Self-avoiding approximate mean curvature flow

Simon Masnou

Camille Jordan Institute Claude Bernard University Lyon 1

joint work with Elie Bretin (INSA Lyon) & Chih-Kang Huang (Univ. Lyon 1)

Conference on Digital Geometry and Discrete Variational Calculus CIRM, Apr 1 2021

Motivation

Many physical systems or engineering models involve interfaces which tend to minimize a geometric energy, involving either the area or the curvatures of interfaces (under various constraints)

We are interested in the numerical simulation of such systems.

Examples: Wetting



Droplet wetting on a lotus leaf (energy = area)

Bubbles







bics

(energy = multiphase area)

Honeycomb



Honeycomb (energy = 2D multiphase perimeter)

Polycrystalline materials



$$E(\Sigma_1,\ldots,\Sigma_N) = \frac{1}{2}\sum_{i,j=1}^N \sigma_{i,j}\operatorname{Area}(\partial\Sigma_i\cap\partial\Sigma_j)$$

 $(\sigma_{i,j} \text{ are surface tensions})$

Nanowires



Nanowires (energy = multiphase anisotropic area)

Lipid bilayer



Blood cell (energy = Helfrich energy $\int (\frac{\kappa}{2}(H - H_0)^2 + \kappa_G K) d\sigma$)

with H = mean curvature, $H_0 =$ spontaneous curvature and K = Gaussian curvature

$$W(S) = \int H^2 d\sigma \quad (-\int K d\sigma)$$
 is the Willmore energy.

Magnetic Resonance Imaging (MRI)

Problem: find a volume containing given slices and having boundary of minimal energy (area or Willmore)





3D reconstruction from 2D slices



Reconstruction of a 3D brain image from real MRI slices

3D reconstruction from 2D slices



Smoothing of a digital shape using the Willmore energy



How to approximate the minimizers?

Pick a representation of the surface:

- Parametric "continuous" surface or graph surface
- Level set
- Phase field approximation

and try to minimize the energy, or an approximation of it using either:

- graph methods (e.g, min flow/max cut)
- a static Euler equation
- a time-dependent Euler equation

This talk focuses on phase field approximation and time-dependent Euler equations, and is motivated by the following issue: can we efficiently minimize while avoiding undesirable topology changes as the surface evolves?



Phase field approximation

A phase field $u_{\varepsilon} : \mathbb{R}^d \to [0, 1]$ is a smooth function which approximates the characteristic function $\mathbb{1}_E$ of a set E.

The set $\{u_{\varepsilon} = \frac{1}{2}\}$ is an approximation of the boundary ∂E .

The area of ∂E is the perimeter of E.



Perimeter approximation



Thus,
$$\int \varepsilon |\nabla u_{\varepsilon}|^2 \mathrm{d}x \approx \frac{1}{\varepsilon} Area \approx \frac{1}{\varepsilon} \varepsilon P(E) = P(E)$$
 as $\varepsilon \to 0$.

Minimizing $\int \varepsilon |\nabla u_\varepsilon|^2 \mathrm{d} x$ is not a good idea: any constant function has zero energy...

How to constrain minimizers to be close to a characteristic function?

Perimeter approximation

Use a double-well potential, for instance $G(s) = \frac{1}{2}s^2(1-s)^2$.



If $\sup_{\varepsilon} \left(\int \frac{1}{\varepsilon} G(u_{\varepsilon}) dx \right) < +\infty$ then $u_{\varepsilon} \to 0$ or 1 a.e. as $\varepsilon \to 0$, i.e. u_{ε} approximates a characteristic function.

The Cahn-Hilliard functional

(Van der Waals)-Cahn-Hilliard energy

The phase-field approximation of perimeter is

$${\mathcal{P}}_{arepsilon}(u) = \int \left(rac{arepsilon}{2} |
abla u|^2 + rac{1}{arepsilon} G(u)
ight) \mathrm{d}x$$



where G is a double-well potential.



e.g., $G(s) = \frac{1}{2}s^2(1-s)^2$

Phase-field approximation of perimeter

Convergence of P_{ε} (Modica, Mortola - 1977)

 P_{ε} Γ -converges to

$$\mathsf{P}(u) = \left\{ egin{array}{cc} \lambda \mathsf{P}(E) & ext{si} \ u = \mathbbm{1}_E \in BV \ +\infty & ext{otherwise} \end{array}
ight.$$

where $\lambda = cst$ depends only on potential G.

