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Shape derivative of the Willmore functional and applications to equilibrium shapes of vesicles

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Abstract: The vesicles constitute a simplified biological model to describe the mechanical behavior of red blood cells. The equilibrium shapes of these vesicles are driven by the bending energy which is given by the Willmore functional. We present a method to compute the shape derivative of the Willmore functional in the level set framework. The equivalence with the method originally introduced by Willmore, where the surface is represented by a parametrization, is established. Finally, some numerical simulations of the relaxation of vesicles towards their equilibrium shapes in three dimensions are presented.

Key-words: Shape optimization, fluid-structure interaction, eulerian, level set, finite differences

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Dérivée de forme de la fonctionnelle de Willmore et applications aux formes d'équilibre des vésicules

Résumé : Les vésicules constituent un modèle biologique simplifié pour la description du comportement mécanique des globules rouges. Les formes d'équilibre de ces vésicules sont pilotées par l'énergie de flexion qui est donnée par la fonctionnelle de Willmore. Nous présentons une méthode pour calculer la dérivée de forme de la fonctionnelle de Willmore avec l'approche level set. Nous montrons l'équivalence avec la méthode initialement introduite par Willmore où la surface est représentée à l'aide d'une paramétrisation. Enfin, quelques simulations numériques de la relaxation de vésicules vers leur formes d'equilibre en trois dimensions sont présentées.

Mots-clés : Optimisation de formes, interaction fluide-structure, eulerien, "level set", differences finies

Introduction

Understanding the blood rheology is a major issue for biomedical applications. We can cite, for example, the prediction of vascular pathologies. The blood is mainly composed of red blood cells, which are responsible of the non Newtonian behavior of the flow. These cells have complex membranes, which are constituted of phospholipids and sprinkled over with proteins. The modelling of both biological and mechanical properties of such cells is then difficult to handle. The vesicles in suspension are composed of a phospholipidic membrane with elastic properties. They constitute a simplified biological model to describe the mechanical behavior of red blood cells *in vitro* .

The strong interaction between the elastic membrane and the fluid leads to a coupled fluid-structure problem. A convenient way to tackle this kind of problem is to use the immersed boundary method introduced by Peskin [22]. The main idea is to describe the fluid-structure medium with an unique continuous velocity. This method involves both Eulerian and Lagrangian variables coupled through Dirac mass. The elastic forces are treated as a source term in the fluid equations. The Lagrangian treatment of the elasticity leads to some drawbacks on the numerical point of view as for instance the treatment of large deformations and the loss of mass. More recently, Cottet and Maitre have introduced in [7, 8] a full Eulerian formulation of the fluid-structure interaction for membranes. The interface is tracked implicitly with a level set function ϕ which does also capture the change of area through $|\nabla\phi|$. This formulation allows to overcome the difficulties inherent to the immersed boundary method.

The membrane of the vesicle responds mechanically only to the change of area and bending. The vesicle is constituted of a fixed amount of molecules so the membrane is nearly inextensible. As a result, the main mode of deformation of the vesicle is bending.

For this reason, we focus in this paper on the derivation of the bending force and its application to the shape equilibrium of vesicles. The bending energy is generally given by the Willmore functional [17, 4, 19]

$$J(\Gamma) = \int_\Gamma H(\Gamma)^2 \, \mathrm{d}s.$$

Here H is the mean curvature of the surface Γ. The Willmore energy has an interesting geometrical interpretation: it captures the deviation of a surface from its local sphericity. Let κ_1,κ_2 be the principal curvatures and $H = \kappa_1 + \kappa_2$, $G = \kappa_1\kappa_2$ denote the respective mean and Gaussian curvatures related by $H^2 - 4G = (\kappa_1 - \kappa_2)^2$. The Gauss-Bonnet theorem ensure that the Gaussian curvature is a topological invariant *ie* $\int_\Gamma G \, \mathrm{d}s$ is constant for a closed surface. Therefore, up to an additive constant, the Willmore energy writes $\int_\Gamma (\kappa_1 - \kappa_2)^2 \, \mathrm{d}s$. As a result, this energy vanishes when $\kappa_1 = \kappa_2$ and captures the deviation of a surface from a sphere. In order to take the bending energy into account, the force linked to the Willmore energy has to be computed. Following the virtual work principle, this force is related to the variation of the functional $J(\Gamma)$. Since Γ is a surface, the problem is recasted as finding the shape derivative of the Willmore functional $J'(\Gamma)$. Two different methods have been

developed for this problem in the literature. While the first one is based on a explicit representation of the surface with a parametrization [28], the second one is based on an implicit representation of the surface with a level set function [20].

In the first method, the surface is represented by a parametrization $\mathbf{X}$ and the Willmore functional is denoted by $\mathbb{J}(\mathbf{X})$. In order to perform the shape derivative, a deformation in the normal direction is introduced. Using differential calculus, $\mathbb{J}'$ writes [28]

$$\mathbb{J}'(\mathbf{X})(\delta) = -\int_\Gamma \Big(2\Delta_\Gamma H + H(H^2 - 4G)\Big)\delta \, \mathrm{d}s, \tag{1}$$

where Δ_Γ is the Laplace-Beltrami operator on the surface Γ. This method is natural since it only involves quantities defined on the surface. This result can be used in the framework of the immersed boundary method since the surface and terms appearing in (1) can be computed with a parametrization. However, when the surface is described by a level set function, a parametrization is not known.

In the second method, the surface is represented by the zero level set of a function ϕ and the Willmore energy is written $\mathcal{J}(\phi) = \displaystyle\int_{\{\phi=0\}} H(\phi)^2 \, \mathrm{d}s$. The derivative with respect to ϕ is tough to handle since the domain of integration depends itself on ϕ. To overcome this difficulty a volumic approximation of $\mathcal{J}(\phi)$ is introduced and the result is the following [20]

$$\mathcal{J}'(\phi)(\delta) = \int_{\{\phi=0\}} \frac{1}{|\nabla\phi|} \operatorname{div}\left(-H(\phi)^2\frac{\nabla\phi}{|\nabla\phi|} + \frac{2}{|\nabla\phi|}\mathbb{P}_{\nabla\phi^\perp}(\nabla(|\nabla\phi|H(\phi)))\right)\delta \, \mathrm{d}s, \tag{2}$$

where $\mathbb{P}_{\nabla\phi^\perp}$ is the projector on the plane which is orthogonal to $\nabla\phi$. This result can be used in an Eulerian framework since it only involves quantities depending on the level set function ϕ.

