# Diffusion redistanciation schemes, Willmore problem and red blood cells.

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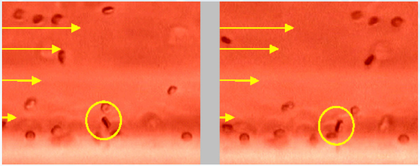
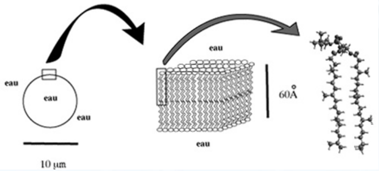
## Fluid-structure interaction in biomechanics

- **Phospholipidic vesicles: red blood cell model**

*Area change and bending energies, membrane shear (for real RBC)*






Behavior at equilibrium and under shear flow: tumbling, tank-treading. Chaouqi Misbah Team, LiPhy.

- **Willmore problem to model RBC shape:**

Find Γ, a curve (in 2D) or surface (3D) of fixed length or area, which encloses a given area (resp. volume) and minimizes the Willmore energy:

$$\inf_{\ell(\Gamma)=\ell_0,\mathcal{A}_e(\Gamma)=A_0} \int_\Gamma H^2 d\sigma$$

where $H$ is the (mean) curvature.

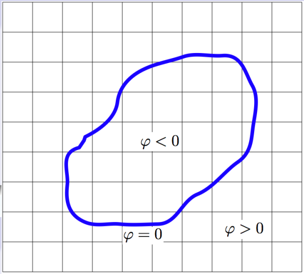
- **The dynamics coupling of RBC with an incompressible flow (plasma)**

# Level set method

## Level Set method (Osher-Sethian)

Let $\Gamma_0$, and $\varphi^0(x) = \epsilon(x)\,\mathrm{dist}(x, \Gamma^0)$ where $\epsilon = -1$ (resp. 1) if $x$ int. (resp. ext.).
To find $(x, t) \to \varphi(x, t)$ such that

$$\Gamma(t) = \{x \in \Omega, \varphi(x, t) = 0\}.$$

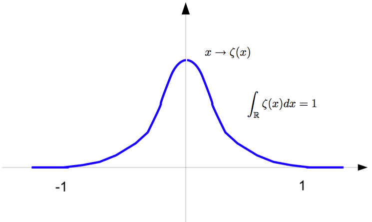



## Spreaded Dirac function

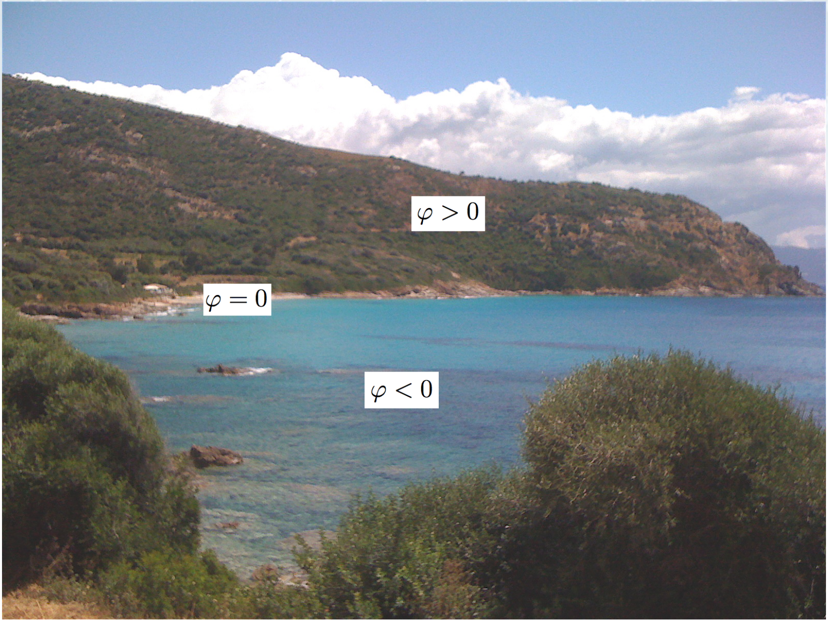
If $\zeta$ is a cut-off function, then under regularity assumptions on $\varphi$,

$$\frac{1}{\varepsilon}\zeta\left(\frac{\varphi}{\varepsilon}\right)|\nabla\varphi| \rightharpoonup \delta_{\{\varphi=0\}} \quad \text{in } \mathcal{M}(\Omega)$$

Warning: this is not scale-independent !



