A STABILIZED MAXIMUM-ENTROPY METHOD FOR THE STOKES PROBLEM COUPLED WITH A PHASE-FIELD MODEL OF BIOMEMBRANES

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Abstract. Vesicles are closed biomembranes consisting of one or several different kinds of lipids. The stationary shapes of the vesicles are usually studied with the Canham-Helfrich bending energy model. We use a phase-field description of the membrane, governed by a fourth-order nonlinear partial differential equation with constraints. We tackle numerically this problem with the Local Maximum-Entropy (LME) approximants, since phase-field solutions benefit from the LME characteristics such as positivity, smoothness and variation diminishing property.

To analyze the dynamic properties of the vesicles, the fluid where they are immersed is commonly modeled as a Stokes flow because of the low Reynold's number. The idea is to apply the same numerical scheme to compute both the phase-field bending energy and the bulk effect of the fluid field surrounding the membrane. It is well-known that the Stokes problem lacks pressure stability if velocity and pressure are described with the same interpolation space. This fact has led to two families of approaches, either using different and compatible spaces for the velocity and the pressure, or stabilizing equal interpolation methods. All these methods have been developed mainly in the context of finite elements. In this work we show stationary shapes of the vesicles computed with the phase-field approach and we present new results regarding the solution of Stokes benchmark problems using stabilized LME methods.

1   INTRODUCTION

Biomembranes or biological membranes have been object of experimental and theoretical investigation for biologists, chemists and physicists during many years. Biomembranes are composed by several kinds of lipids self-assembled in a fluid bilayer, which presents a liquid behaviour in-plane and solid out-of-plane. Vesicles are closed biomembranes which play an important role in biophysical processes and serve as simplified models of cell membranes to study aspects of the interaction between the lipid bilayer structure and the surrounding fluid.

To simulate the dynamic behaviour of a vesicle both biomembrane solid structure and surrounding fluid have to be properly modeled. The Canham-Helfrich bending energy model is normally used to describe the solid behaviour, while the fluid is modeled as a Stokes flow.

Two different approaches can be used to describe the equations for equilibrium shapes of vesicles in the continuum media approach, sharp-interface and phase-field or diffuse-interface models. In this work a phase-field model proposed by Du et al. (Du et al., 2004) is used. This kind of models represent the interface between the inner and outer fluid as a diffuse-interface whose thickness is controlled by a transition parameter ϵ. The derived equations are highly nonlinear and involve fourth-order spatial partial differential operators. The weak form of the equations necessitates piecewise smooth and globally C^1-continuous basis functions because products of second-derivatives are involved in the integration of the variational formulation. The equations are discretized with LME approximation schemes (Arroyo and Ortiz, 2006) because they present interesting features such as positivity, monotonicity, variation diminishing property (the interpolation is not more wiggly than the data) and smoothness (C^∞). Adaptivity strategies are also required to make computationally affordable the phase-field approach.

The fluid is commonly modeled as a Stokes flow because the Reynold's number is low. The idea is to apply the same numerical scheme to compute both the phase-field bending energy and the bulk effect of the fluid field surrounding the membrane. It is well-known that the Stokes problem lacks pressure stability if velocity and pressure are described with the same interpolation space, which demands a stabilization method to handle the problem. We borrowed finite element method (FEM) stabilization strategies to develop a LME stabilizing method.

The structure of this paper is as follows. Section 2 introduces the formulation of the phase-field model and its numerical treatment. The capability of the adaptive strategy is also illustrated. In Section 3, we describe the Stokes flow problem and the stabilizing LME method, whose performance is tested through numerical benchmarks. Some concluding remarks are collected in Section 4.

2   MODEL OF THE BIOMEMBRANE: A PHASE-FIELD APPROACH

In this section we present the problem formulation and its numerical treatment (discretization, nonlinear solver, and adaptivity). We also analyze a numerical example corresponding to an equilibrium shape, known as oblate, to evaluate the performance of the proposed scheme.

