x \in \Sigma(t)$$

Examples of computation of n_φ







Crystalline evolution 2

Existence and uniqueness of the resulting evolution is expected, partial results:

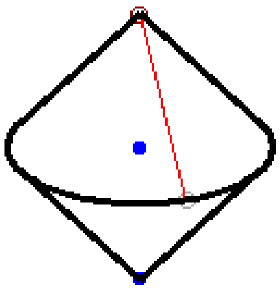
- Existence and uniqueness of evolution starting from a convex initial set [Bellettini-Caselles-Chambolle-Novaga],
- Uniqueness and comparison with the Allen-Cahn [Bellettini-Novaga]

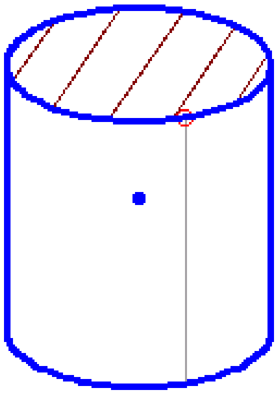
[show numerical simulations, Ctrl-F3, wulffmovies.sh]

- Local velocity is not always determined only by the local shape: nonlocal evolution law

Cylindrical anisotropy

We shall now focus on the **cylindrical** anisotropy, which is of *mixed* type. Frank diagram (left) and Wulff shape (right):



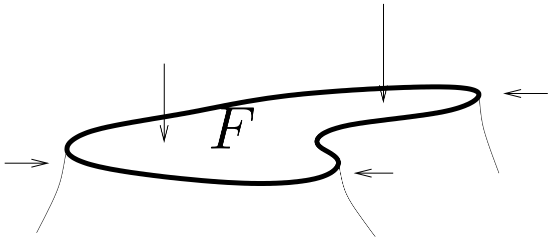


Preferred normals to an evolving surface correspond to the North and South poles and to the equator in the sphere of unit normals. A typical evolution presents plateaus and vertical walls (**Admissible evolution**).

A top face

Let $F = F(t)$ denote a **top** face: a plateau which is a local maximum for the surface. We are interested in the evolution of F.
Two ingredients:

- Erosion from the surrounding walls
- Vertical velocity of F (possible creation of fractures/bending)



On F restriction $n_\varphi \in T^o(\nu_\varphi)$ means n_φ in the top face of the Wulff shape, i.e. $n_\varphi = (\widetilde{n}_\varphi, 1)$ with $\widetilde{n}_\varphi \in \mathbb{R}^2$, $|\widetilde{n}_\varphi| \leq 1$

[show numerical simulation, Ctrl-F3, bendevolution.sh]

Canonical selection

Loosely speaking the evolution is a **gradient flow** with a (not strictly) convex energy. In spite of the apparent freedom in the choice of $n_\varphi \in T^o(\nu_\varphi)$ on the top face F, the evolution law selects a **canonical representative** obtained by solving the minimum problem

$$\int_F |\mathrm{div}\ \xi|^2 \to \text{min}, \qquad \xi \in \mathbb{R}^2, |\xi| \leq 1, \quad \xi = \nu \text{ at } \partial F$$

Let $\bar{\xi}$ by a minimizer. The vertical velocity is then given by $V = -\mathrm{div}\ \bar{\xi}$ [Giga,Gurtin,Matias]

- $\mathrm{div}\ \bar{\xi} =$ constant $\iff$ F does not break/bend

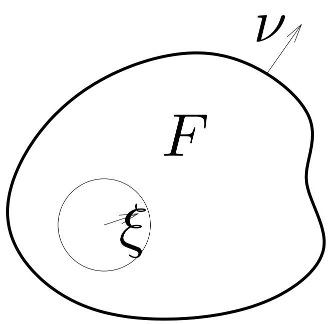
The problem

$F \subset \mathbb{R}^2$ bounded, open, smooth

$\mathcal{K} = \{\xi : F \to \mathbb{R}^2 : \text{div}\, \xi \in L^2, \|\xi\|_{L^\infty} \leq 1, \xi_{|\partial F} = \nu\}$

$\mathcal{F}(\xi) = \frac{1}{2} \int_F |\text{div}\, \xi|^2$

Problem: Find $\min\{\mathcal{F}(\xi) : \xi \in \mathcal{K}\}$



- Convex minimization problem
- Existence of a minimizer $\bar{\xi}$
- Uniqueness up to divergence-free vector fields