The main goal of the paper is to investigate the equivalence of the shape derivatives (1) and (2). This is not straightforward since the two results use different representations of a surface and different differential operators. Moreover, the formula (2) depends *a priori* on ϕ outside the surface $\{\phi = 0\}$ through $|\nabla\phi|$, while (1) depends on both curvature and Laplace-Beltrami operator, which are independent of the parametrization. The equivalence of the approaches will prove that $\mathcal{J}'(\phi)$ is in fact independent of the choice of ϕ outside $\{\phi = 0\}$. Moreover, writing (2) under the form (1) is also relevant for numerical purpose. Indeed, we can focus separately on the approximation of the curvature and the Laplace-Beltrami operator.

The second goal of the paper is to use the formula (1) in the level set framework to study the relaxation of vesicles towards their equilibrium shapes. These shapes can be determined by minimizing the bending energy with two constraints: fixed area (inextensible membrane) and fixed volume (incompressible fluid). The numerical methods used to solve this problem in the literature rely on the finite elements method on surfaces [3, 2] and the phase field methods

[23, 24]. It is worth mentioning the related works [12, 11, 13], which focus on the minimization of the bending energy without constraints. Our approach is to consider an Eulerian model where an elastic membrane is immersed in a incompressible viscous fluid. Taking the hydrodynamics into account is necessary in order to be able to study the dynamics of these vesicles in a flowing fluid. The volume of the vesicle is naturally constraint with the incompressibility of the fluid while the area of the vesicle is constraint with a stiff elastic coefficient. We obtain various equilibrium shapes in three dimensions depending on a volume ratio, which qualitatively agrees with the literature.

The paper is organized as follow. The first section is devoted to the introduction of the tools of differential geometry. The second section deals with the shape derivative of the Willmore energy in the level set framework. The third section is devoted to numerical simulations of equilibrium shapes of vesicles in three dimensions. A simple proof of the Stokes formula for surfaces as well as a different shape derivative method for the Willmore functional will be presented in the Appendix.

1 Preliminaries

The vectors and the matrices will be written in the canonical orthonormal basis of $\mathbb{R}^3$. Let $\mathbf{a}$,$\mathbf{b}$ be two vectors of $\mathbb{R}^3$. We denote by $\mathbf{a}\cdot\mathbf{b} = \sum_i a_i b_i$ the Euclidean scalar product, $|\mathbf{a}|$ the associated norm and $[\mathbf{a}\otimes\mathbf{b}]_{ij} = a_i b_j$ the outer product. Let A be a matrix of $M_3(\mathbb{R})$. We denote by $\mathrm{Tr}(A)$, $\det(A)$ the usual trace and determinant. We denote also by $\mathrm{Tr}(\mathrm{Cof}(A)) = \frac{1}{2}(\mathrm{Tr}(A)^2 - \mathrm{Tr}(A^2))$ the trace of the comatrix. We denote by ∇, div and Δ the usual Euclidean gradient, divergence and Laplace operators, respectively.

1.1 Level set method

Throughout the paper, Γ denotes a smooth connected, oriented and closed surface of $\mathbb{R}^3$. This surface is represented implicitly as the zero level set [21, 25] of a smooth scalar function ϕ

$$\Gamma = \{x \in \mathbb{R}^3 \ / \ \phi(x) = 0\}.$$

Assume that $|\nabla\phi| > 0$ in a neighborhood $\mathcal{V}$ of $\{\phi = 0\}$. The unitary normal is then well defined on $\mathcal{V}$ and given by

$$\mathbf{n}(\phi) = \frac{\nabla\phi}{|\nabla\phi|}. \tag{3}$$

The dependence on ϕ will be dropped in the next sections of the paper. We denote by $\mathcal{U}$ the domain enclosed by the surface Γ. We choose the convention that $\phi < 0$ in $\mathcal{U}$ and $\phi > 0$ outside $\mathcal{U}$ so that $\mathbf{n}$ is the outward normal. The gradient of the relation $|\mathbf{n}|^2 = 1$ writes

$$[\nabla\mathbf{n}]^T\mathbf{n} = 0, \qquad ([\nabla\mathbf{n}]\mathbf{n})\cdot\mathbf{n} = 0. \tag{4}$$

1.2 Tangential operators

It is natural to define differential operators on surfaces to study the variation of scalar and vector fields on Γ. When Γ is represented explicitly by a parametrization, these differential operators are naturally defined with the metric induced by the parametrization [5, 6, 14]. In the case of an implicit representation of Γ with a level set function, the scalar and vector fields are extended to a neighborhood $\mathcal{V}$ of Γ. The differential operators on surfaces named tangential operators are then defined as the projection on the tangent plane of the classical Euclidean differential operators [18, 1, 26, 9, 15]. Let f and $\mathbf{v}$ be smooth scalar and vector fields defined in $\mathcal{V} \subset \mathbb{R}^3$. Then, the tangential operators are defined by

$$\begin{aligned}
\nabla_\Gamma f &= \nabla f - (\nabla f \cdot \mathbf{n})\mathbf{n}, \\
\nabla_\Gamma \mathbf{v} &= \nabla \mathbf{v} - [\nabla \mathbf{v}](\mathbf{n} \otimes \mathbf{n}), \\
\operatorname{div}_\Gamma(\mathbf{v}) &= \operatorname{Tr}(\nabla_\Gamma \mathbf{v}) = \operatorname{div}(\mathbf{v}) - ([\nabla \mathbf{v}]\mathbf{n}) \cdot \mathbf{n}, \\
\Delta_\Gamma f &= \operatorname{div}_\Gamma(\nabla_\Gamma f).
\end{aligned}$$

These definitions are independent of the extension of the quantities outside the surface Γ since the usual differential operators are projected on the tangent plane of Γ. The following identities hold

$$\nabla_\Gamma \phi = 0, \tag{5}$$
$$\nabla_\Gamma f \cdot \mathbf{n} = 0, \tag{6}$$
$$\operatorname{div}_\Gamma(f\mathbf{v}) = f \operatorname{div}_\Gamma(\mathbf{v}) + \nabla_\Gamma f \cdot \mathbf{v}, \tag{7}$$
$$\nabla_\Gamma f \cdot \nabla g = \nabla f \cdot \nabla_\Gamma g = \nabla_\Gamma f \cdot \nabla_\Gamma g, \tag{8}$$
$$[\nabla n]\, n = \frac{\nabla_\Gamma |\nabla \phi|}{|\nabla \phi|}. \tag{9}$$

These properties are simple consequences of the definitions of the tangential operators and (3). We have also the relations

$$([\nabla (\nabla_\Gamma f)]\mathbf{n}) \cdot \mathbf{n} = -\nabla f \cdot ([\nabla \mathbf{n}]\mathbf{n}), \tag{10}$$
$$([\nabla ([\nabla n]\, n)]\mathbf{n}) \cdot \mathbf{n} = -([\nabla n]\, n) \cdot ([\nabla n]\, n). \tag{11}$$

Taking gradient of equality (6) and multiplying by $\mathbf{n}$ leads to (10). Taking the gradient of (4) and multiply the result by $\mathbf{n}$ gives (11).

