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Geometric shape optimization of membrane in the presence of a diffusion field

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Abstract. In this work we study the geometric shape optimization of membrane in the presence of a diffusion field of molecules, such as proteins which have the ability to adsorb on, and to desorb from the membrane. The main idea of this study is to vary the position of the boundaries of a given initial shape of the membrane, without changing its topology which remains the same as the initial shape. We develop a model that includes, molecular diffusion along the membrane as well as the attachment and detachment of molecules to and from the membrane. The numerical simulations based on Level-Set method show that the coupling between the membrane and the molecules makes the membrane suffer from morphological instability.

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1. Introduction

Geometric shape optimization theory based on the boundary variation method, dates back to J. Hadamard in 1907 [1]. It has been very classic since then. The first results of existence of an optimal shape under constraint of geometric regularity are due to D. Chenais [4], F. Murat and J. Simon [2], [3]. More recently, some results of existence under topological constraint for flat shapes have been obtained by V. Sverak [5] for a membrane model, then by A. Chambolle [9] for the elasticity model. There are other types of additional constraints for the existence of optimal shaps. For example, the work of L. Ambrosio and G. Buttazzo [7] where an upper bound on the perimeter is imposed, which prevents the creation of too many holes.

In this work we follow the method of F. Murat and J. Simon [3] based on the study of optimal control problems where the control is the shape of a domain in which the state of the system is defined by a partial differential equation. Compared to other optimization problems, many new difficulties arise. In particular, the mathematical representation of the shape. For example, a shape can be represented by the characteristic function of its domain (which is 1 inside and 0 outside), but in this case, we don't know how we can represent shape variations. Indeed, a linear combination of characteristic functions is not, in general, a characteristic function. Therefore we can not do "variations computation" in the space of the characteristic functions, and

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compute the gradient. This is a typical difficulty in geometric shape optimization that is important to focus on for both theoretical and numerical reasons.

A new numerical implementation of geometric shape optimization problem has been used in this work. It is based on the level set method of S. Osher and J. Sethian [8]. The main idea is to represent the membrane as the set of zero level of a discretized function on a fixed mesh. This method is based on capturing shapes in an Eulerian fixed mesh. The main advantage of this method is that it allows us to considerably reduce the cost of the computations and gives a simple expresssion of the normal vector and the curvature.

We present in this study a model of membrane (Γ_0) in the presence of a diffusion field of molecules c_{Ω_0}. The aim of this work is to understand the effect of molecules on the membrane shape. First we proved the existence of an optimal shape then we computed the first derivative with respect to the domain of the free energy of the membrane in presence of diffusion and finally we did numerical simulation to see the morphological instability of the membrane induced by interaction with molecules.

1.1. Mathematical model. At equilibrium, the membrane (Γ_0) represent the variable part of the border of a reference domain Ω_0 whose border is divided into tow disjointed parts (see figure1)

$$\partial\Omega_0 = \Gamma_0 \cup \Gamma_D$$

where Γ_0(the membrane) is the variable part of the boundary (Neumann boundary condition), Γ_D is the fixed part of the boundary (Dirichlet boundary condition). The two parts of the boundary are assumed to be non-empty. We assumed that the variable part Γ_0 of the border is free of any effort, which means that the membrane is supposed to be impermeable and the molecules can just adsorb on, or desorb from the membrane(homogeneous Neumann boundary condition).

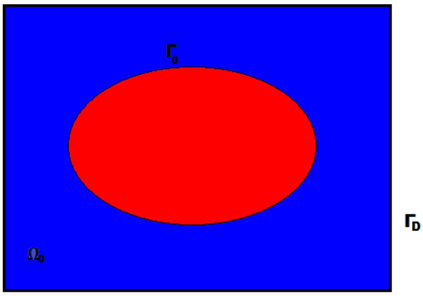

FIGURE 1. The red part is the cell with membrane Γ_0 and the blue part represent the surrounding fluid containing the molecules

The concentration of the molecules in the surrounding fluid (see Figure1: the blue part) verifies the following system

$$\begin{cases} \eta c_{\Omega_0} - d\Delta c_{\Omega_0} = f & \text{in } \Omega_0 \\ \dfrac{\partial c_{\Omega_0}}{\partial n} = 0 & \text{on } \Gamma_0 \\ c_{\Omega_0} = 0 & \text{on } \Gamma_D \end{cases} \tag{1}$$

where
- d is diffusion coefficient
- f is the reaction term
- η is a positive parameter

The total free energy of the membrane is given by [10]

$$E(\Omega_0) = \frac{k}{2}\int_{\partial\Omega_0} (K_{\Omega_0} - K_0)^2 ds - \int_{\partial\Omega_0} k\Lambda K_{\Omega_0} c_{\Omega_0}\, ds + \int_{\partial\Omega_0} \frac{\alpha}{2}(c_{\Omega_0} - c_0)^2 ds. \quad (2)$$

The first term represents the curvature energy of the membrane, the second one represents the coupling term between curvature and surface concentration and the last term represent the concentration deviation of adsorbed molecules from its equilibrium value c_0. Where
- K is the mean local curvature,
- K_0 is the spontaneous curvature ,
- k is the bending rigidity.
- Λ is the molecule size.
- α is supposed to be positive constant.