Remark: $\forall \xi \in \mathcal{K}$ we have $-V_{\text{mean}} := \frac{1}{|F|} \int_F \text{div}\, \xi = \frac{|\partial F|}{|F|}$, hence if there exists $\bar{\xi} \in \mathcal{K}$ with constant divergence (F is **calibrable**), then $\bar{\xi}$ is a minimizer of $\mathcal{F}$

Remarks and questions

- Elasticity problem with a constraint on the deformation vector
- Select a **canonical** minimizer: gradient of a scalar field? **NO** [Giga, Rybka, P.]
- Find a numerical approximation of a solution
- Find equivalent formulations

Numerical approximation

Piecewise affine finite elements:

- T_h triangular mesh; $h > 0$ mesh size; N internal nodes
- $F_h := \cup_{K \in T_h} K \approx F$
- $V_h := \{v \in H^1(F_h) : v_{|K} \in \mathbb{P}_1 \ \ \forall K \in T_h\}$
- $\mathcal{K}_h := [V_h]^2 \cap \mathcal{K}$

Problem: Find $\min\{\int_{F_h} |\mathrm{div}\ \xi_h|^2 : \xi_h \in \mathcal{K}_h\}$

[Novaga, E. Paolini; P.]

Convex minimization problem in dimension $2N$ (in fact: quadratic minimization with quadratic constraints)

Minimization technique

$\xi \in \mathcal{K}_h \implies \xi = \xi_b + \sum_{i=1}^{N} \xi_i \phi_i$
where $\xi_i \in \mathbb{R}^2$ is the nodal value of ξ at the internal node x_i;
$\xi_b \in \mathcal{K}_h$ vanished at all internal nodes; $\{\phi_i\}_i$ is the canonical basis (hat functions) of V_h.

Then $\boxed{\mathcal{F}_h(\xi) = \frac{1}{2} \int_{F_h} |\text{div } \xi_h|^2 = \frac{1}{2} U^t A U - b^t U + c}$

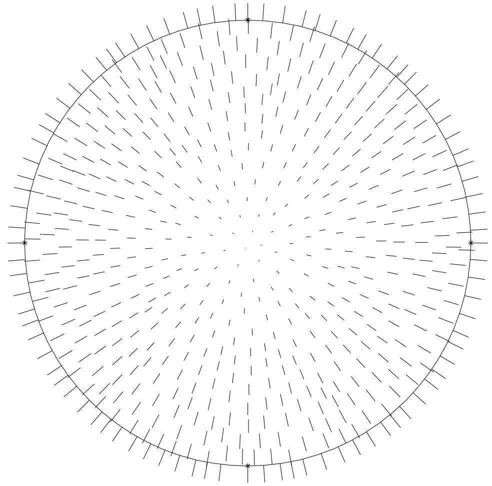
where $U \in \mathbb{R}^{2N}$ is the concatenation of ξ_i, $i = 1, ..., N$;
A is a $2N \times 2N$ matrix (stiffness matrix) made of $N \times N$ blocks $A_{ij} \in M(2)$ defined by $A_{ij} = \int_{F_h} \nabla \phi_i \otimes \nabla \phi_j$, $b \in \mathbb{R}^{2N}$ and $c \in \mathbb{R}$ come from the boundary condition

Matrix A turn out to be symmetric and positive definite
The difficulty then comes from the constraints
$|\xi_i|^2 = \xi_i^t \xi_i \leq 1$, $i = 1, ..., N$