Let f, g be two smooth functions and $\mathbf{v}$ a smooth vector field. Let Q a smooth open set of $\mathbb{R}^3$ and ∂Q its boundary (which is a closed surface of $\mathbb{R}^3$). For the classical Euclidean operators, the Stokes formula for volumes writes

$$\int_Q \operatorname{div}(\mathbf{v}) f \, \mathrm{d}x = -\int_Q \mathbf{v} \cdot \nabla f \, \mathrm{d}x + \int_{\partial Q} f \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}s. \tag{12}$$

For tangential operators, we have the following Stokes formula for closed surfaces

$$\int_\Gamma \operatorname{div}_\Gamma(\mathbf{v}) f \, \mathrm{d}s = -\int_\Gamma \mathbf{v} \cdot \nabla_\Gamma f \, \mathrm{d}s + \int_\Gamma H f \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}s. \tag{13}$$

Note that there is an extra term depending on the mean curvature H if $\mathbf{v}$ has a component in the normal direction. We provide a new simple proof of this formula in the Appendix 1. Taking $\mathbf{v} = \nabla_\Gamma g$ in this formula and using (5) we get

$$\int_\Gamma f \Delta_\Gamma g \, \mathrm{d}s = \int_\Gamma g \Delta_\Gamma f \, \mathrm{d}s. \tag{14}$$

1.3 Curvature

Intuitively, the curvature represents the amount by which a surface deviates from being a plane. Let us introduce the tensor $[\nabla_\Gamma \mathbf{n}]$, the so called extended Wirtinger map [15]. This tensor has the eigenvector $\mathbf{n}$ associated to the eigenvalue 0 since $[\nabla_\Gamma \mathbf{n}]\mathbf{n} = 0$. The remaining eigenvalues are the principal curvatures denoted by κ_1 and κ_2. The mean and Gaussian curvatures are then defined by

$$H = \kappa_1 + \kappa_2 = \mathrm{Tr}([\nabla_\Gamma \mathbf{n}]) = \mathrm{div}_\Gamma(\mathbf{n}), \qquad G = \kappa_1 \kappa_2 = \mathrm{Tr}(\mathrm{Cof}([\nabla_\Gamma \mathbf{n}])). \tag{15}$$

Since $\mathbf{n}$ is extended by (3), we obtain with (4)

$$H = \mathrm{Tr}([\nabla \mathbf{n}]) = \mathrm{div}(\mathbf{n}), \qquad G = \mathrm{Tr}(\mathrm{Cof}([\nabla \mathbf{n}])). \tag{16}$$

The identity $\mathrm{Tr}([\nabla \mathbf{n}]^2) = \kappa_1^2 + \kappa_2^2 = H^2 - 2G$ and (16) prove the following relation

$$\mathrm{div}([\nabla n] \, n) = \nabla H \cdot \mathbf{n} + H^2 - 2G. \tag{17}$$

2 Shape derivative of the Willmore functional

The aim of this section is to compute the shape derivative of the Willmore functional

$$J(\Gamma) = \int_\Gamma H(\Gamma)^2 \, \mathrm{d}s.$$

The original method of Willmore where the surface is represented by a parametrization is presented in section 2.1. The section 2.2 deals with the shape derivative of a general functional in the level set framework with the volumic approach. In the section 2.3, this method is applied for the Willmore functional and the equivalence of the level set and the parametric approaches is proved.

2.1 Shape optimization with a parametrization

In the method described in [28], the surface is parametrized locally by $\mathbf{X} : U \longrightarrow \mathbb{R}^3$ with parameter domain $U \subset \mathbb{R}^2$. We denote by $g_{ij} = \mathbf{X}_{,i} \cdot \mathbf{X}_{,j}$ the coefficients of the first fundamental form, g its determinant and g^{ij} the coefficients of its inverse. The normal is defined by $\mathbf{n} = \dfrac{\mathbf{X}_{,1} \wedge \mathbf{X}_{,2}}{|\mathbf{X}_{,1} \wedge \mathbf{X}_{,2}|}$ and the second fundamental

form by $h_{ij} = \mathbf{X}_{,ij} \cdot \mathbf{n}$. The mean curvature is then given by $H = -\sum_{i,j} g^{ij} h_{ij}$. The Willmore energy is then

$$\mathbb{J}(\mathbf{X}) = \int_U (H(u_1,u_2))^2 \sqrt{g(u_1,u_2)}\, \mathrm{d}u_1 \mathrm{d}u_2.$$

In order to perform the shape derivative, a deformation in the normal direction is introduced with the associate parametrization $\mathbf{X}(t) = \mathbf{X} + t\delta\mathbf{n}$ where δ is a scalar function. This choice is justified by the fact that a deformation in the tangential direction has no influence on the shape derivative. The resulting sequence of perturbed surfaces is denoted by $(\Gamma_t)_{t>0}$ where $\Gamma_0 = \Gamma$. Using differential calculus $\mathbb{J}'$ writes [28]

$$\mathbb{J}'(\mathbf{X})(\delta) := \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \mathbb{J}(\mathbf{X} + t\delta\mathbf{n}) = -\int_\Gamma \Big(2\Delta_\Gamma H + H(H^2 - 4G)\Big)\delta \,\mathrm{d}s, \qquad (18)$$

where $\Delta_\Gamma H = \dfrac{1}{\sqrt{g}} \sum_{i,j} (\sqrt{g} g^{ij} H_{,j})_{,i}$ is the Laplace Beltrami operator on the surface Γ. This operator and the curvature involved in (18) can be computed with a parametrization of the surface. However, this formula cannot be used directly in a level set framework since a parametrization is not known.