The geometric shape optimization problem is written as follows

$$\inf_{\Omega\in\mathcal{D}_{ad}} E(\Omega) \quad (3)$$

where it remains to define the set of admissible shapes $\mathcal{D}_{ad}$.

We organised this work as follows. In the next section (section 2) we will consider the existence of the optimal shape under some regularity constraints. The section 2 will also introduce a framework for mathematical shape representation that will be useful to define a notion of derivation with respect to the domain. In Section 3 we will develop this derivation theory which will allow us to write the optimality conditions, and construct numerical simulation that will be presented in Section 4 and finally conclusion in section 5.

2. Existence of optimal solution

The problem is rather the absence of an optimal shape than its existence. However, if additional constraints of a regularity nature are added, then there exist an optimal shape in a restricted class of admissible shapes.

2.1. Existence under a condition of regularity. We give here some notions of topology on a domain of regular boundary, using the perturbations of the identity. Taking inspiration from the approach developed in [2] and [3] to demonstrate the existence result. We will take this framework further to establish a concept of derivation with respect to the domain.

Let Ω_0 be a reference domain, which we assumed to be a connected bounded open set of $\mathbb{R}^n$, of the classe $W^{2,\infty}$. As in the introduction, we suppose that the border of Ω_0 is divided into tow disjointed parts (not empty)

$$\partial\Omega_0 = \Gamma_0 \cup \Gamma_D$$

where Γ_D is fixed and only Γ_0 is variable.

The main idea is to define a set of admissible shapes $\mathcal{D}_{ad}$ from which any element Ω is obtained by applying a regular diffeomorphism to the reference domain Ω_0. Thus the space of admissible shapes is very significantly restricted, but we gain a very simple representation of the shape in terms of diffeomorphisms.

Let us first remind that, $W^{2,\infty}(\mathbb{R}^n,\mathbb{R}^n)$ is the space of Lipschitz functions ϕ from $\mathbb{R}^n$ to $\mathbb{R}^n$ such that ϕ, $\nabla\phi$, and $\Delta\phi$ are uniformly bounded in $\mathbb{R}^n$ to which we associate the following norm wich makes it a Banach space

$$\| \varphi \|_{W^{2,\infty}(\mathbb{R}^n,\mathbb{R}^n)}= \sup_{x\in\mathbb{R}^n} ess \left(\Sigma_{0<|\alpha|\leq 2} \mid D^\alpha\varphi(x) \mid^2_{\mathbb{R}^n}\right)^{\frac{1}{2}}. \tag{4}$$

We define a space of diffeomorphisms as follows

$$\tau^{2,\infty} = \Big\{T \text{ such that } (T - Id) \in W^{2,\infty}(\mathbb{R}^n,\mathbb{R}^n), \big(T^{-1} - Id\big) \in W^{2,\infty}(\mathbb{R}^n,\mathbb{R}^n)\Big\}. \tag{5}$$

Somehow we can see diffeomorphisms of $\tau^{2,\infty}$ as perturbations of the identity. Now we can then introduce a space of admissible shapes obtained by deformation of Ω_0

$$\mathcal{D}^{2,\infty}_{\Omega_0} = \Big\{\Omega \text{ such that } \exists T \in \tau^{2,\infty}, \Omega = T(\Omega_0)\Big\}. \tag{6}$$

Each admissible shape $\Omega \in \mathcal{D}^{2,\infty}_{\Omega_0}$, is represented by a diffeomorphism $T \in \tau^{2,\infty}$. This representation is not unique because it is possible that two diffeomorphisms $T \neq T_2$ in $\tau^{2,\infty}$ lead to the same open set $\Omega = T(\Omega_0) = T_2(\Omega_0)$. Since the functions of $W^{2,\infty}(\mathbb{R}^n,\mathbb{R}^n)$ are continuous, the applications T of $\tau^{2,\infty}$ are also homomorphisms, which implies that they preserve the topology of the domains to which they are applied. Thus, all admissible shapes of $W^{2,\infty}(\mathbb{R}^n,\mathbb{R}^n)$ have the same topology as Ω_0. Therefore this approach is not helpful to optimize the topology (number of holes or connected components of the boundary). We can then introduce a pseudo-distance on $\mathcal{D}^{2,\infty}_{\Omega_0}$ (it verifies only a weak version of the triangular inequality)

$$d^{2,\infty}(\Omega,\Omega_2) = \inf_{T\in\tau|T(\Omega)=\Omega_2} \left(\| T - Id \|_{W^{2,\infty}(\mathbb{R}^n,\mathbb{R}^n)} + \| T^{-1} - Id \|_{W^{2,\infty}(\mathbb{R}^n,\mathbb{R}^n)}\right). \tag{7}$$