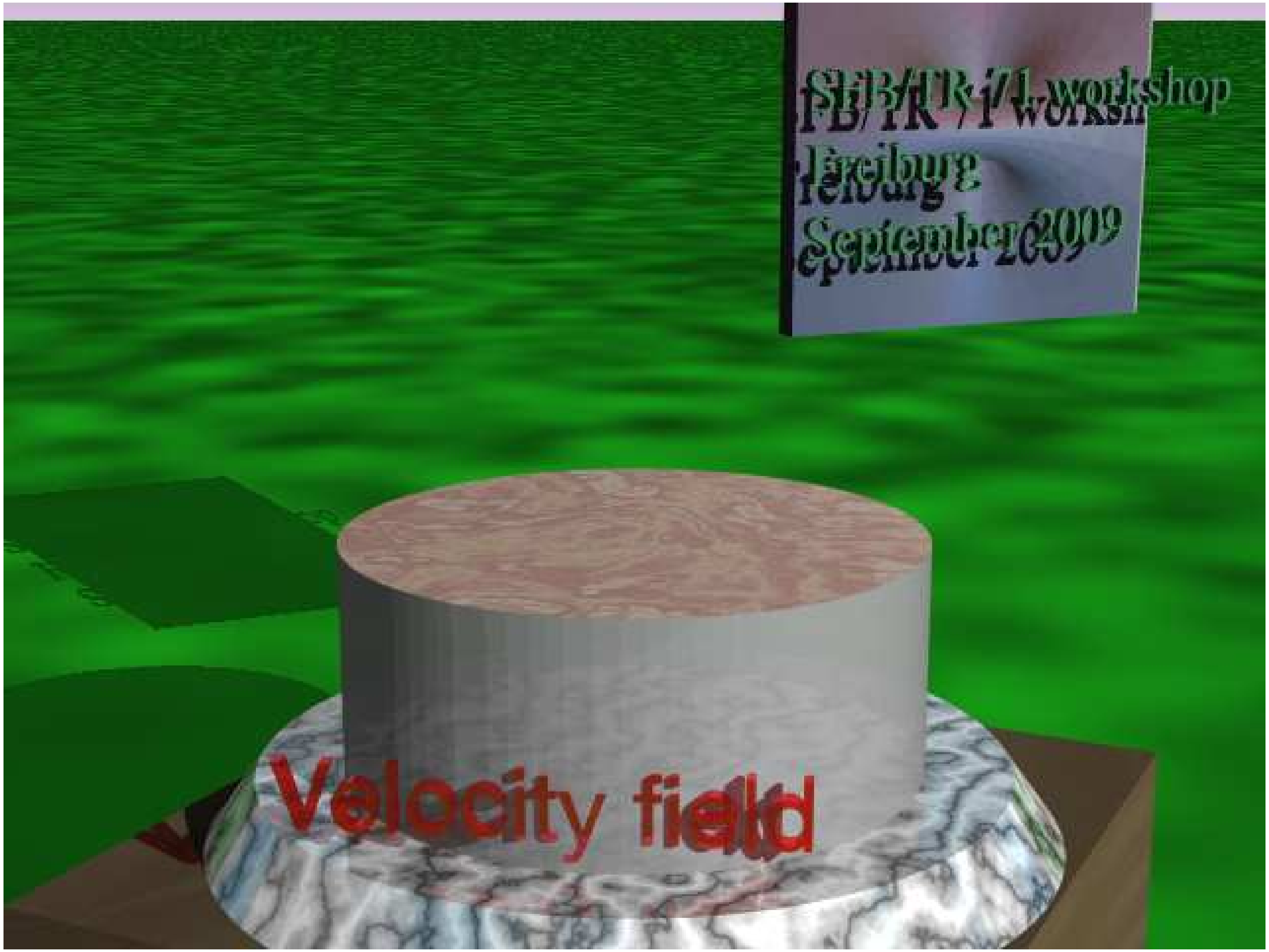
Minimization technique (2)

- First we solve $AU = b$ (unconstrained global minimizer) with conjugate gradient and project the result on the constraint
- Then we iterate with a (projected) gradient method with a projection on the constraint after each iteration.

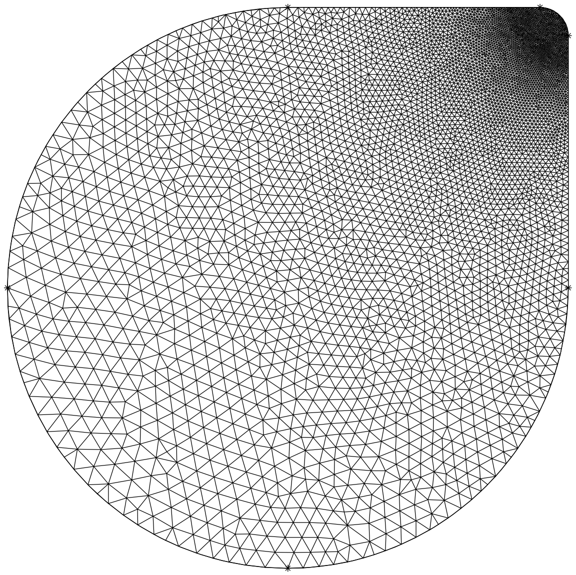
Test example F is the unit circle $h = 0.07$, $N = 480$, 210 conjugate gradient steps, no gradient iterations. F is calibrable, hence the constraint is not involved. $\mathrm{div}\,\bar{\xi}$ ranges from 1.996247 to 2.002405