Γ-convergence and minimizers

Let (F_n) equicoercive, Γ -converging to F. If, $\forall n, u_n$ is a minimizer of F_n , then every cluster point u of (u_n) is a minimizer of F and $F(u) = \lim F_n(u_n)$.

Optimal profile

The phase-field optimal profile associated with E and P(E) is:

$$u_{\varepsilon}(x) = q\left(rac{d_s(x,E)}{arepsilon}
ight) \qquad ext{with} \quad q(s) = rac{1}{2}(1- anh(rac{s}{2}))$$



Signed distance $d_s(x, E) = d(x, E) - d(x, \mathbb{R}^N \setminus E)$

where
$$q = \operatorname{argmin}_{arphi} \{ \int_{\mathbb{R}} [rac{|arphi'(t)|^2}{2} + G(arphi(t))] dt, \ arphi(-\infty) = 1, \ arphi(\infty) = 0 \}$$

Convergences

For a bounded set E

• $u_{\varepsilon} \rightarrow \mathbb{1}_{E}$

•
$$P_{\varepsilon}(u_{\varepsilon}) \rightarrow \lambda P(E)$$
 if E has finite perimeter

as $\varepsilon \to 0$.

Phase field approximation of the Willmore energy

The L^2 -gradient of P_{ε} satisfies

$$-\nabla_{L^2} P_{\varepsilon}(u) = \varepsilon \Delta u - \frac{1}{\varepsilon} G'(u).$$

The gradient flow of perimeter is the mean curvature flow and $-\nabla_{L^2} P_{\varepsilon}(u_{\varepsilon})$ approximates the mean curvature of ∂E in the transition zone of u_{ε} when $u_{\varepsilon} \approx \mathbb{1}_E$.

Approximation of the Willmore energy

In \mathbb{R}^2 and $\mathbb{R}^3,$ the energy

$$u\mapsto P_{\varepsilon}(u)+W_{\varepsilon}(u)=P_{\varepsilon}(u)+\int rac{1}{2\varepsilon}\left(\varepsilon\Delta u-rac{1}{\varepsilon}G'(u)
ight)^{2}\mathrm{d}x$$

 Γ -converges to $E \mapsto \lambda(P(E) + W(E))$ if E is C^2 and compact

• De Giorgi + Bellettini, Paolini (1993) + Röger, Schätzle (2006)

Optimal profile

With the same phase-field profile associated with E

$$u_{\varepsilon}(x) = q\left(\frac{1}{\varepsilon}d_{s}(x,E)\right)$$

one has

Convergences

For a bounded set E

- $u_{\varepsilon} \rightarrow \mathbb{1}_{E}$
- $P_{\varepsilon}(u_{\varepsilon}) \rightarrow \lambda P(E)$ if E has finite perimeter
- $W_{\varepsilon}(u_{\varepsilon}) \rightarrow \lambda W(E)$ if ∂E is C^2

as $\varepsilon \to 0$.

Phase field mean curvature flow: numerical approximation

The L^2 -gradient flow of the Cahn-Hilliard energy gives the time-dependent Allen-Cahn equation

$$u_t = \Delta u - \frac{1}{\varepsilon^2} G'(u)$$

Given a time-step δ_t , solutions can be numerically approximated with the scheme

$$\frac{u^{n+1}-u^n}{\delta_t} = \Delta u^{n+1} - \frac{1}{\varepsilon^2} G'(u^{n+1})$$

 u^{n+1} can be computed using Picard iterations to find fixed points of the map $v \mapsto (I_d - \delta_t \Delta)^{-1} \left(u^n - \frac{\delta_t}{\varepsilon^2} G'(v) \right)$

Implementation with Fourier series and periodic boundary conditions, which guarantee a high spatial accuracy.