We can now define a condition of uniform regularity of the admissible shapes by being limited to open sets Ω close to Ω_0 in the sense of this pseudo-distance $d^{2,\infty}$. More precisely, for $R > 0$ we define

$$\mathcal{D}_{ad} = \Big\{\Omega \in \mathcal{D}^{2,\infty}_{\Omega_0} \;/\; d^{2,+\infty}(\Omega,\Omega_0) \leq R,\ \Gamma_0 \cup \Gamma_D \subset \partial\Omega_0,\ \mid \Omega \mid= V_0\Big\}, \tag{8}$$

The choice of the regularity constant R is arbitrary as well as the choice of the reference domain Ω_0.

Theorem 2.1. *If we assume that*

$$\begin{cases} \Omega_0 \textit{ is a connected bounded open set of } \mathbb{R}^n \textit{ of the class } W^{2,\infty}, \\ f \in L^2(\mathbb{R}^n), \quad K_0 \in H^1(\mathbb{R}^n) \quad \textit{and} \quad c_0 \in H^1(\mathbb{R}^n). \end{cases} \tag{9}$$

There exists an optimal shape Ω^*, such that

$$\Omega^* \in \mathcal{D}_{ad}, \qquad E(\Omega^*) \leqslant E(\Omega), \qquad \forall\Omega \in \mathcal{D}_{ad}. \tag{10}$$

Remark 2.1. The proof of this theorem rests on a compactness argument. The essential idea is that the admissible shapes of $\mathcal{D}_{ad}$ can not change their topology, and the uniform regularity bound R prevents the boundaries of the Ω shape from being too oscillating.

Proof. Let Ω_0 be a fixed connected bounded open set of $\mathbb{R}^n$ of the class $W^{2,\infty}$ such that $\mid \Omega_0 \mid = V_0$, every domain $\Omega \in \mathcal{D}^{2,\infty}$ is a connected bounded open set of the class $W^{2,\infty}$ [3]. We will proove that:

- $\mathcal{D}_{ad}$ is a compact of $\mathcal{D}^{2,\infty}$,
- $E(\Omega)$ is a continuous functional of $\mathcal{D}^{2,\infty}$.

For the compacity of $\mathcal{D}_{ad}$, let $\Omega \in \mathcal{D}_{ad}$ and $R \geq 0$ fixed. For all sequence $\{\Omega_n\}_{n\in\mathbb{N}}$ of $\mathcal{D}_{ad}$ such that $d^{2,+\infty}(\Omega_n, \Omega) \leq R$ and $\mid \Omega_n \mid = V_0$, we can extract a subsequence that we can also call Ω_n that converges to $\Omega_* \in \mathcal{D}^{2,\infty}$ such that $d^{2,+\infty}(\Omega_*, \Omega) \leq R$ [3](theorem 2,4), it remains to show that $\mid \Omega_* \mid = V_0$. Let K_1 and K_2 be closed subsets of $\mathbb{R}^n$ such that $K_1 \subset \Omega_*$ and $K_2 \subset \mathbb{R}^n - \overline{\Omega}_*$.Then, according to the definition of the Hausdorff distance, $K_1 \subset \Omega_n$ and $K_2 \subset \mathbb{R}^n - \overline{\Omega}_n$ for n large enough.

We consider closed subsets reduced to a single point, since $mes(\partial\Omega_*) = 0$ it results that

$$\chi(\Omega_n) \longrightarrow \chi(\Omega_*) \quad a.e \quad \text{in} \quad \mathbb{R}^n.$$

Using Lebesgue's theorem, Ω_* is bounded and the sequence Ω_n is bounded in $L^\infty(\mathbb{R}^n)$ it comes that

$$\chi(\Omega_n) \longrightarrow \chi(\Omega_*) \quad \text{in} \quad L^\infty(\mathbb{R}^n) \quad \text{star weak and} \quad \text{strongly in} \quad L^p(\mathbb{R}^n) \ 1 \leq p < \infty$$

wich means that $\mid \Omega_* \mid = V_0$ and so $\Omega_* \in \mathcal{D}_{ad}$. Hence the compacity of $\mathcal{D}_{ad}$.

For the continuity of the functional E we will use the variable change $\Omega = T(\Omega_0)$, $T \in \tau^{2,\infty}$, where $\Omega \in \mathcal{D}^{2,\infty}$ is a connected bounded open set of the class $W^{2,\infty}$, such that $\mid \Omega \mid = V_0$.