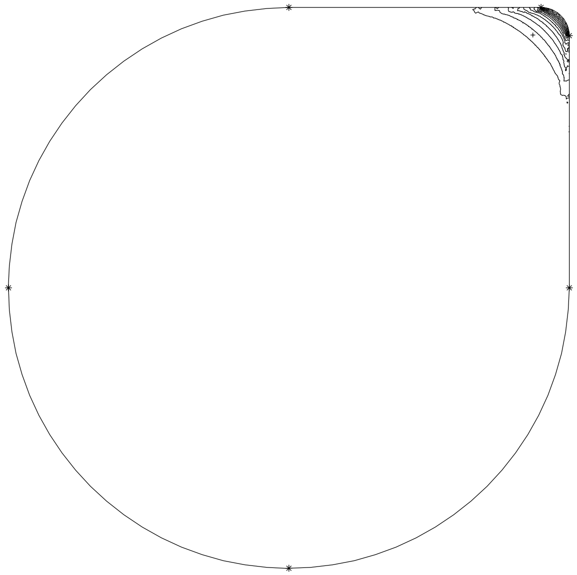


Velocity field for the circle



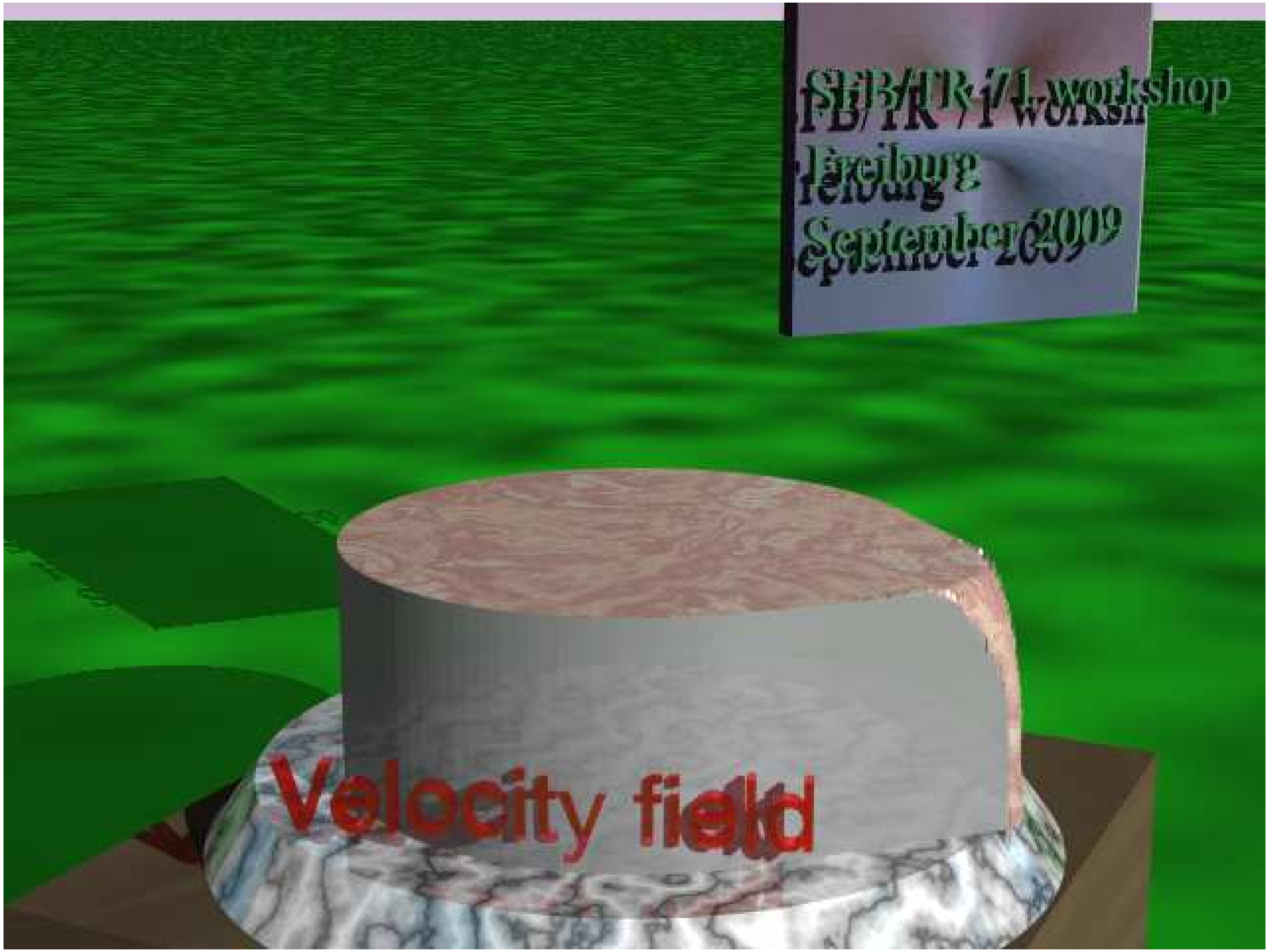
Example with corner





5484 internal nodes, 3829 C.G. iterates, 9243 gradient steps, divergence ranges from 1.18 to 12.7