2.2 Shape optimization in the level set framework

In an Eulerian framework, the surface Γ is represented implicitly as the zero level set of a function ϕ. We consider the generalized functional

$$\mathcal{I}(\phi) = \int_{\{\phi=0\}} f[\phi] \,\mathrm{d}s, \qquad (19)$$

where $f[\phi]$ denotes a function depending on the spatial derivatives of ϕ. For instance, in the case of the Willmore functional we have $f[\phi] = \mathrm{div}\left(\dfrac{\nabla\phi}{|\nabla\phi|}\right)^2$. To perform the shape derivative, we deform the surface assuming that ϕ satisfies the transport equation

$$\phi_t + \mathbf{u} \cdot \nabla\phi = 0, \qquad (20)$$

where $\mathbf{u}$ is a vector field. We denote then $\Gamma_t = \{x \in \mathbb{R}^3 \ / \ \phi(x,t) = 0\}$ and $\Gamma_0 = \Gamma$. The shape derivative is then given by $\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \mathcal{I}(\phi)$ denoted by $(\mathcal{I}(\phi))_t$. The major difficulty to compute $(\mathcal{I}(\phi))_t$ relies in the fact that the domain of integration is a surface which depends on time. To overcome this difficulty, an idea introduced in [8] is to approximate the surface integral on a fixed domain of $\mathbb{R}^3$ with the following lemma.

Lemma: Let be ζ a smooth positive cut-off function with support in $[-1,1]$ and $\int_{\mathbb{R}} \zeta = 1$. Assume that ϕ is a smooth function with $|\nabla\phi| > 0$ in a neighborhood of $\{\phi = 0\}$. Let Q be a an open set of $\mathbb{R}^3$ such that $\{x \in \mathbb{R}^3 / \phi(x) \leq 1\} \subset Q$,

$0 < \varepsilon < 1$ and $f[\phi]$ a smooth scalar function which depends on ϕ and its derivatives. Then

$$\mathcal{I}_\varepsilon(\phi) := \int_Q f[\phi]|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\,\mathrm{d}x \underset{\varepsilon\longrightarrow 0}{\longrightarrow} \int_{\{\phi=0\}} f[\phi]\,\mathrm{d}s. \tag{21}$$

A proof of this lemma involves the co-area formula and is given in [8]. We now use this lemma to give a simple proof of the shape derivative $(\mathcal{I}(\phi))_t$.

The derivative of $\mathcal{I}_\varepsilon(\phi)$ with respect to t gives three terms

$$(\mathcal{I}_\varepsilon(\phi))_t = \int_Q (f[\phi])_t\,|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\,\mathrm{d}x + \int_Q f[\phi]\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\frac{\nabla\phi}{|\nabla\phi|}\cdot\nabla\phi_t\,\mathrm{d}x + \int_Q f[\phi]|\nabla\phi|\frac{1}{\varepsilon^2}\zeta'\left(\frac{\phi}{\varepsilon}\right)\,\phi_t\,\mathrm{d}x. \quad (*)$$

The Stokes formula for volumes (12) gives

$$\int_Q f[\phi]\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\frac{\nabla\phi}{|\nabla\phi|}\cdot\nabla\phi_t\,\mathrm{d}x = -\int_Q \mathrm{div}\left(f[\phi]\frac{\nabla\phi}{|\nabla\phi|}\right)\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\phi_t\,\mathrm{d}x - \int_Q f[\phi]\frac{\nabla\phi}{|\nabla\phi|}\cdot\nabla\phi\,\frac{1}{\varepsilon^2}\zeta'\left(\frac{\phi}{\varepsilon}\right)\phi_t\,\mathrm{d}x, \quad (**)$$

since the term on ∂Q vanishes. Indeed, we have $\zeta\left(\frac{\phi}{\varepsilon}\right) = 0$ for $|\phi| > \varepsilon$ because the support of ζ is in $[-1,1]$. As $\{x\in\mathbb{R}^3/\phi(x)\le 1\}\subset Q$ and $\varepsilon<1$ we get $\zeta\left(\frac{\phi}{\varepsilon}\right) = 0$ on ∂Q. Therefore, inserting $(**)$ in $(*)$ and using the transport equation (20) leads to

$$(\mathcal{I}_\varepsilon(\phi))_t = \int_Q \Big((f[\phi])_t + \mathrm{div}\,(f[\phi]\mathbf{n})\,u\cdot n\Big)|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\,\mathrm{d}x. \tag{22}$$

Note that $u\cdot n$ appears in (29). Hence, the tangential component of $\mathbf{u}$ has no influence in the shape derivative.

The following section is devoted to the computation of the shape derivative of the Willmore functional with the volumic approach. We introduce the scalar function $A:\mathbb{R}\longrightarrow\mathbb{R}$ and the generalized Willmore functional[1]

$$\mathcal{J}(\phi) = \int_{\{\phi=0\}} A(H(\phi))\,\mathrm{d}s. \tag{23}$$

2.3 Shape derivative with a volumic approximation

We consider the volumic approximation (21) of the Willmore functional (23)

$$\mathcal{J}_\varepsilon(\phi) = \int_Q A(H(\phi))|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\,\mathrm{d}x.$$

[1] The choice $A(r) = (r-c_0)^2$ is widely used in the applications (c_0 is the spontaneous curvature).

We apply the general volumic approximation formula (22) with $f = A(H)$ to obtain

$$(\mathcal{J}_\varepsilon(\phi))_t = \int_Q \Big(A'(H)H_t + \operatorname{div}\left(A(H)\mathbf{n}\right) u\cdot n\Big)|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\,\mathrm{d}x.$$

As the mean curvature depends on the variation of the normal, we start by computing the derivative of the normal. We get from (20) and (9)

$$\mathbf{n}_t = \left(\frac{\nabla\phi}{|\nabla\phi|}\right)_t = \frac{\nabla_\Gamma\phi_t}{|\nabla\phi|} = -\nabla_\Gamma(u\cdot n) - ([\nabla n]\,n)u\cdot n. \tag{24}$$

As before there will be no contribution on ∂Q in the Stokes formula for volumes since $\zeta\left(\frac{\phi}{\varepsilon}\right) = 0$ on ∂Q.