Let Ω_n be a sequence of $\mathcal{D}^{2,\infty}_{\Omega_0}$ that converges to $\Omega \in \mathcal{D}^{2,\infty}_{\Omega_0}$, as a result of [3] (theorem 2.4) we can extract a subsequence Ω_m, then we have

$$\Omega_m = T_m(\Omega_0), \ \Omega = T(\Omega_0), \quad \text{where} \quad T_m, T \in \tau^{2,\infty}. \tag{11}$$

Now we need the continuity of the state transport c_{Ω_m} to the fixed domain Ω_0. The function c_{Ω_m} is a unique solution of the following equation in the domain $\Omega_m = T_m(\Omega_0)$

$$\begin{cases} c_{\Omega_m} \in H^1(\Omega_m), \\ \displaystyle\int_{\Omega_m} d\nabla c_{\Omega_m} \nabla\varphi + \eta c_{\Omega_m}\varphi = \int_{\Omega_m} f\varphi, \qquad \forall\varphi \in H^1(\Omega_m). \end{cases} \tag{12}$$

Applying the change of variable T_m to equation (12) in order to return back to the fixed domain Ω_0, we deduce that [3] (lemma 4.1).

$$\begin{cases} c(\Omega_m) \circ T_m \in H^1(\Omega_0), \\ \displaystyle\int_{\Omega_0} d < {}^t[T'_m]^{-1}\nabla(c(\Omega_m) \circ T_m), {}^t[T'_m]^{-1}\nabla\varphi \\ \qquad > \mid det[T'_m] \mid + \eta < c(\Omega_m) \circ T_m, \varphi > \mid det[T'_m] \mid \\ \qquad = \displaystyle\int_{\Omega_0} < f \circ T_m, \varphi > \mid det[T'_m] \mid, \qquad \forall\varphi \in H^1(\Omega_0). \end{cases} \tag{13}$$

As a result [3] (lemma 4.2, 4.3 and 4.4)

$$\begin{cases} {}^t[T'_m]^{-1} \longrightarrow {}^t[T']^{-1} \quad \text{in} \quad L^\infty(\mathbb{R}^n, \mathbb{R}^{2n}), \\ \mid det[T'_m] \mid \longrightarrow \mid det[T'] \mid \quad \text{in} \quad L^\infty(\mathbb{R}^n, \mathbb{R}^{2n}), \\ f \circ T_m \longrightarrow f \circ T \quad \text{in} \quad L^2(\Omega_0). \end{cases} \tag{14}$$

The continuity of the solution of equation (13) with respect to its coefficients coupled with (14) and the fact that $\Omega_m \longrightarrow \Omega$ implies that

$$c_{\Omega_m} \circ T_m \longrightarrow c_\Omega \circ T \quad \text{in} \quad H^1(\Omega_0).$$

The uniform ellipticity of the equation (13) in m gives

$$\begin{cases} \|^t\, [T'_m]^{-1} \|_{W^{1,\infty}(\mathbb{R}^n,\mathbb{R}^{2n})} \leq C, \quad \forall \quad m, \\ \mid det[T'_m] \mid_{W^{1,\infty}(\mathbb{R}^n)} \leq C, \quad \forall \quad m, \\ \| f \circ T_m \|_{L^2(\Omega_0)} \leq C, \quad \forall \quad m. \end{cases} \tag{15}$$

Since Ω_0 is a bounded open set of the class $W^{2,\infty}$, the sequence $c_{\Omega_m} \circ T_m$ is bounded in $H^2(\Omega_0)$. We have then

$$c_{\Omega_m} \circ T_m \longrightarrow c_\Omega \circ T \quad \text{in} \quad H^2(\Omega_0) \quad \text{weak.} \tag{16}$$

Let us now verify the continuity of the functional E. We denote by n_Ω the exterior normal vector to $\partial\Omega$, we have

$$E(\Omega_m) = \int_{\partial\Omega_m} \frac{k}{2}(K_{\Omega_m} - K_0)^2 - k\Lambda K_{\Omega_m} c_{\Omega_m} + \frac{\alpha}{2}(c_{\Omega_m} - c_0)^2 ds, \tag{17}$$

where $K_{\Omega_m} = div(n_{\Omega_m})$. We apply the variable change $\Omega_m = T_m(\Omega_0)$

$$\begin{aligned} E(\Omega_m) = \int_{\partial\Omega_0} \Big[&\frac{k}{2}(K_{\Omega_m} \circ T_m - K_0 \circ T_m)^2 - k\Lambda K_{\Omega_m} \circ T_m c_{\Omega_m} \circ T_m \\ &+ \frac{\alpha}{2}(c_{\Omega_m} \circ T_m - c_0 \circ T_m)^2 \Big] \times \mid det[T'_m] \mid \mid^t\, [T'_m]^{-1} n(\Omega_0) \mid_{\mathbb{R}^n} ds. \end{aligned} \tag{18}$$

The convergence results of (14) also holds in $L^\infty(\partial\Omega_0)$, since T_m and T are $C^1(\mathbb{R}^n, \mathbb{R}^n)$. Furthermore, we have

$$\mid^t\, [T'_m]^{-1} n(\Omega_0) \mid_{\mathbb{R}^n} \geq \frac{1}{\| [T'_m] \|_{L^\infty(\mathbb{R}^n,\mathbb{R}^{2n})}} \qquad a.e. \quad \text{on} \quad \partial\Omega_0.$$