## An example of level-set function



# Some facts about Level Set framework (Osher, Sethian, Süssman and others)

## Geometry (regularity assumptions needed):

Normal $\mathbf{n} = \frac{\nabla\varphi}{|\nabla\varphi|}$, curvature $H = \mathrm{div}(\mathbf{n})$, enclosed area (resp. volume) $\mathcal{A}_e[\varphi] = \int_{\{\varphi<0\}} dx$ length (resp. area) $\ell[\varphi] = \int_{\{\varphi=0\}} d\sigma$, Willmore energy $\mathcal{W}[\varphi] = \frac{1}{2}\int_{\{\varphi=0\}} H^2 d\sigma$

## Derivatives of Enclosed area, Length and Willmore energy (the latter in 2D):

$$d\mathcal{A}_e[\varphi](\psi) = -\int_{\{\varphi=0\}} \psi|\nabla\varphi|^{-1} d\sigma, \quad d\ell[\varphi](\psi) = -\int_{\{\varphi=0\}} H\psi|\nabla\varphi|^{-1} d\sigma,$$

$$d\mathcal{W}[\varphi](\psi) = \int_{\{\varphi=0\}} \left(\Delta_{\{\varphi=0\}} H + \frac{1}{2}H^3\right)\psi d\sigma$$

## Kinematics:

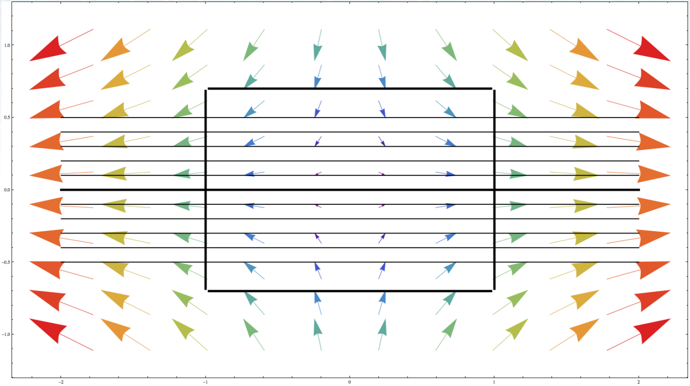
Moving with velocity $u$ is expressed as $\partial_t\varphi + u\cdot\nabla\varphi = 0$

## Divergence-free $u$

Area (3D) or length (2D) variations $= |\nabla\varphi|$ (Cottet-Maitre 06, generalization for compressible case Beale-Strain 07, Bresch et al 08)

# Area variation in the levet set context

Let $\varphi$ a function advected by the velocity field $u$, $\partial_t \varphi + u \cdot \nabla \varphi = 0$. If $u$ is incompressible then $|\nabla \varphi|$ captures the area variation

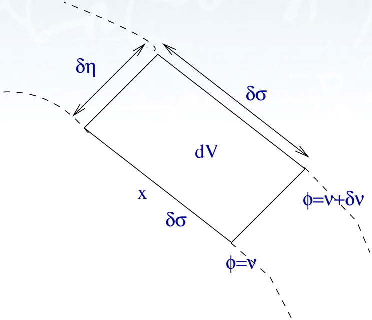


# Variations of area recorded in $|\nabla\varphi|$ ?

For a divergence free $u$: $dV = \delta\sigma\delta\eta$ with
$\delta\nu = \varphi(x + \delta\eta\frac{\nabla\varphi}{|\nabla\varphi|}) - \varphi(x) = \delta\eta|\nabla\varphi| + o(\delta\eta)$. Thus $\delta\nu = |\nabla\varphi|\delta\eta$ and

$$dV = |\nabla\varphi|^{-1}\delta\sigma\delta\nu$$

But $dV$ is conserved in the flow and $\delta\nu$ too ($\varphi$ is advected) thus $|\nabla\varphi|$ varies as $\delta\sigma$.