We obtain with the derivative of the normal (24)

$$(\mathcal{J}_\varepsilon(\phi))_t = \int_Q \left(A'(H)\operatorname{div}\left(\frac{\nabla_\Gamma\phi_t}{|\nabla\phi|}\right) + \operatorname{div}\left(A(H)\mathbf{n}\right) u\cdot n\right)|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\,\mathrm{d}x. \tag{25}$$

The first term denoted by $(\mathcal{J}_{1,\varepsilon}(\phi))_t$. The Stokes formula for volumes (12) and the symmetry relation (8) are used to obtain

$$\begin{aligned}(\mathcal{J}_{1,\varepsilon}(\phi))_t &= -\int_Q \frac{\nabla_\Gamma\phi_t}{|\nabla\phi|}\cdot\nabla\left(A'(H)|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\right)\,\mathrm{d}x\\ &= -\int_Q \frac{\nabla\phi_t}{|\nabla\phi|}\cdot\nabla_\Gamma\left(A'(H)|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\right)\,\mathrm{d}x.\end{aligned}$$

Using (5), we have the relation $\nabla_\Gamma\left(\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\right) = \frac{1}{\varepsilon^2}\zeta'\left(\frac{\phi}{\varepsilon}\right)\nabla_\Gamma\phi = 0$. This property is used to develop the term involving ∇_Γ and a Stokes formula for volumes gives

$$\begin{aligned}(\mathcal{J}_{1,\varepsilon}(\phi))_t &= -\int_Q \frac{\nabla\phi_t}{|\nabla\phi|}\cdot\nabla_\Gamma\left(A'(H)|\nabla\phi|\right)\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\,\mathrm{d}x\\ &= \int_Q \operatorname{div}\left(\frac{1}{|\nabla\phi|}\nabla_\Gamma\left(A'(H)|\nabla\phi|\right)\right)\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\Big)\,\phi_t\,\mathrm{d}x.\end{aligned}$$

With the relation (6), we get

$$\nabla_\Gamma(A'(H)|\nabla\phi|)\cdot\nabla\left(\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\right) = \frac{1}{\varepsilon^2}\zeta'\left(\frac{\phi}{\varepsilon}\right)|\nabla\phi|\nabla_\Gamma(A'(H)|\nabla\phi|)\cdot\mathbf{n} = 0.$$

We use this property to develop the divergence term. Since $\phi_t = -|\nabla\phi|u\cdot n$ with the transport equation (20), we get

$$(\mathcal{J}_\varepsilon(\phi))_t = \int_Q \operatorname{div}\left(A(H)\mathbf{n} - \frac{1}{|\nabla\phi|}\nabla_\Gamma\left(A'(H)|\nabla\phi|\right)\right)u\cdot n|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\,\mathrm{d}x.$$

At this point we find the result (2) when ε goes to 0 with (21) and $\delta = -|\nabla\phi|u\cdot n$. This formula has the drawback to depend on ϕ outside $\{\phi = 0\}$. We go further to obtain a more intrinsic result depending only on curvature and tangential operators. Following (9) we get

$$\mathrm{div}\left(\frac{1}{|\nabla\phi|}\nabla_\Gamma(A'(H)|\nabla\phi|)\right) = \mathrm{div}(A'(H)[\nabla n]\ n) + \mathrm{div}(\nabla_\Gamma(A'(H))).$$

For the first term we use (17)

$$\mathrm{div}(A'(H)[\nabla n]\ n) = A'(H)\ (\nabla H\cdot\mathbf{n} + H^2 - 2G) + \nabla(A'(H))\cdot([\nabla n]\ n).$$

For the second term we use (10)

$$\begin{aligned}\mathrm{div}(\nabla_\Gamma(A'(H))) &= \mathrm{div}_\Gamma(\nabla_\Gamma(A'(H))) + ([\nabla(\nabla_\Gamma(A'(H)))]\ \mathbf{n})\cdot\mathbf{n}\\ &= \Delta_\Gamma(A'(H)) - \nabla(A'(H))\cdot([\nabla n]\ n).\end{aligned}$$

Combining these expressions gives

$$\mathrm{div}\left(\frac{1}{|\nabla\phi|}\nabla_\Gamma(A'(H)|\nabla\phi|)\right) = \Delta_\Gamma(A'(H)) + A'(H)\ (\nabla H\cdot\mathbf{n} + H^2 - 2G).$$

According to (16), we have the relation

$$\mathrm{div}(A(H)\mathbf{n}) = A(H)H + A'(H)\nabla H\cdot\mathbf{n},$$

and using the transport equation (20), we finally get

$$(\mathcal{J}_\varepsilon(\phi))_t = \int_Q \Big(A(H)H - \Delta_\Gamma(A'(H)) - A'(H)(H^2-2G)\Big)u\cdot n|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\,\mathrm{d}x. \tag{26}$$

When ε goes to 0, we obtain with the lemma (21)

$$(\mathcal{J}(\phi))_t = \int_{\{\phi=0\}} \Big(A(H)H - \Delta_\Gamma(A'(H)) - A'(H)(H^2-2G)\Big)u\cdot n\,\mathrm{d}s. \tag{27}$$

This result does not depends on ϕ outside $\{\phi = 0\}$ because it involves only curvature and tangential operators. We propose in the Appendix 2 another proof of this result based on direct computations on the surface. In the particular case $A(r) = r^2$ we find the result (18) obtained with a parametrization of the surface. This result allow us to construct more efficients numerical schemes to approximate the bending force. Indeed, we can focus separately on the approximation of the curvature and the Laplace-Beltrami operator.

3 Numerical simulations of equilibrium shapes

Vesicles are closed membranes of lipids suspended in an aqueous solution. The membrane can be considered as a two-dimensional fluid since there is no stress response to shear deformation. The membrane is also nearly inextensible and thus the equilibrium shapes of vesicles is driven by the bending energy. An important ingredient is the volume ratio given by

$$\tau = \frac{V}{\frac{4}{3}\pi\left(\frac{S}{4\pi}\right)^{\frac{3}{2}}}, \tag{28}$$

where V is the volume and S the area of the vesicle. This parameter measures the ratio between the volume of the vesicle and the volume of the sphere with the same area.

Our approach is to consider an Eulerian fluid-structure model where an elastic membrane is immersed in an incompressible viscous fluid. Two energies will be introduced to take the change of area and the bending into account. The volume of the vesicle is naturally constraint with the incompressibility of the fluid while the area of the vesicle is constraint with a stiff elastic coefficient.