2.1 Problem formulation and numerical treatment

The phase-field approach to compute the equilibrium shapes for vesicles can be possed as an energy constrained-minimization problem:

$$
\begin{aligned}
\text{Minimize} \quad & E(\phi) = f_E \frac{k}{2\epsilon} \int_\Omega \left[\epsilon \Delta \phi + \left(\frac{1}{\epsilon} \phi + C_0 \sqrt{2} \right) \left(1 - \phi^2 \right) \right]^2 \, d\Omega \\
\text{subject to} \quad & V(\phi) = \frac{1}{2} \left(Vol(\Omega) + \int_\Omega \phi \, d\Omega \right) = V_0 \\
& A(\phi) = f_A \int_\Omega \left[\frac{\epsilon}{2} |\nabla \phi|^2 + \frac{1}{4\epsilon} (\phi^2 - 1)^2 \right] \, d\Omega = A_0 \\
& M(\phi) = \int_\Omega \phi \, (z - z_0) \, d\Omega = 0
\end{aligned}
\tag{1}
$$

where ϕ is the phase-field, ϵ the transition parameter, C_0 the spontaneous curvature, $f_E = \frac{3}{8\sqrt{2}}$, $f_A = \frac{3}{2\sqrt{2}}$, k the bending rigidity, V_0 and S_0 the volume and area constraints, respectively.

We discretize these equations with LME approximation schemes and apply augmented Lagrangian methods to impose the linear and nonlinear constraints, and L-BFGS and Newton-Rahpson techniques to solve the nonlinear problem. We also propose an adaptive algorithm based on Centroidal Voronoi Tesselations (Du et al., 1999) to reduce the computational cost. We refer to see (Rosolen et al., 2010) for a detailed explanation about the approximants, the discretization procedure, the numerical strategy to solve the problem, and the adaptive algorithm.

2.2 Numerical example

This selected example illustrates how positivity, smoothness and convex properties of LME approximants can be exploited to deal with non-structured grid of points and to be combined with adaptivity strategies.

The accuracy of phase-field results is intrinsically associated to the value of the transition parameter ϵ, which is in turn directly related with the size of the discretization. It motivates to study two relevant aspects of the proposed method: (i) the convergence for a fixed transition parameter ϵ and uniform grid of points, and (ii) the convergence to a sharp model for variable ϵ and adapted grid of points.

(i) Convergence for fixed transition parameter ϵ and uniform grid of points

The energies computed for the oblate equilibrium shape considering different values of ϵ and several level of refinement for the grid of points are shown in Table 1. The identification code and the number of nodes for each grid are indicated in the first and the second column, respectively. As the grids are not perfectly uniform, the values of the average nodal spacing $\bar{h}$ (average element size in finite element terminology) are denoted in the third column. The remaining columns correspond to the values of energies for different values of transition parameter ϵ. The minimum value for the transition parameter is related with the discretization size: we consider that the relation $\epsilon \geq 2h$ is quite reasonable. It can be appreciated that values of energy converge for each fixed ϵ (columns) and, if we take as reference the value of the grid O7, the error becomes gradually less as the grid of points is refined. The largest errors are presented by the values of the upper supra-diagonal, and it happens because they do not fulfill the mentioned relation between the transition paremeter and the discretization size. We can also observe that the values of the energy converge to the sharp-interface value $E_{oblate} = 9.12657$ as

the value of ϵ decreases.

ID	# nodes	h	$\epsilon = 0.05$	$\epsilon = 0.04$	$\epsilon = 0.03$	$\epsilon = 0.02$	$\epsilon = 0.01$
O1	6124	0.024	9.71279	9.59056	–	–	–
O2	12271	0.017	9.72137	9.59446	9.43775	–	–
O3	24597	0.012	9.72671	9.59553	9.43483	9.29532	–
O4	49145	0.0084	9.73203	9.59786	9.43515	9.28938	–
O5	98388	0.0059	9.73536	9.59901	9.43481	9.28674	9.22082
O6	146545	0.0048	9.73716	9.59948	9.43422	9.28378	9.19139
O7	296344	0.0034	9.73989	9.60053	9.43437	9.28326	9.18627

Table 1: Energies of the oblate equilibrium shape for different uniform grids of points and several values of ϵ. The size of the computational domain is $[0, 1.5] \times [0, 2]$.