Phase field Willmore flow: numerical approximation

• The classical phase field Willmore flow is

$$\begin{cases} \partial_t u = \Delta v - \frac{1}{\varepsilon^2} G''(u) v \\ v = \frac{1}{\varepsilon^2} G'(u) - \Delta u. \end{cases}$$

• Implicit discretization in time

$$\begin{cases} u^{n+1} = \delta_t \left[\Delta v^{n+1} - \frac{1}{\varepsilon^2} G''(u^{n+1}) v^{n+1} \right] + u^n \\ v^{n+1} = \frac{1}{\varepsilon^2} G'(u^{n+1}) - \Delta u^{n+1}, \end{cases}$$

• Use Picard iterations for approximating a fixed point of:

$$\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} I_d & -\delta_t \Delta \\ \Delta & I_d \end{pmatrix}^{-1} \begin{pmatrix} u^n - \frac{\delta_t}{\varepsilon^2} G''(u)v \\ \frac{1}{\varepsilon^2} G'(u) \end{pmatrix}$$

Implement it with Fourier series in space.

• Stability :

$$\delta_t \leq C \min\left\{\varepsilon^4, \delta_x^2 \varepsilon^2\right\}.$$

Phase field Willmore flow

$$\partial_t u = -\Delta\left(\Delta u - \frac{1}{\varepsilon^2}G'(u)\right) + \frac{1}{\varepsilon^2}G''(u)\left(\Delta u - \frac{1}{\varepsilon^2}G'(u)\right),$$



Phase field Willmore flow

$$\partial_t u = -\Delta\left(\Delta u - \frac{1}{\varepsilon^2}G'(u)\right) + \frac{1}{\varepsilon^2}G''(u)\left(\Delta u - \frac{1}{\varepsilon^2}G'(u)\right),$$



Phase field Willmore flow

$$\partial_t u = -\Delta\left(\Delta u - \frac{1}{\varepsilon^2}G'(u)\right) + \frac{1}{\varepsilon^2}G''(u)\left(\Delta u - \frac{1}{\varepsilon^2}G'(u)\right),$$



Lawson-Kusner surface of genus 4

Key aspects of phase field approximation

- Replace singular energies with smooth energies
- **F**-convergence can be proven
 - I for area: Modica-Mortola'77
 - If for Willmore 2D, 3D: De Giorgi'91 Bellettini-Paolini'93, Röger-Schätzle'06, Nagase-Tonegawa'07
- Smooth minimizers approximate sharp minimizers
- Efficient numerical schemes can be designed
- Do phase field flows approximate sharp flows? (as long as they are smooth)
 - If or area: well-posedness, convergence → YES [Chen'92, de Mottini-Schatzman'95, Bellettini-Paolini'95]
 - If or Willmore:
 - well-posedness (YES [Colli-Laurençot'12], [Bretin-Huang-M.'19]),
 - * convergence (formally YES [Loreti-March'00, Bretin-M.-Oudet'17], rigorously YES [Fei-Liu'19]) Willmore flow: $V_n = \Delta_S H + |A|^2 H - \frac{1}{2}H^3$ where $|A|^2 = \sum \kappa_i^2$.

Issue: the classical phase field Willmore flow may develop undesirable singularities



The classical phase field Willmore flow may develop undesirable singularities



The classical phase field Willmore flow may develop undesirable singularities



Such configuration has infinite relaxed Willmore energy

 $\overline{\mathcal{W}}(\Omega) = \inf \{ \liminf \mathcal{W}(\Omega_h), \ \partial \Omega_h \in \mathrm{C}^2, \ \Omega_h \to \Omega \text{ in } \mathrm{L}^1(\Omega) \}.$



If $\overline{\mathcal{W}}(E) < +\infty$, then a non-oriented tangent must exist everywhere on the boundary of *E*, [Bellettini-Dal Maso-Paolini'93], [Bellettini-Mugnai'04]

Explanation: existence of smooth Allen-Cahn solutions with singular nodal set

• Existence of smooth solutions [Dang Fife Peletier 92], [Kowalczyk Pacard 2012] to the Allen-Cahn equation

$$\Delta u_{arepsilon} - rac{1}{arepsilon^2} G'(u_{arepsilon}) = 0,$$

such that $u_{arepsilon} o \chi_{E}$ with $\overline{\mathcal{W}}(E) = +\infty$

• Example of Allen-Cahn solutions





Mugnai's approximation of the Willmore energy in 2D

- Let A = second fundamental form
- In 2D, $H^2 = ||A||^2$ • if $u_{\varepsilon} = q\left(\frac{\text{dist}(x,\Omega)}{\varepsilon}\right)$, then