3.1 Eulerian model

We consider the Eulerian fluid-structure model introduced in [7, 8]. Let Q be a domain containing an incompressible fluid where the vesicle is immersed. The motion of the interface is captured by a level set function ϕ which is advected by the fluid velocity. A part of the elasticity, the change of area, is recorded in $|\nabla\phi|$ and we introduce the associated regularized energy

$$\mathcal{E}_e(\phi) = \int_Q E(|\nabla\phi|)\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\,\mathrm{d}x,$$

where ζ is a cut-off function used to spread the interface near $\{\phi = 0\}$. We use in our simulations the following expression $\zeta(r) = \frac{1}{2}(1+\cos(\pi r))$ on $[-1,1]$ and $\zeta(r) = 0$ elsewhere. The parameter ε is equal to $1.5\Delta x$ in the simulations where Δx is the grid size. The constitutive law $r \mapsto E'(r)$ describe the response of the membrane to the change of area. We use in our simulations the linear law $E'(r) = \lambda(r-1)$ where λ is elastic modulus. The associated force is given by

$$\mathbf{F}_e(\phi) = \Big(\nabla_\Gamma(E'(|\nabla\phi|)) - E'(|\nabla\phi|)H(\phi)\mathbf{n}(\phi)\Big)|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right).$$

To take the bending energy into account, we introduce the regularized energy

$$\mathcal{E}_c(\phi) = \int_Q A(H(\phi))|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\,\mathrm{d}x,$$

where A is a constitutive law for the bending energy. We use in our simulations the Helfrich law $A(r) = \alpha r^2$ where α is the bending modulus. The principle of virtual works claims that $(\mathcal{E}_c(\phi))_t = -\displaystyle\int_Q \mathbf{F}_c(\phi)\cdot\mathbf{u}\,\mathrm{d}x$. Using the result (26), we get

$$\mathbf{F}_c(\phi) = \alpha\Big(2\Delta_\Gamma(H(\phi)) + H(\phi)(H(\phi)^2 - 4G(\phi))\Big)|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\mathbf{n}(\phi).$$

The model is then given by the incompressible Navier-Stokes equations with the bending and elastic forces as a source term coupled with a transport equation for the level set. Let L, U, ρ_{ref} and μ_{ref} represent the respective characteristic length, velocity, density and viscosity scales. The dimensionless equations writes

$$\left\{\begin{array}{rcl} R_e(\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u}) - \Delta\mathbf{u} + \nabla p &=& \frac{1}{W_e}\mathbf{F}_e(\phi) + \frac{1}{W_c}\mathbf{F}_c(\phi), \\ \phi_t + \mathbf{u}\cdot\nabla\phi &=& 0, \\ \text{div}(\mathbf{u}) &=& 0, \end{array}\right.$$

where

$$R_e = \frac{LU\rho_{\text{ref}}}{\mu_{\text{ref}}}, \qquad W_e = \frac{\mu_{\text{ref}}U}{\lambda}, \qquad W_c = \frac{\mu_{\text{ref}}UL^2}{\alpha},$$

are respectively the Reynolds, Weissenberg and bending numbers. In this model, the fluid viscosity and the density are the same in the two fluids. Moreover we have neglected the mass of the membrane. These equations are completed with appropriate initial and boundary conditions.

The transport equation is discretized with fifth order WENO scheme in space [16] and explicit Euler scheme in time. A projection method is used to decoupled the pressure and the velocity in time in the Navier-Stokes equations. The resolution of the Poisson equation for the pressure is performed with FFT. An implicit scheme in time is used for the diffusion to avoid a restrictive stability condition on the time step for low Reynolds numbers. The others terms are discretized in space with classical centered schemes of order two. Since the level set function is used through its gradient to compute the stretching, we do not perform the redistancing. Instead, we use the renormalization $\frac{\phi}{|\nabla\phi|}$ to measure the distance to interface. Thus, $|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)$ is replaced by $\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{|\nabla\phi|\varepsilon}\right)$. This approach was proved in [8] to be efficient from the point of view of both volume conservation and interface force calculations.

3.2 Numerical results

The domain $Q = [0,1]^3$ is discretized on a Cartesian mesh with 64 points in each direction. We choose $R_e = 0.01$ to reproduce the typical regime of the flow , $W_e = 0.0001$ to constraint the change of area and $W_c = 0.3$. We impose zero velocity for the initial and boundary conditions. We consider the relaxation of two initial shapes with different volume ratio (28). In the following simulations we represent the evolution of the zero level set of ϕ and slices of the pressure at the center of the domain.

In the first simulation, we choose an ellipsoid represented by the level set function $\phi(x,y,z) = \left(\frac{x-0.5}{a}\right)^2 + \left(\frac{y-0.5}{b}\right)^2 + \left(\frac{z-0.5}{c}\right)^2$ with the parameters $a =$

$0.35, b = 0.35, c = 0.1$. We perform initially a redistancing on this level set function. The associated volume ratio is $\tau = 0.6$. The results are presented on Fig 1.