Finally by the results obtained in (15) and the continuity Lemma 4.4 i)[3] we have

$$K(\Omega_m) \circ T_m \longrightarrow K(\Omega) \circ T \quad \text{in} \quad L^2(\partial\Omega_0) \quad \text{strongly}$$

$$K_0 \circ T_m \longrightarrow K_0 \circ T \quad \text{in} \quad L^2(\partial\Omega_0) \quad \text{strongly}$$

$$c(\Omega_m) \circ T_m \longrightarrow c(\Omega) \circ T \quad \text{in} \quad L^2(\partial\Omega_0) \quad \text{strongly}$$

which implies that

$$E(\Omega_m) \longrightarrow E(\Omega).$$

This convergence lies for all sequences $\{\Omega_n\}_{n\in\mathbb{N}}$ which ends the proof. □

3. Differentiability with respect to domain

In this section we take again the shape representation introduced in section 2, which will allow us to naturally define a notion of derivation with respect to the domain. Once we are able to differentiate, we can write the optimality conditions that we will use to characterize the optimal shape and compute the gradient to implement a numerical optimization method. It is therefore a fundamental concept both from the theoretical and practical point of view.

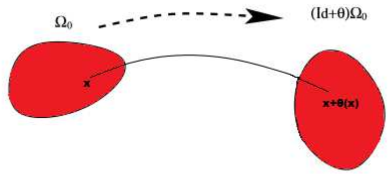

FIGURE 2. Definition of a domain transported by a vector field θ.

Let Ω_0 (reference doamin) be a regular bounded open set of $\mathbb{R}^n$. We consider the class of admissible shapes $\mathcal{D}^{2,\infty}_{\Omega_0}$ as defined before. It is natural to consider the variable θ defined by

$$T = Id + \theta \quad \text{where} \quad \theta \in W^{2,\infty}(\mathbb{R}^n, \mathbb{R}^n) \text{ small enough.}$$

With this notation Ω is defined by

$$\Omega = (Id + \theta)(\Omega_0).$$

We can see $\theta(x)$ as a vector field which transports or displaces the reference domain Ω_0(see figure5). In other words, each admissible shape $\Omega \in \mathcal{D}^{2,\infty}_{\Omega_0}$ is represented by a vector field $\theta(x)$ of $\mathbb{R}^n$ in $\mathbb{R}^n$. We can then define a notion of differentiability in Ω_0 by using the derivation with respect to $\theta(x)$.

Remark 3.1. - If $\theta(x)$ is small enough then $T = Id + \theta$ belongs to the set $\tau^{2,\infty}$ of diffeomomorphisms on $\mathbb{R}^n$.
- A function E defined in $\mathcal{D}^{2,\infty}$ is differentiable at Ω_0 if the function $\theta \longrightarrow E((I + \theta)(\Omega_0) = E(\Omega)$ is Frechet differentiable (in the usual sense) from $W^{2,\infty}$ to $\mathbb{R}$ in 0, and its derivative is defined by

$$\frac{\partial E}{\partial \Omega}(\Omega_0) = \frac{\partial E((I+\theta)(\Omega_0))}{\partial \theta}(0) \in \mathcal{L}_c(W^{2.\infty}(\mathbb{R}^n, \mathbb{R}^n), \mathbb{R}).$$

We consider the equation defined by (1) in Ω which admits a unique solution $c_\Omega \in H^1(\Omega)$. The variational formulation of (1) in Ω is to find $c \in H^1(\Omega)$ such that

$$\begin{cases} c \in H^1(\Omega), \\ \int_\Omega d\nabla c \nabla \varphi + \eta c \varphi = \int_\Omega f\varphi, \qquad \forall \varphi \in H^1(\Omega). \end{cases} \tag{19}$$

Theorem 3.1. *Let Ω_0 be a regular open set. The total free energy of the membrane $E(\Omega_0)$, defined by (2), is differentiable from $\mathcal{D}^{2,\infty}$ to $\mathbb{R}$, and it's derivative with respect to the domain is defined by:*

$$E'(\Omega_0)(\theta) = \int_{\partial\Omega_0} (\theta.n)\left\{\eta c p + d\nabla c \nabla p - fp + k(K - K_0 - \Lambda c)\frac{\partial K}{\partial n} + \frac{k}{2}K(K-K_0)^2 - k\Lambda K^2 c + \frac{\alpha}{2}K(c-c_0)^2 + k(\Delta_{\partial\Omega_0}K - \Lambda\Delta_{\partial\Omega_0}c)\right\},$$

where n is the normal vector, $\Delta_{\partial\Omega_0}$ is the Laplace Beltrami operator defined by $\Delta_{\partial\Omega_0}c_{\Omega_0} = \Delta c_{\Omega_0} - K\frac{\partial c_{\Omega_0}}{\partial n} - \frac{\partial^2 c_{\Omega_0}}{\partial n^2}$ on Γ_0, and p_{Ω_0} is the solution of the adjoint *state*

$$\begin{cases} \eta p_{\Omega_0} - d\Delta p_{\Omega_0} = 0 & in \quad \Omega_0 \\ d\dfrac{dp_{\Omega_0}}{dn} = k\Lambda K - \alpha(c_{\Omega_0} - c_0) & on \quad \Gamma_0 \\ p_{\Omega_0} = 0 & on \quad \Gamma_D \end{cases} \tag{20}$$

where $\partial\Omega_0 = \Gamma_0 \cup \Gamma_D$.