$$\frac{1}{\varepsilon} \left| \varepsilon \nabla^2 u_{\varepsilon} - \frac{1}{\varepsilon} G'(u_{\varepsilon}) \frac{\nabla u_{\varepsilon}}{|\nabla u_{\varepsilon}|} \otimes \frac{\nabla u_{\varepsilon}}{|\nabla u_{\varepsilon}|} \right|^2 = |\nabla^2 \operatorname{dist}(x, \Omega)|^2 \frac{1}{\varepsilon} q' \left(\frac{\operatorname{dist}(x, \Omega)}{\varepsilon} \right)^2 \longrightarrow ||A(x)||^2 c_G \mathcal{H}^{N-1} \sqcup \partial \Omega \quad \text{as } \varepsilon \to 0$$

Definition (Mugnai's approximation in 2D) $\mathcal{W}_{\varepsilon}^{M}(u) = \frac{1}{2\varepsilon} \int \left| \varepsilon \nabla^{2} u - \frac{1}{\varepsilon} G'(u) \frac{\nabla u}{|\nabla u|} \otimes \frac{\nabla u}{|\nabla u|} \right|^{2} dx$

Gradient flow

Energy

$$\mathcal{W}_{\varepsilon}^{\mathcal{M}}(u) = \frac{1}{2\varepsilon} \int \left| \varepsilon \nabla^2 u - \frac{1}{\varepsilon} G'(u) \frac{\nabla u}{|\nabla u|} \otimes \frac{\nabla u}{|\nabla u|} \right|^2 dx.$$

• Its L^2 -gradient flow is

$$\begin{cases} \varepsilon^2 \partial_t u = \Delta \psi - \frac{1}{\varepsilon^2} G''(u) v + G'(u) B(u) \\ v = G'(u) - \varepsilon^2 \Delta u, \end{cases}$$

where

$$B(u) = \operatorname{div}\left(\operatorname{div}\left(\frac{\nabla u}{|\nabla u|}\right)\frac{\nabla u}{|\nabla u|}\right) - \operatorname{div}\left(\nabla\left(\frac{\nabla u}{|\nabla u|}\right)\frac{\nabla u}{|\nabla u|}\right)$$

• Well-posedness and existence at fixed parameter ε ? Requires presumably a regularization of B(u) (which is done in practice numerically).

Formal asymptotic expansion in the smooth case

• Formal expansion

$$egin{split} u_arepsilon(x,t) &\simeq q\left(rac{d(x,\Omega^arepsilon(t))}{arepsilon}
ight)+arepsilon^2rac{A^2}{2}\eta_1\left(rac{d(x,\Omega^arepsilon(t))}{arepsilon}
ight)\ v_arepsilon(x,t) &\simeq -arepsilon\mathsf{H}q'\left(rac{d(x,\Omega^arepsilon(t))}{arepsilon}
ight)+arepsilon^2\mathsf{A}^2\eta_2\left(rac{d(x,\Omega^arepsilon(t))}{arepsilon}
ight), \end{split}$$

• Front speed:

$$V^{\varepsilon} = \Delta_{S}H + III^{3} - \frac{1}{2}H|A|^{2} + O(\varepsilon),$$

with $III^3 = \sum \kappa_i^3$.

• It coincides with the Willmore flow in dimensions 2, 3, as long as it is smooth.

A self-avoiding approximate Willmore flow



A self-avoiding approximate Willmore flow



About the reaction term B(u)

Lemma

Let
$$u \in C^2$$
 with $\nabla u \neq 0$. Consider the normal field $n = \frac{\nabla u}{|\nabla u|}$. Then:
 $B(u) = \operatorname{div}(\operatorname{div}(n)n) - \operatorname{div}((\nabla n)n) = 2 \sum_{1 \leq i,j \leq N} \left(\frac{\partial n_i}{\partial x_i} \frac{\partial n_i}{\partial x_j} - \frac{\partial n_j}{\partial x_i} \frac{\partial n_i}{\partial x_j} \right)$.
In particular, when $\mathbf{N} = \mathbf{2}$, $B(u) = 2 \operatorname{det}(\nabla n) = \mathbf{0}$ (because $||n|| = 1$).