(ii) Convergence for variable transition parameter ϵ and adapted grid of points

In Table 2 we indicate the bending energies of the oblate equilibrium shape for uniform and adapted grids of 6124 points. The first and last rows give information about the uniform grids of points. The other three rows correspond to the adapted grids computed in each loop of the adaptive strategy. The first column of the table gives an identification code for the grids of points, which are illustrated in Figure 1. The minimum possible value for the transition parameter ϵ_{min} in each loop of the adaptive strategy is determined by the nodal spacing distribution. It can be appreciated that the energies converge to those indicated in Table 1, which demonstrate the well performance of the adaptive strategy.
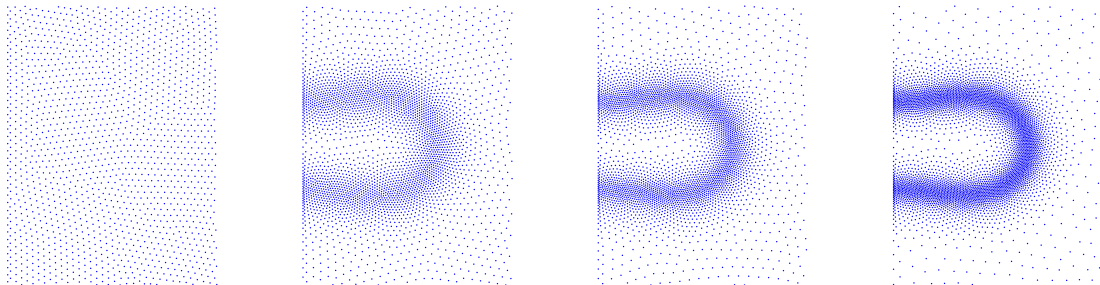

Figure 1: Detail of the uniform and adapted grid of 6124 points (oblate equilibrium shape). From left to rigth: O1, O11, O12 and O13. The features of each grid of points are indicated in Table 2.

ID	Description	$\epsilon = 0.04$	$\epsilon = 0.03$	$\epsilon = 0.025$	$\epsilon = 0.02$	$\epsilon = 0.015$	$\epsilon = 0.01$
O1	Uniform	9.59056	–	–	–	–	–
O11	Adapted	9.59678	9.44002	–	–	–	–
O12	Adapted	–	9.43506	9.35810	9.28849	–	–
O13	Adapted	–	–	9.35970	9.28701	9.22588	9.18703
O7	Uniform	9.60053	9.43437	9.35488	9.28326	9.22399	9.18627

Table 2: Energies of the oblate equilibrium shape for several values of ϵ and uniform and adapted grids of 6124 points.
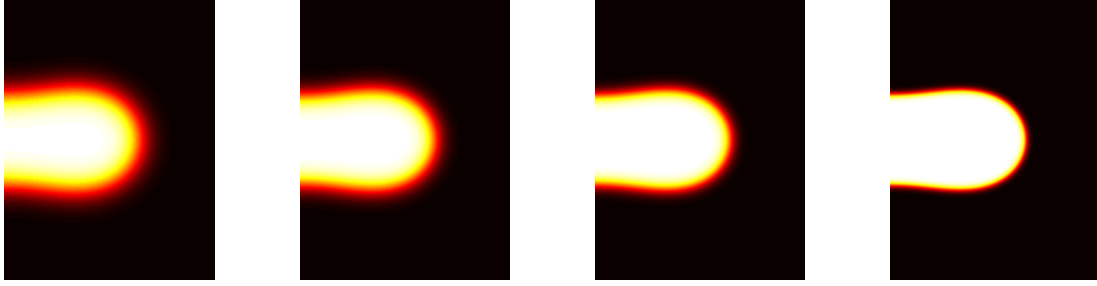
Figure 2: Phase-field density for different grids of 6124 points (oblate equilibrium shape). From left to rigth: O1 with $\epsilon = 0.04$, O11 with $\epsilon = 0.03$, O12 with $\epsilon = 0.02$, and O13 with $\epsilon = 0.01$. The values of energy for each solution and the features of the grids of points are indicated in Table 2.