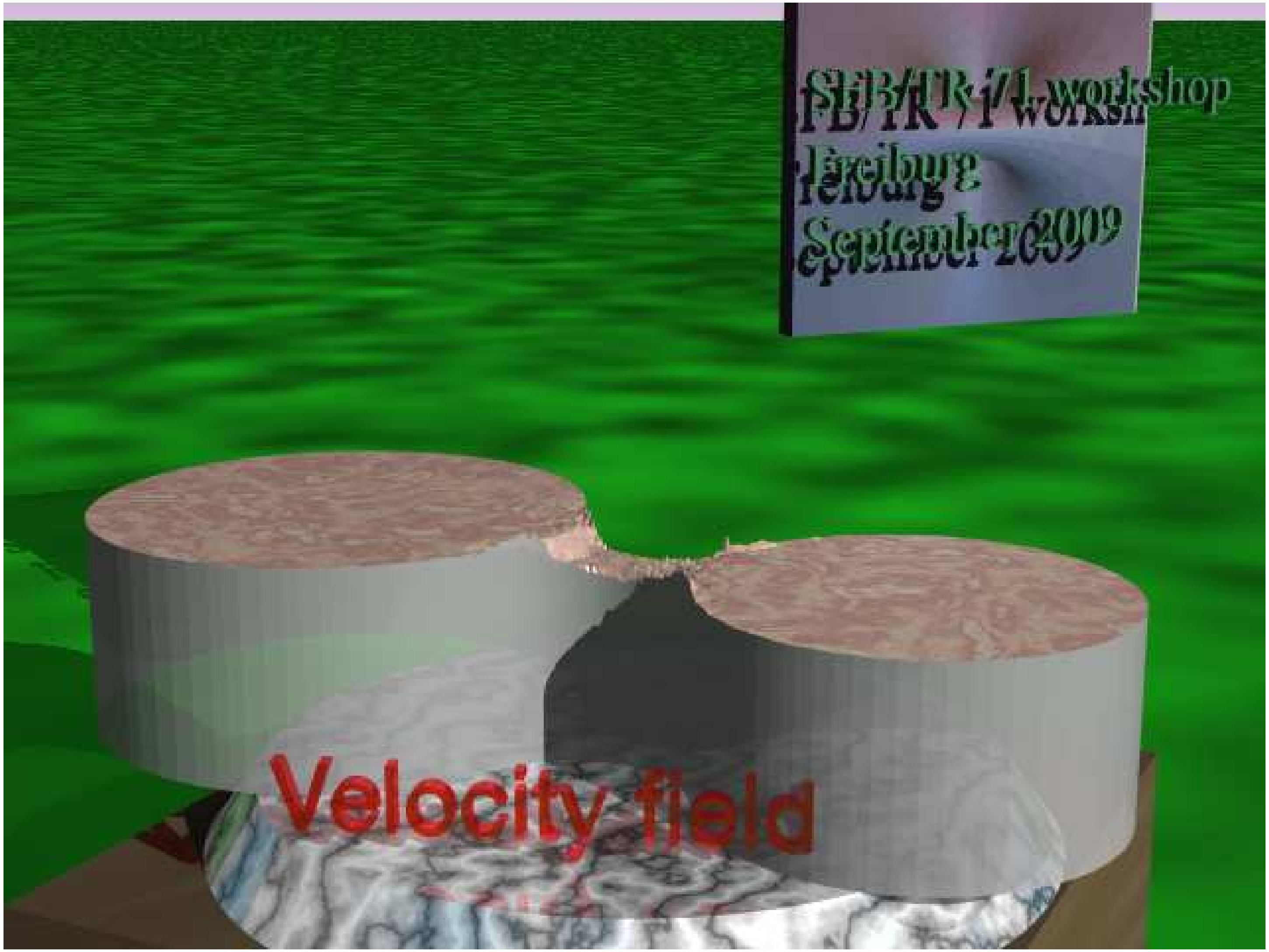
Velocity field for the corner



Nonconvex example

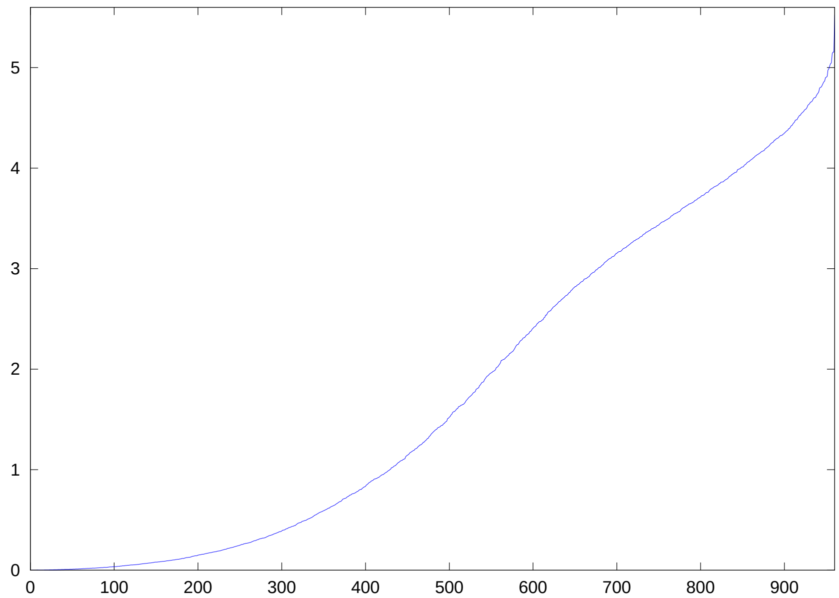
2564 internal nodes, 2299 C.G. iterates, 22675 gradient steps, divergence ranges from 0.90 to 4.22

Velocity field for the nonconvex example



Why is A positive definite?

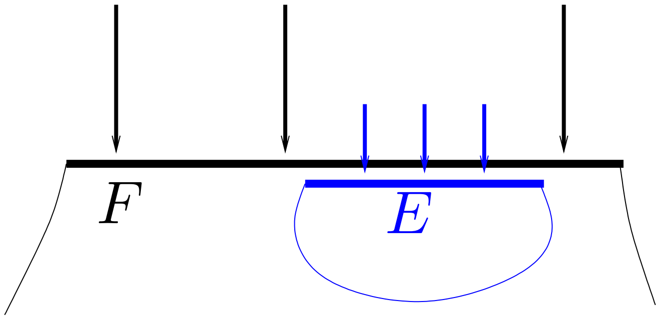
The continuous problem is highly degenerate, due to the invariance w.r.t. divergence-free vector fields; we should expect roughly half of the eigenvalues of A to vanish. This does not happen due to the choice of the finite element space that does not contain divergence-free vector fields (except the trivial constant ones).



Circular domain. Plot of the 960 eigenvalues of A

Calibrability of face $F = F(t)$

- F does not break/bend at time t during evolution
- There esists $\xi : F \to \mathbb{R}^2$ such that
  - $|\xi| \leq 1$
  - $\xi_{|\partial F} = \nu$ (outward normal to ∂F)
  - $\mathrm{div}\ \xi$ is constant
- For all $E \subseteq F$:
  $\frac{|\partial E|}{|E|} \geq \frac{|\partial F|}{|F|} =: \bar{\lambda}$ (comparison principle)



- (if F is convex) F is calibrable $\iff$ $\max_{x \in \partial F} \kappa_{\partial F}(x) \leq \bar{\lambda}$

Prescribed curvature problem

- For $\lambda \in \mathbb{R}$ solve a **prescribed curvature** problem $\mathcal{F}_\lambda(E) = |\partial E| - \lambda |E| \to \min$, $E \subseteq F$. Set $M(\lambda) := \min_{E \subseteq F} \mathcal{F}_\lambda(E)$