What happens when the normal field n is less regular? Numerical simulations show that B(u) charges singular sets of n, more precisely:

- singular sets of dimension 0,
- but also sets of dimension > 0, however inconsistently (depends on the boundary configuration, on the regularization kernel, etc.)

Can we use the simpler term $det(\nabla n)$ in all dimensions to charge singular sets consistently?

No: Brézis-Coron-Lieb proved that the distributional Jacobian of $n \in W^{1,N-1}(\mathbb{R}^N, \mathbb{S}^{N-1})$ is a weighted sum of Dirac masses, i.e. charges only sets of dimension 0.

Can we design a more consistent term for charging the singular sets of n?

Remark: mean curvature flow with a forcing term

• Consider the Allen-Cahn equation with an additional forcing term

$$\partial_t u^{\varepsilon} = \Delta u^{\varepsilon} - \frac{G'(u^{\varepsilon})}{\varepsilon^2} (1 + f^{\sigma})$$

• The speed of the limit sharp interface is:

$$V = H + \frac{\nabla f^{\sigma} \cdot \mathbf{n}}{2(1+f^{\sigma})}$$

• Can we design f^{σ} to impose a distance δ between the interface and its skeleton to prevent topology changes?



Examples of sets and their skeletons

Skeleton = singular set of the signed distance function, i.e. where it is not differentiable.

Some sets...



and the support of their skeletons



Localization of the skeleton of a set E using a jump term

• A normal vector field associated with the signed distance function $dist(\cdot, E)$ is

$$n = \nabla \operatorname{dist}(\cdot, E)$$

• *n* satisfies ||n|| = 1 thus

$$\partial_n \|n\|^2 = 2(\nabla n \ n) \cdot n = 0,$$

where it is smooth.

• Let $k \in C_c^{\infty}(\Omega)$ denote a smooth kernel such that $\int_{\Omega} k = 1$, let $\sigma > 0$, $k^{\sigma} = \frac{1}{\sigma^N} k\left(\frac{\cdot}{\sigma}\right)$ and $n^{\sigma} = k^{\sigma} * n$

Define the (regularized) jump term Sn^{σ} of *n* as

$$Sn^{\sigma} = \langle n^{\sigma}, (\nabla n^{\sigma})n^{\sigma} \rangle = \sum_{1 \leq i,j \leq N} n_i^{\sigma} (\partial_j n_i^{\sigma})n_j^{\sigma}$$

• $\lim_{\sigma\to 0} Sn^{\sigma} \to 0$ where *n* is smooth. What happens when *n* is not smooth? Does $\lim_{\sigma\to 0} Sn^{\sigma}$ charge the singularities of *n*, i.e. the skeleton?

Limit of the regularized jump term

 $\mathrm{SBV} =$ space of special functions of bounded variation (e.g., the characteristic function of a set of finite perimeter)

Theorem

Let $n \in SBV(\mathbb{R}^N, S^{N-1})$ with C^1 discontinuity set Σ oriented by the unit normal vector ν . Then

$$Sn^{\sigma}
ightarrow rac{1}{12} |[n]|^2 \langle [n],
u
angle \, \mathcal{H}^{N-1} igsqcap \Sigma \qquad ext{ in } D'(\Omega) ext{ as } \sigma
ightarrow 0,$$
 (1)

where [n] denotes the jump of n.



Conjecture

The asymptotic analysis of various configurations leads to the conjecture:

$$Sn^{\sigma} \sim \sum_{j=0}^{N-1} \sigma^j \alpha_j \mathcal{H}_{|\Sigma_j}^{N-1-j}$$

where

- α_j are density functions;
- Σ_j are (N-1-j)-dimensional sets;
- the discontinuity set of *n* satisfies $\Sigma(n) = \bigcup_j \Sigma_j$

Allen-Cahn equation with topology penalization

• Consider the Allen-Cahn equation with an additional jump term :

$$\partial_t u^{\varepsilon} = \Delta u^{\varepsilon} - \frac{G'(u^{\varepsilon})}{\varepsilon^2} (1 + f_{u^{\varepsilon}}^{\sigma}),$$

where

$$f_{u^{arepsilon}}^{\sigma} = c(k^{\sigma} * |Sn_{u^{arepsilon}}^{\sigma}|), \quad ext{and} \quad n_{u^{arepsilon}}^{\sigma} = k^{\sigma} * rac{
abla u^{arepsilon}}{|
abla u^{arepsilon}|}.$$