3 MODEL OF THE FLUID: STOKES FLOW

In this section we introduce the Stokes flow problem and explain the LME stabilizing method, whose performance is illustrated for a classical benchmark test.

3.1 Introduction

The Stokes problem can be set in general form as:

$$
\begin{aligned}
-\nu \triangle u + \nabla p &= f \quad \text{in } \Omega \\
\nabla \cdot u &= 0 \quad \text{in } \Omega \\
u &= u_d \quad \text{on } \Gamma_d
\end{aligned}
\tag{2}
$$

where v is the velocity, p the pressure, f the vector of body forces, ν the kinematic viscosity, and $\Omega \subset \mathbb{R}^d$.

Let be $V = H_0^1(\Omega)^d$ and $Q = L_2(\Omega)/\mathbb{R}$ the velocity and pressure spaces, respectively. Then, the weak form is set to find $u \in V$ and $p \in Q$ such that:

$$
\begin{aligned}
a(u, v) - b(p, v) &= l(v) \quad v \in V \\
b(q, u) &= 0 \quad q \in Q
\end{aligned}
\tag{3}
$$

This weak form is well-known and widely studied in literature. The main conclusions from the mathematical point of view are the ones that concern to the existence and uniqueness of the solution of the system, condensed in the Ladyzhenskaya-Babuška-Brezzi (LBB) condition. This rule states that the following inf-sub condition has to be fulfilled to guarantee the stability of the system (matrix of the system derived non singular):

$$
\inf_{q \in Q} \sup_{v \in V} \frac{b(q, v)}{\|q\|_Q \|v\|_V} \geq K_b > 0
\tag{4}
$$

This condition holds true if $b(q, v) = (q, \nabla \cdot v)$, $q \in Q = L_2(\Omega)/\mathbb{R}$ and $v \in V = H_0^1(\Omega)^d$, meaning that the existence and uniqueness of solution is proved for Stokes problem at a continuous level. Unfortunately, when the equations are discretized with restrictive spaces, that is, $Q_h \subset Q$ and $V_h \subset V$, the LBB condition can fail and the pressure become unbounded. In particular, it is proven that using the same discretization space for both pressure and velocity

results in a loss of stability, which is the cardinal issue of numerical methods for solving the Stokes problem.

3.2 Stabilization of Stokes equations

Main strategies to deal with this obstacle are mixed formulations and stabilization of Stokes equations. The mixed formulations tackle the problem by seeking admissible pairs of spaces that fulfill the inf-sup condition. The main drawback of this strategy is the necessity of using two different discretizations for pressure and velocity, hence increasing the calculation effort.

The stabilization strategy faces the loss of stability inheriting the techniques developed for convection-diffussion problems, adding terms to the original weak form to stabilize the resulting matrix for a discretization based on a single space for both pressure and velocity. These techniques have undergone a large and satisfactory development in the FEM context (Codina, 1998). We develop a LME stabilization method inspired in FEM stabilization ideas. Because of the noticeable differences between FEM and LME, the application of the FEM based methods is not direct and redefinition of parameters is needed. The discretization of the Stokes problem leads to the following system:

$$
\begin{bmatrix} K & -D^T \\ D & 0 \end{bmatrix} \begin{bmatrix} U \\ P \end{bmatrix} = \begin{bmatrix} F \\ 0 \end{bmatrix} \tag{5}
$$