Remark 3.2. The rigorous computation of the derivative of an objective function requires the ability to derive the solution of the equation of state (c) even though this derivative ($\tilde{C}$(Eulerian derivative of c) or $\bar{C}$(Lagrangian derivative of c)) does not appear in the final result [3]. There is a certain waste, especially since the computation of $\tilde{C}$ or $\bar{C}$ is quite delicate and tedious. Fortunately, there is a method faster to derive (at least formally) an objective function called the Lagrangian method, developed by J. Cea in [11].

Proof. The proof of this theorem is based on the Lagrangian method.

$$E(\Omega) = \int_{\partial\Omega} \frac{k}{2}(K - K_0)^2 - k\Lambda K u + \frac{\alpha}{2}(u - u_0)^2. \tag{21}$$

We suppose first that u is a solution of (1) in Ω wich means that u verifies (18) $\forall q \in H^1(\Omega)$. We introduce the Lagrangian which is the sum of the objective function and the variational formulation of the equation of state

$$\mathcal{L}(\Omega, u, q) = E(\Omega) + \int_\Omega \eta u q + d\nabla u \nabla q - f q dx, \tag{22}$$

with u and q in $H^1(\mathbb{R}^n)$. It is important to note that the space $H^1(\mathbb{R}^n)$ does not depend on Ω then the three variables of the Lagrangian $\mathcal{L}$ are independent. The partial derivative of $\mathcal{L}$ with respect to q in the direction $\phi \in H^1(\mathbb{R}^n)$ is

$$< \frac{\partial \mathcal{L}}{\partial q}(\Omega, u, q), \phi >= \int_\Omega \eta u q + d\nabla u \nabla q - f q dx, \tag{23}$$

which, when it vanishes, gives (by construction) the variational formulation of the equation of state (1). The partial derivative of $\mathcal{L}$ with respect to u in the direction $\phi \in H^1(\mathbb{R}^n)$ is

$$< \frac{\partial \mathcal{L}}{\partial u}(\Omega, u, q), \phi >= \int_\Omega \eta\phi q - d\phi\Delta q dx + \int_{\partial\Omega} d\frac{dq}{dn}\phi ds + \int_{\partial\Omega} \alpha(u - u_0)\phi - k\Lambda K\phi ds. \tag{24}$$

which, when it vanishes, gives nothing else than the variational formulation of the adjoint state equation (20). Finally, the derivative of $\mathcal{L}$ with respect to the domain, evaluated by assuming that u and q are fixed (i.e. as a partial derivative), in the direction θ is

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, u, q)(\theta) = \int_{\partial\Omega_0} (\theta.n) \Big\{ & \eta u q + d\nabla u \nabla q - f q + K(\frac{k}{2}(K - K_0)^2 - k\Lambda K u \\ & + \frac{\alpha}{2}(u - u_0)^2) + \frac{\partial}{\partial n}(\frac{k}{2}(K - K_0)^2 - k\Lambda K u + \frac{\alpha}{2}(u - u0)^2) \Big\} ds \\ & + \int_{\partial\Omega_0} k((K - K_0) - \Lambda u)\frac{\partial K}{\partial \Omega}(\Omega_0)(\theta) ds, \end{aligned}$$

where (see for exemple[12])

$$\frac{\partial K}{\partial \Omega}(\Omega_0)(\theta) = \frac{\partial(div(n))}{\partial \Omega}(\Omega_0)(\theta) = div(\frac{\partial n}{\partial \Omega}(\Omega_0)(\theta)) = -\nabla.(\nabla_{\partial\Omega_0}(\theta.n))$$

and

$$\frac{\partial}{\partial n}(\frac{k}{2}(K-K_0)^2 - k\Lambda K u + \frac{\alpha}{2}(u-u0)^2) = k(K-K_0-\Lambda u)\frac{\partial K}{\partial n}.$$

When it comes to evaluate this derivative at the state c_{Ω_0} and the adjoint state p_{Ω_0}, we find exactly the value of the derivative of the objective function

$$\frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, c, p)(\theta) = E'(\Omega_0). \tag{25}$$