# Area change in level-set

- Let $(x,t) \to X(x,t)$ the forward characteristics of $u$, and $(x,t) \to Y(x,t)$ the backward ones, defined respectively by

$$\partial_t X = u(X,t),\ X(x,0) = x, \quad \text{and} \quad \partial_t Y + u \cdot \nabla Y = 0,\ Y(x,0) = x.$$

- Then $X(Y(x,t),t) = x$ and $Y(X(x,t),t) = x$. Let $J(x,t) = \det \nabla Y(x,t)$.
- There holds $\partial_t J + u \cdot \nabla J = -J \operatorname{div} u,\ J(x,0) = 1$. In incompressible case $J = 1$.

## Proposition

*Let $u : \mathbb{R}^d \times [0,T] \to \mathbb{R}^d$ of class $\mathcal{C}^1$ and $\varphi$ a $\mathcal{C}^1$ solution of $\partial_t \varphi + u \cdot \nabla \varphi = 0$, $\varphi = \varphi_0$ with $|\nabla \varphi| \geq \alpha > 0$ in a neighborhood of $\{\varphi = 0\}$. Then for all $f$ continuous with compact support,*

$$\int_{\{\varphi_0(\xi)=0\}} f(\xi) |\nabla \varphi_0|^{-1}(\xi) d\sigma(\xi) = \int_{\{\varphi(x,t)=0\}} f(Y(x,t)) J(x,t) |\nabla \varphi|^{-1}(x,t) d\sigma(x) \qquad (1)$$

*which means that $J^{-1}|\nabla\varphi|/|\nabla\varphi_0|$ records the area change of $\Gamma_t$ wrt $\Gamma_0$.*

*[Cottet-Maitre 06 for $J = 1$, Beale-Strain 07, Bresch et al 07]*

NB: in measure theory we would write $Y \# J |\nabla \varphi|^{-1} \delta_{\{\varphi=0\}} = |\nabla \varphi_0|^{-1} \delta_{\{\varphi_0=0\}}$.

# Defining energies

- Length penalizing and curvature energies

$$\mathcal{E}[\varphi] = \int_{\{\varphi=0\}} E(|\nabla\varphi|)\frac{1}{|\nabla\varphi|}d\sigma \quad \mathcal{G}[\varphi] = \int_{\{\varphi=0\}} G(H)d\sigma$$

where $E(r) = \frac{\lambda}{2}(r-1)^2$, $G(r) = \frac{\kappa}{2}r^2$ are usually chosen.

- Regularization by a cut-off $\zeta$:

$$\mathcal{E}_\varepsilon[\varphi] = \int_\Omega E(|\nabla\varphi|)\frac{1}{\varepsilon}\zeta\left(\frac{\varphi}{\varepsilon}\right)dx \quad \mathcal{G}_\varepsilon[\varphi] = \int_\Omega G(H)|\nabla\varphi|\frac{1}{\varepsilon}\zeta\left(\frac{\varphi}{\varepsilon}\right)dx$$

- Differentiating along $\partial_t\varphi + u\cdot\nabla\varphi = 0$ gives for $\mathcal{E}_\varepsilon$:

$$F_\varepsilon[\varphi] = \operatorname{div}\left(E'(|\nabla\varphi|)|\nabla\varphi|(\mathbb{I} - \frac{\nabla\varphi\otimes\nabla\varphi}{|\nabla\varphi|^2})\frac{1}{\varepsilon}\zeta\left(\frac{\varphi}{\varepsilon}\right)\right)$$

- Sharp interface: see T. Milcent Thesis.