where K comes from the Laplacian velocity and it is definite positive, while D corresponds to the pressure terms and introduces the inestability to the total matrix. To stabilize the system we need to add an extra term to the weak form (Codina, 1998):

$$
\int_\Omega \boldsymbol{\tau} \, \mathcal{P}(w, q) \, \mathcal{R}(u, p) \, d\Omega \tag{6}
$$

where $\mathcal{R}(u, p)$ is the residual or strong form of the problem (which ensures the consistency of the new weak form), τ is a parameter which controls the measure of the stabilization to be applied and $\mathcal{P}$ is a partition of the differential operator. Different choices of this partition lead to different stabilization methods.

To summarize the effect of the stabilization methods and to provide an integrated way of implementation in the code, the following general term becomes adequate from now on (Barth et al., 2004):

$$
\int_\Omega \tau_1 \left(-\alpha \nu \Delta w + \beta_1 \nabla q \right) \left(-\nu \Delta u + \nabla p - f \right) d\Omega \tag{7}
$$

where α and β_1 are parameters that take values $1, 0, -1$ the former, and $1, -1$ the latter. The different combinations of the values enable the user to jump from one stabilization method to another while mantaining the same term structure.

This last expression can be developed in a larger group of terms to add their discretized matrices to the original matrix form of the Stokes problem, resulting:

$$
\begin{bmatrix} K + \alpha K_{st} & -D^T - \alpha D_{st}^T \\ \beta_2 D - \beta_1 D_{st} & \beta_1 L_{st} \end{bmatrix} \begin{bmatrix} U \\ P \end{bmatrix} = \begin{bmatrix} F - \alpha F'_{st} \\ \beta_1 F''_{st} \end{bmatrix} \tag{8}
$$

where $\beta_2 = -\beta_1$ and L_{st} is a positive definite matrix since comes from a pressure Laplacian. This matrix gives to the global matrix the stabilization needed to be non singular and subsequently provide a solution for the system.

3.3 Numerical example

We select and apply the GLS-LME stabilization technique ($\alpha = 1$ and $\beta_1 = 1$) to the classical Poiseouille and Colliding flows benchmark tests for the Stokes problem. Here we only illustrate the performance of the method for the Colliding flows, but similar results were obtained for the Poiseouille problem.

The essential boundary conditions of the problem are plotted in Figure 3(left). The velocity field is illustrated in the Figure 4 without the application of stabilizing method (left) and after stabilization (right). Although we have illustrated the solutions corresponding to a coarse grid of points for clearness purposes, the observed patterns are maintained in refined grids. The velocity stabilized solutions do no present a strange physical behaviour when compared with the analytical one. This fact is reflected in the recovery of the optimal rate for L_2 norm convergence after the stabilization, as it is illustrated in the Figure 3(right).
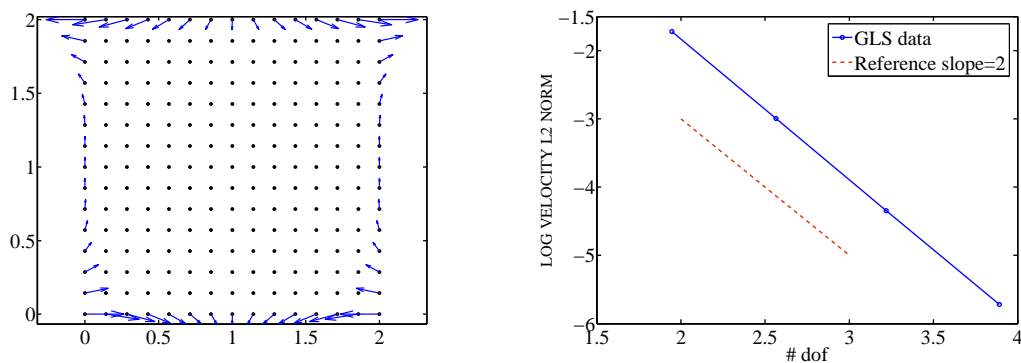