The boundary $\partial E \cap F$ of a minimizer has curvature λ and has tangential contact with ∂F

Set $\boxed{\bar{\lambda} = \frac{|\partial F|}{|F|}}$ and $\boxed{\lambda^* = \inf_{E \subseteq F} \frac{|\partial E|}{|E|}}$ $\quad$ ($\lambda^* \leq \bar{\lambda}$)

- $\forall \lambda \ M(\lambda) \leq 0$, $M(\lambda)$ is nonincreasing in λ
- $\lambda \leq \lambda^* \implies M(\lambda) = 0$
- $\lambda > \lambda^* \implies M(\lambda) < 0$
- F is calibrable $\iff \lambda^* = \bar{\lambda} \iff M(\bar{\lambda}) = 0$

Finding the contours of the velocity field

- Find $M(\bar{\lambda})$ (by solving a prescribed curvature problem). If result is 0 then **STOP** (the velocity field is constant $= \bar{\lambda}$)
- Decrease λ and find $M(\lambda)$ untill the result is zero (bisection method). Let λ^* be the limiting value
- Let E^* minimize $\mathcal{F}_{\lambda^*}(E)$, i.e. $\mathcal{F}_{\lambda^*}(E^*) = 0$, then the velocity field is λ^* in E^*
- Find the minimizer for $\mathcal{F}_{\lambda}(E)$ for $\lambda > \lambda^*$ and obtain the level set where velocity is λ (boundary of the minimizer)

Prescribed curvature problem 2

Identifying E with its characterestic function v we have equivalently

$$\mathcal{F}_\lambda(v) = \int_F |Dv| - \int_F \lambda v + \int_{\partial F} v, \qquad v \in BV(F; \{0,1\})$$

Using the coarea formula $\mathcal{F}_\lambda$ can be equivalently minimized on $K = BV\{F; [0,1]\}$ which is a convex set

Numerical solution: convex minimization algorithm using P^1 finite elements plus regularization $|Dv| \approx \sqrt{\epsilon^2 + |\nabla v|^2}$.

[Bellettini-P-Verdi]

A capillarity problem

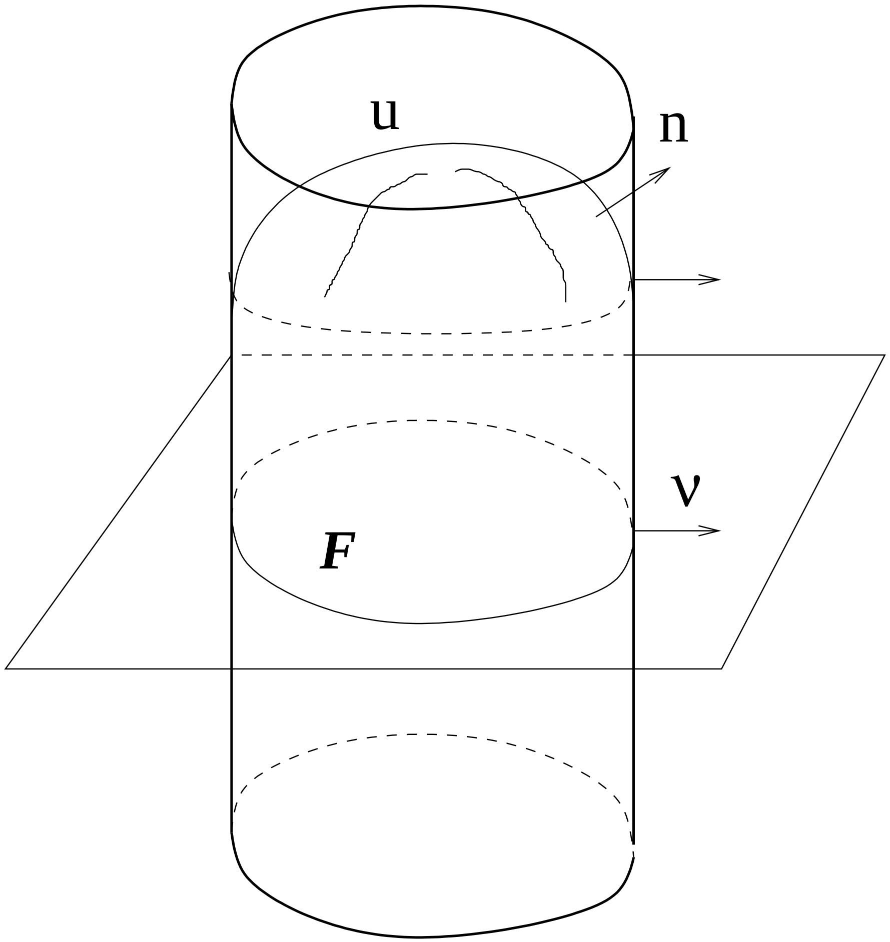
Vessel $F \times [-L, L]$, L large enough, containing a fluid with surface tension and tangential contact + microgravity