## Complex fluid form

- The fluid-structure coupling then reads:

$$\begin{cases} \rho(\varphi)(\partial_t u + u\cdot\nabla u) - \operatorname{div}(\mu(\varphi)D(u) - E'(|\nabla\varphi|)|\nabla\varphi|\frac{\nabla\varphi\otimes\nabla\varphi}{|\nabla\varphi|^2}\frac{1}{\varepsilon}\zeta\left(\frac{\varphi}{\varepsilon}\right)) + \nabla\pi = 0 \\ \operatorname{div} u = 0 \\ \partial_t\varphi + u\cdot\nabla\varphi = 0 \end{cases}$$

which is a generalized Korteweg model (Sy et al 06). Regularization does not induce extra dissipation:

$$\frac{1}{2}\int_\Omega \rho_\varepsilon(\varphi(x,T))u^2(x,T)dx + \int_0^T\int_\Omega \mu(\varphi)D(u)^2 dxdt + \int_\Omega E(|\nabla\varphi|)\frac{1}{\varepsilon}\zeta(\frac{\varphi}{\varepsilon})dx$$
$$= \frac{1}{2}\int_\Omega \rho_\varepsilon(\varphi_0(x))u_0^2(x)dx + \int_\Omega E(|\nabla\varphi_0|)\frac{1}{\varepsilon}\zeta(\frac{\varphi_0}{\varepsilon})dx$$

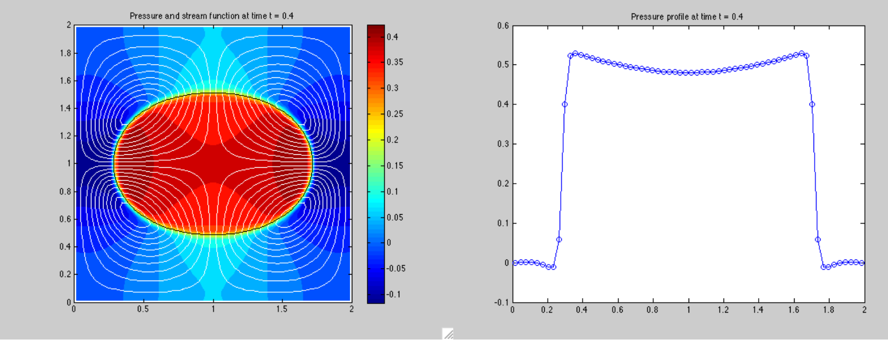
**Theorem (Cottet-Maitre-Milcent)**

*Let $\Omega$ be a open bounded connected and regular domain of $\mathbb{R}^3$. Let $p > 3$, and $\varphi_0 \in W^{2,p}(\Omega)$, such that $|\nabla\varphi_0| \geq \alpha > 0$ in a neighborhood of $\{\varphi_0 = 0\}$, and $u_0 \in W_0^{1,p}(\Omega)\bigcap W^{2,p}(\Omega)$, with* $\operatorname{div} u_0 = 0$. *Then $\exists T^*(u_0,\varphi_0,\varepsilon) > 0$ and $\varphi \in L^\infty(0,T^*;W^{2,p}(\Omega))$, $u \in L^\infty(0,T^*;W_0^{1,p}(\Omega)) \cap L^p(0,T^*;W^{2,p}(\Omega)), \nabla\pi \in L^p(0,T^*;L^p(\Omega))$ solution of the multiphysics problem.*

# Pros/Cons of this complex fluid formulation

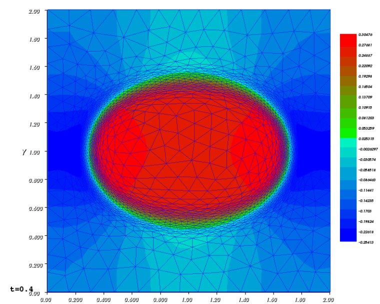
- Simple to implement starting from a fluid solver (projection method). See the software section of my homepage `http://ljk.imag.fr/membres/Emmanuel.Maitre` for an elementary yet functional Matlab/Octave implementation.