This equation is not a coincidence. Indeed, for all $q \in H^1(\mathbb{R}^n)$

$$\mathcal{L}(\Omega, c_\Omega, q)(\theta) = E(\Omega). \tag{26}$$

Since c_Ω verifies the variational formulation of the state system (1) witch depends on Ω, but not q, by deriving this expression and using the composite derivative theorem, it comes

$$E'(\Omega_0) = \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, c(\Omega_0), q)(\theta) + < \frac{\partial \mathcal{L}}{\partial u}(\Omega_0, c(\Omega_0), q), c'(\Omega_0)(\theta) > . \tag{27}$$

Taking $q = p_{\Omega_0}$ solution of the adjoint state (20), the last term vanishes and we obtain

$$\begin{aligned} E'(\Omega_0) &= \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, c_{\Omega_0}, p_{\Omega_0})(\theta) \\ &= \int_{\partial\Omega_0} (\theta.n) \Big\{ \eta c_{\Omega_0} p_{\Omega_0} + d\nabla c_{\Omega_0} \nabla p_{\Omega_0} - f p_{\Omega_0} + \frac{k}{2} K(K-K_0)^2 - k\Lambda K^2 c_{\Omega_0} \\ &\quad + \frac{\alpha}{2} K(c_{\Omega_0} - c_0)^2 + k(K - K_0 - \Lambda c_{\Omega_0})\frac{\partial K}{\partial n} \Big\} ds \\ &\quad + \int_{\partial\Omega_0} k((K-K_0) - \Lambda c_{\Omega_0})(-\nabla.(\nabla_{\partial\Omega_0}(\theta.n)))ds \\ &= \int_{\partial\Omega_0} (\theta.n) \Big\{ \eta c_{\Omega_0} p_{\Omega_0} + d\nabla c_{\Omega_0} \nabla p_{\Omega_0} - f p_{\Omega_0} + \frac{k}{2} K(K-K_0)^2 - k\Lambda K^2 c_{\Omega_0} \\ &\quad + \frac{\alpha}{2} K(c_{\Omega_0} - c_0)^2 + k(K - K_0 - \Lambda c_{\Omega_0})\frac{\partial K}{\partial n} + k(\Delta_{\partial\Omega_0} K - \Lambda \Delta_{\partial\Omega_0} c_{\Omega_0}) \Big\} ds. \end{aligned} \tag{28}$$

Thanks to this simple computation, we obtain a "good" result for $E'(\Omega_0)$ without going through the Eulerian derivative or material derivative which are rather complicated to establish. However, this quick calculation of the derivative $E'(\Omega_0)$ is only formal. In fact, it assumes that we already know the differentiability of c with respect to the domain, and that we can apply the rule of composed derivation. □

4. Numerical analysis

4.1. Level-set method. In order to evoluates the shape we will consider the variable part of the border Γ and look for a function ϕ such that $\Gamma = \{x \in \mathbb{R}^2 / \phi(x) = 0\}$. So, instead of deforming the shape by studying the evolution of Γ, we will transform the function ϕ into $\widetilde{\phi}$ then take as a new border the set $\Big\{x \in \mathbb{R}^2 / \widetilde{\phi(x)} = 0\Big\}$. The advantage is that many geometric properties of Γ are expressed more easily using ϕ. For example, the vector normal to Γ is defined by $n = \dfrac{\nabla\phi}{\parallel \nabla\phi \parallel}$ and the mean curvature defined by $K = \nabla.\left(\dfrac{\nabla\phi}{\parallel \nabla\phi \parallel}\right)$. We ask ϕ to be negative inside Γ and positive outside. In practice, we choose a function whose gradient does not vanishes on Γ. In fact, we try to work with a function close to the signed distance function at Γ.

We want to evaluate a shape Ω_0 with border $\Gamma_0 = \left\{x \in \mathbb{R}^2 / \phi_0(x) = 0\right\}$ allong the vector field

$$\overrightarrow{V} = V.\frac{\nabla\phi_0}{\parallel \nabla\phi_0 \parallel},$$

where V is obtained by theorem(3.1)(equation (28)) as follows

$$\begin{aligned} V = \quad & \eta cp + d\nabla c\nabla p - fp + k(K - K_0 - \Lambda c)\frac{\partial K}{\partial n} + \frac{k}{2}K(K-K_0)^2 \\ & -k\Lambda K^2 c + \frac{\alpha}{2}K(c-c_0)^2 + k(\Delta_{\partial\Omega_0}K - \Lambda\Delta_{\partial\Omega_0}c). \end{aligned} \tag{29}$$

For that we will solve the system:

$$\begin{cases} \partial_t\Phi + \overrightarrow{V}.\nabla\Phi = 0 & , \\ \Phi(t_0, 0) = \phi_0 & . \end{cases} \tag{30}$$

As a new border we will take $\Gamma = \left\{x \in \mathbb{R}^2 / \phi(x) = 0\right\}$, where $\phi = \Phi(t_0 + \Delta t, .)$.