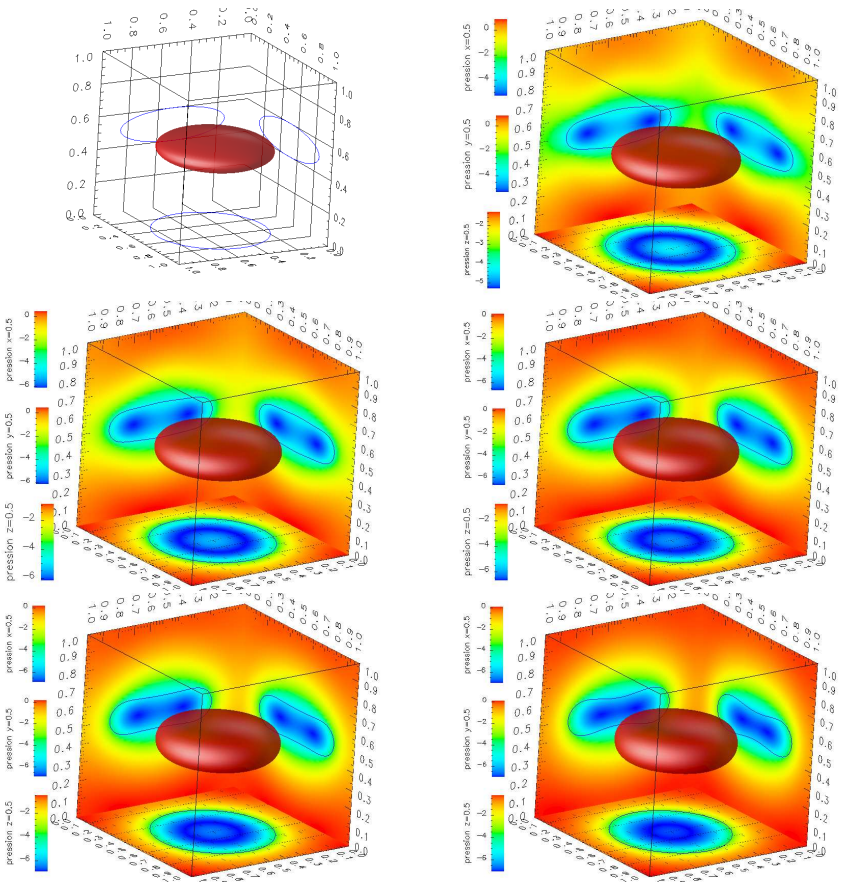

Figure 1: Evolution of the ellipsoid at time $0, 0.5, 1, 1.5, 2$ and 4.5.

In the second simulation, we choose a "dumbbell" represented by the level set function $\phi(x, y, z) = \min(\phi_1(x, y, z), \phi_2(x, y, z), \phi_3(x, y, z))$ with

$$\begin{aligned}
\phi_1(x, y, z) &= \sqrt{x^2 + y^2 + (z + \alpha)^2)} - r, \\
\phi_2(x, y, z) &= \sqrt{x^2 + y^2 + (z - \alpha)^2)} - r, \\
\phi_3(x, y, z) &= \max(|z| - \alpha, \sqrt{x^2 + y^2} - w).
\end{aligned}$$

and the parameters $\alpha = 0.22, w = 0.13, r = 0.18$. The volume ratio is $\tau = 0.77$. We perform initially a redistancing on this level set function. The results are presented on Fig 2.

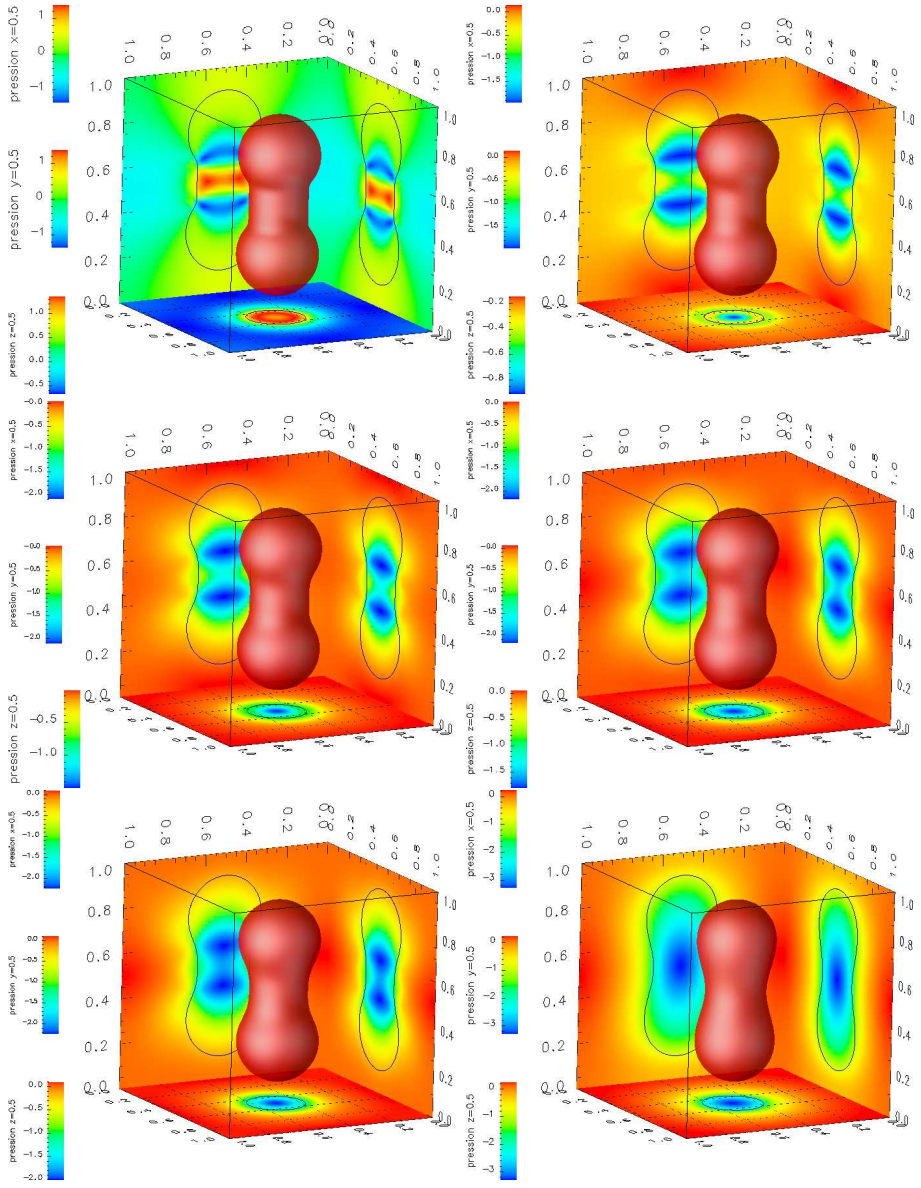

Figure 2: Evolution of the dumbbell at time $0, 0.05, 0.1, 0.15, 0.2$ and 2.

Note that the initial shapes are close to the optimal shapes in order to avoid local minimums. These shapes qualitatively agree with the results presented in the literature [3, 2, 23, 24].

4 Conclusion and forthcoming works

In this paper, we have introduced a method to compute the shape derivative of the Willmore functional in the level set framework. This approach relies on

the approximation of surface integrals on a fixed domain and allow to use the standard differential calculus in $\mathbb{R}^3$. We have proved that this method leads to a geometrical result involving the curvature and the Laplace-Beltrami operator. The equivalence with the method originally introduced by Willmore, where the surface is represented by a parametrization, is established. The level set bending force associated to the Willmore energy is then added on an Eulerian fluid-structure model where an elastic membrane is immersed in a viscous fluid. The discretization on a fixed Cartesian mesh of the level set function allows to overcome the difficulties inherent to a Lagrangian tracking of the interface, as for instance the treatment of large deformations. We have presented some numerical simulations related to the relaxation of vesicles toward their equilibrium shapes in three dimensions. The various shapes obtained are in good agreement with the results presented in the literature. These numerical results are a first step to understand the behavior of vesicles in the blood flow. A ongoing work concern the simulation of dynamics of vesicles in a shear flow.