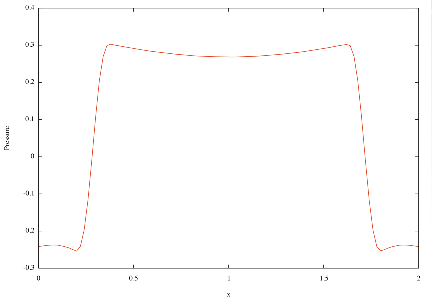
  *Use the Navier-Stokes solver of Benjamin Seibold (MIT), and WENO advection from Level-Set package of Baris Sumengen (included in the code so that it is standalone). Two versions: Diffusion is treated implicitly, with constant time-step and Choleski factorization, or diffusion is explicit with adaptive time-step.*



# Pros/Cons of this complex fluid formulation

- FreeFEM++ Code with adaptative mesh refinement.




- Fast method on fixed mesh with FFT.
- Dimension independent formulation.
- Stability issues (see below). Less accurate than BIM and ALE at a given number of DOF. Full membrane elasticity not recorded in $\varphi$.

## Origin of instabilitties

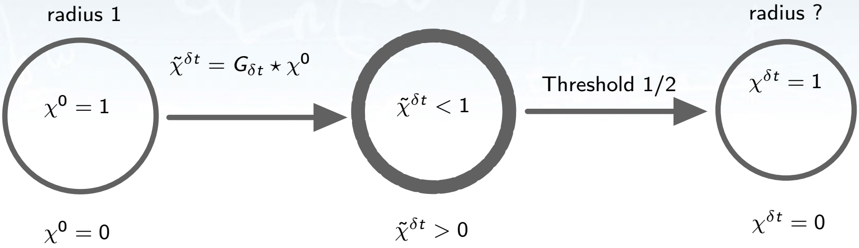
- High stiffness of interface (area conservation)
- High order on derivatives of $\varphi$ due to $\Delta_\Gamma H$.
- Idea: device a fast predictor motion following the Willmore flow and correct it to get the right area and enclosed volume.
- In a former study (Cottet-Maitre JCP'16) we used a predictor based on a rough linearization of the elastic force.
- Arnaud's work is about exploring potential of other schemes to approach geometric motions.

## Principles of diffusion-truncature schemes (Merriman-Bence-Osher JCP'94)

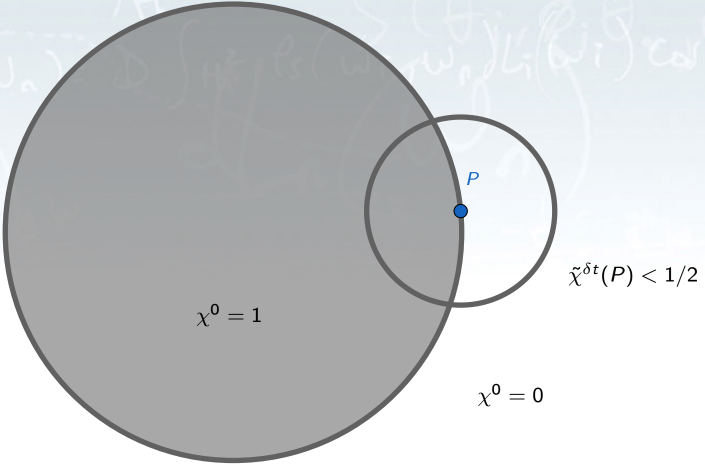
Aim: a fast algorithm to solve mean curvature flows. In level-set, that would need solving:

$$\partial_t \varphi = \operatorname{div} \frac{\nabla \varphi}{|\nabla \varphi|} |\nabla \varphi|$$

**Idea:** given a set and its charateristic function, apply a diffusion kernel for $\delta t$ and threshold at 1/2.



## Principles of diffusion-truncature schemes (Merriman-Bence-Osher JCP'94)

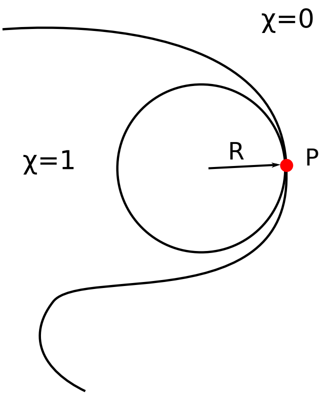


## Principles of diffusion-truncature schemes (Merriman-Bence-Osher JCP'94)

In cylindrical coordinates centered on the osculating circle at a point $P$, the heat equation can be written as

$$\partial_t \chi + \frac{1}{r}\partial_r \chi - \partial_{rr}\chi = 0$$

since $\theta$ derivatives are vanishing. This means that point $P$ will be moving at speed $\frac{1}{R}$ which is the curvature.