• Numerical scheme: use a quasi-static approach. Define $u^{n+1} = v(\cdot, \delta t)$ with v a solution to

$$\begin{cases} \partial_t v = \Delta v - \frac{G'(v)}{\varepsilon^2} (1 + f_{u^n}^{\sigma}) \\ v(\cdot, 0) = u^n \end{cases}$$

Numerical experiments: the dumbbell

Without jump term:



With jump term:



Numerical experiments: the circle case

Numerical experiment:



Formal analysis of the velocity:

$$V = \frac{R}{\delta^2} \left(1 - \frac{1}{\sqrt{1 - \frac{\delta^2}{R^2}}} \right) n(s) \simeq -\frac{1}{2R} \left(1 + O\left(\frac{\delta^2}{R^2}\right) \right) n,$$

Numerical experiments: evolution of filaments

Case of one simple filament:

Case of two connected filaments:



 \Rightarrow Mean curvature flow of codimension 2?

Numerical experiments: evolution of a filament (1)



Evolution of a filament (2)



Evolution of a filament (3) using reduced constraints



Application to the Steiner's problem

Steiner's problem: find, for a given collection of points x_0, \dots, x_N , a compact connected set K containing all the x_i 's and having minimal length.





Some phase field models have been recently introduced to approximate solutions to Steiner's or Plateau's problems [Bonnivard-Lemenant-Santambrogio],[Chambolle-Ferrari-Merlet], [Bonafini-Orlandi-Oudet], [Bonnivard-Bretin-Lemenant]

Application to Steiner's problem

Let $K_{\sigma} = K \oplus B_{\sigma}$ be a σ -thickening of K.

• The length of K is approximated by the perimeter of K_{σ} :

 $Per(K_{\sigma}) \simeq 2\pi\sigma \mathcal{H}^{1}(K).$

• The property that K contains all points x_i is replaced by the inclusion constraint

 $\cup_{i=1}^{\mathsf{N}} B(x_i, \sigma) \subset K_{\sigma},$

• Consider the optimization problem:

min {Per(K_{σ}), K_{σ} connected, σ -thick, and $\cup_{i=1}^{N} B(x_i, \sigma) \subset K_{\sigma}$ }.

Application to Steiner's problem

- Use the phase field mean curvature flow with the self-avoiding term.
- Define

$$u_{in}^{\varepsilon}(x) = q\left(\frac{\operatorname{dist}(x,\cup_{i=1}^{N}\{x_i\}) - \sigma}{\varepsilon}\right),$$

where q is the classical profile associated to the double well G.

The inclusion constraint of all $x'_i s$ is easily obtained by considering the inequality constraint

$$u_{in}^{\varepsilon} \leq u.$$

Numerical Steiner set (1) : vertices of a cube



Numerical Steiner set (2) : 50 random points



Soap films: Plateau's problem



Application to Plateau's problem

• Use a $\sigma\text{-tubular}$ thickening of the boundary Γ

$$\Gamma_{\sigma} := \left\{ x, \mathsf{dist}(x, \Gamma) \leq \sigma \right\},\,$$

• Requires an additional volume penalization term.



• Consider the optimization problem:

 $\min\left\{\mathsf{Per}(\mathit{E}_{\sigma})+\frac{\mathsf{c}}{\sigma}\mathsf{Vol}(\mathit{E}_{\sigma}),\ \mathit{E}_{\sigma} \text{ connected, } \sigma\text{-thick, and } \Gamma_{\sigma}\subset \mathit{E}_{\sigma}\right\}.$

Numerical experiments: influence of the initial set



Case of non oriented surfaces and triple line junction



A hybrid minimal "surface"...



Conclusion

We introduced a reaction term which promotes topology conservation for phase field approximations of some geometric flows in various dimensions and codimensions.

This reaction term is introduced in the context of phase field approximation, but it can be easily extended to:

- Level set methods or volume graph methods involving the signed distance function;
- Recent methods for shape representation using a neural network which learns the signed distance function, see e.g. DeepSDF (Park et al'19).