Figure 3: (Left) Definition of the Colliding flow problem, and (right) Velocity convergence with GLS-LME stabilized, $\gamma = 1.0$, and 36, 144, 225, 625 nodes.
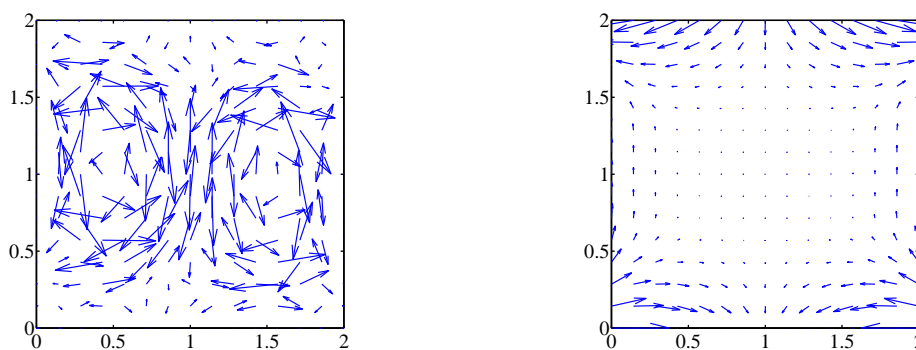

Figure 4: Colliding flow velocity stabilization: (left) Velocity field with no stabilization computed with 225 nodes, and (right) Velocity field stabilized computed with GLS-LME, 225 nodes and $\gamma = 1.0$.

In the Figure 5(left) we plot the pressure for the solution without stabilization. Disproportionate values of pressure and oscillations are observed. This anomalous behaviour dissapears after the stabilization and the obtained solution recovers the smoothness, matching the analytical field.
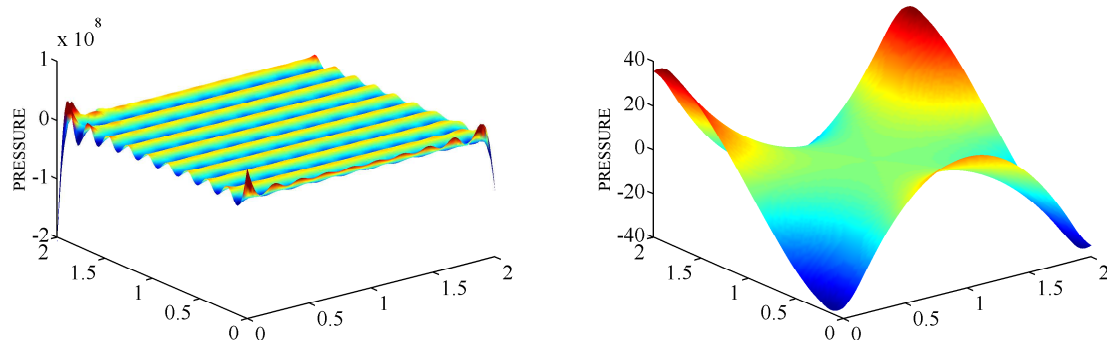
Figure 5: Colliding flow pressure stabilization: (left) Pressure field with no stabilization computed with 625 nodes, and (right) Pressure field stabilized computed with GLS-LME, 625 nodes and $\gamma = 1.0$.

4 CONCLUSIONS

We explain how the biomembranes structural behaviour can be modeled through an energy constrained-minimization phase-field problem. We indicate algorithms to solve the problem and also propose an adaptive strategy based on LME approximants and Centroidal Voronoi Tessellations. We illustrate the performance of the proposed method with a representative example.

We propose a stabilization technique inspired in the well-known FEM stabilization methods to solve the Stokes problem with LME. We illustrate the capability of the proposed scheme in the classical Colliding flows benchmark problem.

The future work involves the coupling of the phase-field model and the Stokes flow to simulate the dynamics of a vesicle.

ACKNOWLEDGEMENTS

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