**Algorithm (Mean curvature flow)**

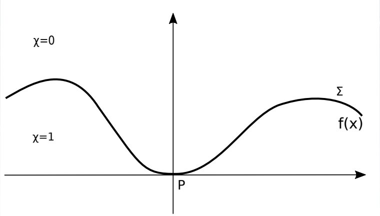
*Given the characteristic function $\chi^n$ of set at time step n:*

1) *Solve $\partial_t \chi - \Delta \chi = 0$ with initial condition $\chi(0) = \chi^n$ for $\delta t$.*
2) *Set $\chi^{n+1} = \mathbf{1}_{\{\chi(\delta t) > \frac{1}{2}\}}$.*

## Higher order motion (Esedoglu,Ruuth,Tsai '08 / Gzhibovskis, Heintz '08)

Later, expansion were computed:

- Locally the interface near a point $P$ can be considered as the graph of a function $f$.
- Without loss of generality one can consider that the origin is at point $P$ and the normal to interface is the $y$ axis.




The following expansion was obtain (in 2D, see second article for 3D):

$$G_{\delta t} \star \mathbf{1}_{\{y<f(x)\}}(0,y) = \frac{1}{2} - \frac{1}{2\sqrt{\pi}} y \delta t^{-\frac{1}{2}} + \frac{1}{2\sqrt{\pi}} H \delta t^{\frac{1}{2}} + \frac{1}{4\sqrt{\pi}} W \delta t^{\frac{3}{2}} + \mathcal{O}(\delta t^{\frac{5}{2}}).$$

where $H$ is the (mean in 3D) curvature, and $W$ is the Willmore term.
Theresholding at $\frac{1}{2}$, we see that interface $y = 0$ becomes

$$y = H\delta t + \frac{1}{2} W \delta t^2 + \mathcal{O}(\delta t^{\frac{3}{)}}.$$

## Higher order motion (Esedoglu,Ruuth,Tsai '08 / Gzhibovskis, Heintz '08)

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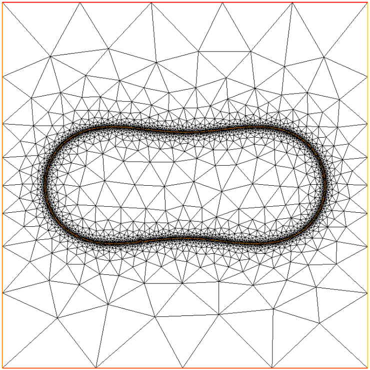
Theresholding at $\frac{1}{2}$, we see that interface $y = 0$ becomes

$$y = H\delta t + \frac{1}{2} W \delta t^2 + \mathcal{O}(\delta t^3).$$

Moreover, we see that if we combine two different time steps $\delta t_1$ and $\delta t_2$ we can get rid of lower order terms and obtain higher order geometric motion.

- We tried this for our RBC problem (thus with conserved enclosed area and fixed length), and succeeded in compute with FreeFEM++ the shape, but at the expense of a local adaptive remeshing.
- Indeed, with a coarse grid, the characteristic function is too rough to capture a descent interface, and the thresholdong scheme often does not move at all interface.



## Diffusion-redistancing schemes (Esodoglu,Ruuth,Tsai '10 in 2D)

The idea is to apply a diffusion step to a signed distance to an interface and look to which geometrical quantities we could access to. Then we could move the zero level set according to this geometric quantities and redistance the function. We have the following proposition :

### Proposition

*In 2D, we have the local expansion for the signed distance function near the interface :*

$$G_{\delta t} \star d^n = d^n + H\delta t + \frac{1}{2}\left[\Delta_\Sigma H + H^3\right]\delta t^2 + \mathcal{O}\left(\delta t^3\right) \tag{2}$$