4.2. Numerical algorithm.

Remark 4.1. To know the evolution of ϕ in time. In practice, the problem lies from the fact that if x is a mesh node, $x + \overrightarrow{V}(t, x)$ is not necessarily one. However, we prefer to work with a fixed mesh. That's why we will use the operator Convect.

If the solution is $\phi_0$at time t_0, then we get $\phi = \Phi(t_0 + \Delta t, .)$ by:

$$\phi = convect\left(\left[-\overrightarrow{V}.e_x, -\overrightarrow{V}.e_y\right], \Delta t, \phi_0\right). \tag{31}$$

This technique will also be used in the program to reset the function delimiting the domain Ω.

Remark 4.2. When we modify a function that serves only to delimit the curve $\left\{x \in \mathbb{R}^2 : \phi(x) = 0\right\}$. ϕ can become less suitable than other functions delimiting the same curve. We denote ϕ_{old} the function that we want to improve and we solve the equation whose stationary solution is the signed distance at Γ:

$$\begin{cases} \partial_t\Phi + sign(\phi_{old})(\parallel \nabla\Phi \parallel -1) = 0 & , \\ \Phi(t_0, 0) = \phi_{old} & . \end{cases} \tag{32}$$

Then we replace ϕ_{old} by $\phi = \Phi(t_0 + \Delta t, .)$. So on the set $\left\{x \in \mathbb{R}^2 : \phi_{old}(x) = 0\right\}$ as $sign(\phi_{old}) = 0$, the equation reduces to $\partial_t\Phi = 0$ and the curve$\left\{x \in \mathbb{R}^2 : \phi(x) = 0\right\}$ is then equal to $\left\{x \in \mathbb{R}^2 : \phi_{old}(x) = 0\right\}$, the border of the shape remains unchanged by this modification. Moreover, in a neighborhood of this curve, $\partial_t\Phi$ is weak so the gradient is almost unit. To solve this system, we start by linearizing the equation by the following approximation:

$$\partial_t\Phi + sign(\phi_{old})\left(\frac{\nabla\phi_{old}}{\parallel \nabla\phi_{old} \parallel}.\nabla\Phi - 1\right) = 0.$$

Then we proceed in two steps, we solve the equation without the source term then we add $dt \times sign(\phi_{old})$ to the solution found. By repeating this process, we get a function closer to the signed distance at Γ.

Algorithm 1 Representation of the shape of the membrane by Level Set method

1.Initialization of the level set function ϕ_0 by solving (32)
2.Iteration until convergence for $k \geq 1$:
  (a) Compute the direct stat c_{Ω_0} solution of (1) and the ajoint stat p_{Ω_0} solution of (20) for the shape ϕ_k.
  Deduce the shape gradient = normal velocity $=V_k$ (29)
  (b) Advect the shape with V_k (solving the Hamilton Jacobi equation (31)) to obtain a new shape ϕ_{k+1}.

4.3. Numerical results. In this section we give numerical results obtained in graphical form. The figure 3 represents the intial shape of the membrane at rest that we choose to be an ellipse. The evolution in time of the deformation of the membrane shape under the effect of molecular diffusion and adsorption phenomenon is given in figure 4 using numerical algorithm based on level set method (Algorithm1). In figure 5 we can see the final state of the membrane shape at equilibrum where the simple coupling between the membrane and adsorbed molecules lead to a morphological instability.

5. Conclusion

Using geometrical shape optimisation we have analyzed the coupling of the membrane to a diffusion field, we prove the existence of the optimal shape of a membrane in a presence of the diffusion field and we compute its first derivative with respect to the domain. We have focused on the situation where the system is in global equilibrium. When the membrane is stable we have analyzed the effect of the various processes on the membrane fluctuations by using level-set method.

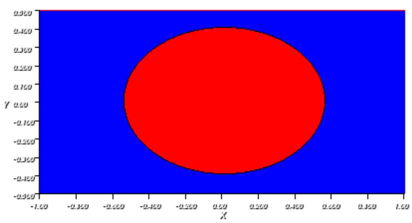

FIGURE 3. Initial shape.

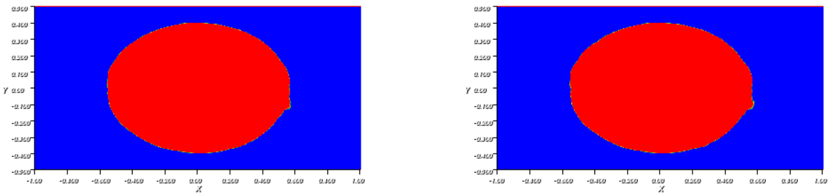

FIGURE 4. Shape evolution in time.

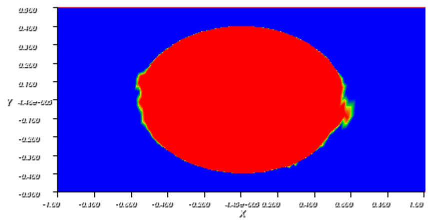

FIGURE 5. Final shape.

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