To find an equilibrium configuration we minimize the surface energy subject to volume constraint of the fluid:

constant mean curvature $= \bar{\lambda}$

(Lagrange multiplier)

$\bar{\lambda} = \frac{|\partial F|}{|F|}$



Capillarity 2

If the surface can be represented by a function $u : F \to \mathbb{R}$ then

$$\xi = \frac{-\nabla u}{\sqrt{1 + |\nabla u|^2}}$$

is the horizontal component of the normal vector, we have

- $|\xi| \leq 1$ in F
- $\xi = \nu$ at ∂F
- $\mathrm{div}\ \xi = \bar{\lambda}$ is constant in F

then ξ is a calibration of F

There exists a *graph-like* solution iff F is calibrable!

[Concus-Finn]

Total variation flow

Strong connections with the "minimizing total variation flow" (gradient flow for $\int_\Omega |Du|$) defined by Caselles et al.

[Ballester-Caselles-...] [Bellettini-Novaga-Caselles]

We seek an *entropy solution* of

$$u_t = \mathrm{div}\left(\frac{Du}{|Du|}\right)$$

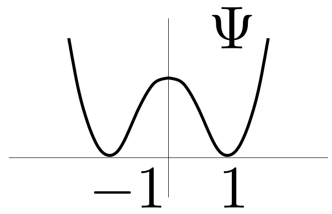
Starting from the characteristic function $u_0 = \chi_F$ of F

F is calibrable $\iff$ the solution is of the form $u(t) = \sigma(t)u_0$

for an appropriate rescaling scalar function σ

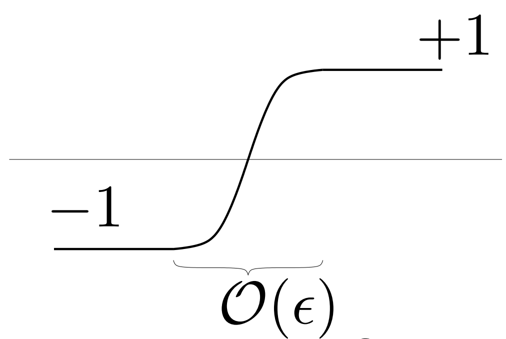
Anisotropic Allen-Cahn

$\epsilon > 0$ singular perturbation parameter,
$\Psi : \mathbb{R} \to \mathbb{R}^+$ a *double well* potential
(e.g. $\Psi(s) = (1 - s^2)^2$), $\psi = \Psi'$



$$\begin{cases} \epsilon \frac{\partial u}{\partial t} - \epsilon \mathrm{div}\, T^o(\nabla u) + \frac{1}{\epsilon}\psi(u) = 0 \\ \text{+ initial and boundary conditions} \end{cases}$$

Typical profile of u:



If $T^o = Id$ then $\Sigma_\epsilon = \{u = 0\}$ approximates a surface evolving by mean curvature
[Evans-Soner-Souganidis, De Mottoni-Schatzman,...]
with an error of order $\mathcal{O}(\epsilon^2 |\log \epsilon|^2)$
[Bellettini-Nochetto-P-Verdi,...]

Identifying the singular limit

Now we can identify the singular limit of the anisotropic Allen-Cahn when T^o is regular (nonlinear)

The zero level set Σ_ϵ of u (solution of the anisotropic Allen-Cahn) approximates (with an error $\mathcal{O}(\epsilon^2|\log\epsilon|^2)$) a surface evolving by anisotropic mean curvature flow
$\mathbf{V} = -\kappa_\varphi n_\varphi$

[Elliott-Schätzle-P, Bellettini-Colli Franzone-P, ...]

Anisotropic Allen-Cahn is well defined also for **crystalline** anisotropy (T^o is a maximal monotone graph, and the equation must be interpreted suitably); what is the singular limit?

Thank you

Thank you!