*In 3D, we have the local expansion for the signed distance function near the interface :*

$$G_{\delta t} \star d^n = d^n + 2H\delta t + \left[\Delta_\Sigma H + 4H\left(H^2 - K\right)\right]\delta t^2 + \mathcal{O}(\delta t^3). \tag{3}$$

Sketch of calculation. Let $d$ solution of:

$$\begin{cases} \partial_t d(t,x) - \Delta d(t,x) = 0 \text{ in } \Omega \\ d(0,x) = d^n(x) \end{cases} \tag{4}$$

Then an expansion gives:

$$\begin{aligned} G_{\delta t} \star d^n = d(t+\delta t, x) &= d^n(x) + \delta t \partial_t d^n(x) + \frac{\delta t^2}{2}\partial_{tt} d^n(x) + \mathcal{O}(\delta t^3) \\ &= d^n(x) + \delta t \Delta d^n(x) + \frac{\delta t^2}{2}\Delta^2 d^n(x) + \mathcal{O}(\delta t^3) \end{aligned} \tag{5}$$

We shall now express the terms $\Delta d$ and $\Delta^2 d$ in geometric quantities involving the mean curvature and the gaussian curvature.

## Diffusion-redistancing schemes: algorithm

A classical result give in $\mathbb{R}^N$ (see Gilbarg-Trudinger):

$$(N-1)\Delta d = H$$

and a more involved calculation produces:

$$\text{3D: } \Delta^2 d = 2\Delta_\Gamma H + 8H(H^2 - K) \qquad \text{2D: } \Delta^2 d = \Delta_\Gamma H + H^3$$

This gives the following algorithm for Willmore flow:

**Algorithm (Willmore flow in 2D)**

*Given the signed distance function $d^n$ of interface at time step $n$:*

1) *Compute $G_{\sqrt{\delta t}} \star d^n$ and $G_{\sqrt{2\delta t}} \star d^n$ (two heat equations)*
2) *Compute $A = 2G_{\sqrt{\delta t}} \star d^n - G_{\sqrt{2\delta t}} \star d^n$ and $B = (G_{\sqrt{\delta t}} \star d^n - d^n)^3$.*
3) *Set $d^{n+1} = \mathrm{redist}(A + \frac{B}{2})$ (using redistancing scheme of Dapogny&Frey)*

Problem: what about length and enclosed area constraints ?

## Diffusion-redistancing schemes: constraints

Let us write the full Lagrangian corresponding to our Willmore optimisation problem:

$$L(\varphi, \lambda, \mu) = \frac{1}{2}\int_{\{\varphi=0\}} H^2 d\sigma + \lambda\left(\int_{\{\varphi=0\}} d\sigma - \ell_0\right) + \mu\left(\int_{\{\varphi<0\}} dx - A_0\right)$$

Differentiating wrt $\varphi$ gives:

$$dL(\varphi, \lambda, \mu)(\psi) = \int_{\{\varphi=0\}} \left(\Delta_{\{\varphi=0\}} H + \frac{1}{2}H^3\right) \psi d\sigma - \lambda \int_{\{\varphi=0\}} H\psi d\sigma - \mu \int_{\{\varphi=0\}} \psi d\sigma$$

- We know already how to find the right gradient direction $\Delta_{\{\varphi=0\}} H + \frac{1}{2}H^3$ thank to our diffusion-redistancing scheme.
- We have to correct this direction by adding something like $\lambda H + \mu$, where normally $\lambda$ and $\mu$ depend on the unknown $\varphi$ in a non linear way.
- Instead, we act as follows: we first move the distance function along the gradient to get a $\hat{d}$, and then compute $\lambda, \mu$ so that $\hat{d} + \lambda H + \mu$ fulfills the contraints.
- This can be done analytically. We found

$$\mu = \frac{A_0 - A_e(\hat{d})}{\ell(\hat{d})}, \qquad \lambda = \frac{\ell_0 - \ell(\hat{d})}{\int_{\{\varphi=0\}} (H - \bar{H}^2)^2 d\sigma}$$

# Numerical example using FEEL++ (A. Sengers)