5 Appendix 1: Stokes formula for surfaces

The aim of this first Appendix is to present a new proof of the Stokes formula for surfaces based on the volumic approximation of functionals.

Let Q be an open set of $\mathbb{R}^3$, f, g smooth functions and $\mathbf{v}, \mathbf{w}$ smooth vector fields. Assume that $\mathbf{w}$ vanishes on ∂Q. As a result, a Stokes formula for volumes and the definition of tangential divergence give

$$\int_Q \mathrm{div}_\Gamma(\mathbf{w})\ \mathrm{d}x = \int_Q \mathrm{div}(\mathbf{w}) - [\nabla \mathbf{w}] : \mathbf{n}\otimes\mathbf{n}\ \mathrm{d}x = \int_Q \mathrm{div}(\mathbf{n}\otimes\mathbf{n})\cdot\mathbf{w}\ \mathrm{d}x.$$

Taking $\mathbf{w} = \mathbf{v}|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)$ (which vanishes on ∂Q) and using the properties (7) and (16), we obtain

$$\begin{aligned}\int_Q \mathrm{div}_\Gamma(\mathbf{v})|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\ \mathrm{d}x = &-\int_Q \nabla_\Gamma\left(|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\right)\cdot\mathbf{v}\ \mathrm{d}x \\ &+\int_Q\Big(H\mathbf{n} + [\nabla n]\ n\Big)\cdot\mathbf{v}|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\ \mathrm{d}x\end{aligned}$$

Using (5) and (9), we have

$$\nabla_\Gamma\left(|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\right) = \nabla_\Gamma\left(|\nabla\phi|\right)\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right) = [\nabla n]\ n|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)$$

Therefore

$$\int_Q \mathrm{div}_\Gamma(\mathbf{v})\ |\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\ \mathrm{d}x = \int_Q H\ \mathbf{v}\cdot\mathbf{n}\ |\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\ \mathrm{d}x.$$

When ε goes to 0 we obtain with the lemma (21)

$$\int_\Gamma \mathrm{div}_\Gamma(\mathbf{v})\ \mathrm{d}s = \int_\Gamma H\ \mathbf{v}\cdot\mathbf{n}\ \mathrm{d}s.$$

Replace $\mathbf{v}$ by $f\mathbf{v}$ gives with (7)

$$\int_\Gamma f\,\mathrm{div}_\Gamma(\mathbf{v})\ \mathrm{d}s = -\int_\Gamma \nabla_\Gamma f\cdot\mathbf{v}\ \mathrm{d}s + \int_\Gamma fH\mathbf{v}\cdot\mathbf{n}\ \mathrm{d}s.$$

6 Appendix 2 : Another proof of the shape derivative of the Willmore functional

This second Appendix is devoted to a different proof of the shape derivative of the Willmore functional. The major difference with the volumic approach is that the computations are performed directly on the surface $\{\phi = 0\}$.

The starting point is the volumic shape derivative (22)

$$(\mathcal{I}_\varepsilon(\phi))_t = \int_Q \Big((f[\phi])_t + \mathrm{div}\,(f[\phi]\mathbf{n})\,u\cdot n\Big)|\nabla\phi|\frac{1}{\varepsilon}\zeta\left(\frac{\phi}{\varepsilon}\right)\ \mathrm{d}x.$$

When ε goes to 0 we get with the lemma (21)

$$(\mathcal{I}(\phi))_t = \int_{\{\phi=0\}} (f[\phi])_t + \mathrm{div}\,(f[\phi]\mathbf{n})\,u\cdot n\ \mathrm{d}s. \tag{29}$$

We obtain the general shape derivative formula for surface integral which can be found in [1, 18]. We consider the Willmore functional

$$\mathcal{J}(\phi) = \int_{\{\phi=0\}} A(H(\phi))\ \mathrm{d}s.$$

We apply (29) with $f = A(H)$ to obtain

$$(\mathcal{J}(\phi))_t = \int_{\{\phi=0\}} A'(H)H_t + \mathrm{div}(A(H)\mathbf{n})\ u\cdot n\ \mathrm{d}s. \tag{30}$$

We choose the definition $H = \mathrm{div}_\Gamma(\mathbf{n})$ of the mean curvature (15) in order to introduce the tangential operators. Then a Stokes formula for surfaces (14) which involves tangential operators will be used to get the final result.

We have with the definition of tangential operators and (4)

$$\begin{aligned} H_t &= (\mathrm{div}(\mathbf{n}))_t - (([\nabla n]\ n)\cdot\mathbf{n})_t,\\ &= \mathrm{div}(\mathbf{n}_t) - ([\nabla\mathbf{n}_t]\ \mathbf{n})\cdot\mathbf{n} - ([\nabla\mathbf{n}]\ \mathbf{n}_t)\cdot\mathbf{n} - ([\nabla\mathbf{n}]\ \mathbf{n})\cdot\mathbf{n}_t,\\ &= \mathrm{div}_\Gamma(\mathbf{n}_t) - ([\nabla n]\ n)\cdot\mathbf{n}_t. \end{aligned}$$

Inserting (24) in the previous expression and developing the tangential divergence with (7) gives

$$H_t = -\Delta_\Gamma(u\cdot n) - \mathrm{div}_\Gamma([\nabla n]\ n)\ u\cdot n + ([\nabla n]\ n)\cdot([\nabla n]\ n)\ u\cdot n.$$

Using the relations (17) and (11) for the second term gives

$$H_t = -\Delta_\Gamma(u \cdot n) - (\nabla H \cdot \mathbf{n} + H^2 - 2G)\, u \cdot n.$$

We have also with (16) the relation

$$\mathrm{div}(A(H)\mathbf{n}) = A(H)H + A'(H)\nabla H \cdot \mathbf{n}.$$

Using the Stokes formula for surfaces (14) we finally obtain

$$(\mathcal{J}(\phi))_t = \int_{\{\phi=0\}} \Big(A(H)H - \Delta_\Gamma(A'(H)) - A'(H)(H^2 - 2G)\Big) u \cdot n \, \mathrm{d}s. \quad (31)$$

We obtain the same shape derivative (27) obtained with the volumic approach.

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