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John W. Barrett, Harald Garcke and Robert Nürnberg

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Finite Element Approximation for the Dynamics of Asymmetric Fluidic Biomembranes

John W. Barrett[†] Harald Garcke[‡] Robert Nürnberg[†]

Abstract

We present a parametric finite element approximation of a fluidic membrane, whose evolution is governed by a surface Navier–Stokes equation coupled to bulk Navier–Stokes equations. The elastic properties of the membrane are modelled with the help of curvature energies of Willmore and Helfrich type. Forces stemming from these energies act on the surface fluid, together with a forcing from the bulk fluid. Using ideas from PDE constrained optimization, a weak formulation is derived, which allows for a stable semi-discretization. An important new feature of the present work is that we are able to also deal with spontaneous curvature and an area-difference elasticity contribution in the curvature energy. This allows for the modelling of asymmetric membranes, which compared to the symmetric case lead to quite different shapes. This is demonstrated in the numerical computations presented.

Key words. fluidic membranes, incompressible two-phase flow, parametric finite elements, Helfrich energy, spontaneous curvature, area difference elasticity (ADE), local surface area conservation, Boussinesq–Scriven surface fluid

AMS subject classifications. 65M60, 65M12, 76M10, 76Z99, 92C05, 35Q35, 76D05

1 Introduction

Biomembranes and vesicles typically consist of lipid bilayers, which have elastic properties that can be modelled with the help of curvature energies. Already in equilibrium one observes a variety of shapes, and we refer to the overview by Seifert (1997) for a detailed account of the arising forms. The membranes typically are in a fluidic state, and they are locally incompressible. Hence the incompressible surface Navier–Stokes equations

[†]Department of Mathematics, Imperial College London, London, SW7 2AZ, UK
[‡]Fakultät für Mathematik, Universität Regensburg, 93040 Regensburg, Germany

describe the flow on the membrane. These surface Navier–Stokes equations have to be coupled to bulk Navier–Stokes equations, which model the evolution of the surrounding bulk fluid. Stresses resulting from the bulk fluid act on the membrane, as well as forces stemming from the first variation of the curvature energy. The underlying elastic energy is a generalization of the Willmore energy, see Willmore (1993), which is proportional to the integral of the squared mean curvature. Due to the bilayer structure of the membrane, often a top-down asymmetry arises, which makes it necessary to generalize the Willmore curvature model. One example of such a generalized model is the spontaneous curvature model, in which the Willmore energy $\frac{1}{2}\int_\Gamma \varkappa^2$ is replaced by $\frac{1}{2}\int_\Gamma (\varkappa - \overline{\varkappa})^2$ where $\varkappa$ is the mean curvature and $\overline{\varkappa}$ is a given constant. This model goes back to Helfrich (1973) and Canham (1970), and it is by now widely used. We refer to Martens and McMahon (2008) and Kamal *et al.* (2009) for recent discussions and experiments related to this model.

A typical phenomenon is that the two layers of the membrane bilayer have a different number of molecules. Since the distance d between the two layers is small, one can approximate the area difference between the two layers by $d\int_\Gamma \varkappa$. Based on this, Miao *et al.* (1994) introduced a curvature model which still assumes that the mid-plane between the two layers is incompressible. However, the two layers themselves can slightly compress or expand under stress. The area difference between the two layers then leads to the fact that a certain value for $\int_\Gamma \varkappa$ is energetically favorable. In the area-difference elasticity (ADE) model of Miao *et al.* (1994), see also Seifert (1997), a contribution which is proportional to $(\int_\Gamma \varkappa - M_0)^2$, where M_0 is the relaxed area difference, is added to the elastic curvature energy. For more details on this curvature elasticity model we refer to the excellent overview by Seifert (1997), and for more information on fluid vesicles and membranes in fluids, we refer to the recent work of Abreu *et al.* (2014).

The overall dynamical model studied in this paper is given by the coupled bulk and surface Navier–Stokes equations, as discussed above, while taking a forcing from the curvature elasticity energy into account. Without the ADE-contribution this model goes back to Arroyo and DeSimone (2009). A mathematical analysis, also considering well-posedness issues of variants of this model, has been performed by Köhne and Lengeler (2015) and Lengeler (2015). The dynamics of lipid membranes and vesicles have been studied numerically by many authors. We only refer to the work of Aland *et al.* (2014); Arroyo and DeSimone (2009); Barrett *et al.* (2008b, 2014b); Bonito *et al.* (2010, 2011); Du *et al.* (2004); Elliott and Stinner (2010); Franke *et al.* (2011); Hu *et al.* (2014); Krüger *et al.* (2013); Laadhari *et al.* (2014); McWhirter *et al.* (2009); Mercker *et al.* (2013); Rahimi and Arroyo (2012); Rodrigues *et al.* (2014); Salac and Miksis (2012); Shi *et al.* (2014). The above mentioned papers used different evolution laws (L^2–gradient flow, simplified fluid models, phase field evolutions, particle-based hydrodynamic evolutions, etc.), and often simplified curvature elasticity models, or substituted the curvature contributions by a spring type model.

Due to the complexity of the model, results on the numerical analysis of this type of problem is limited. In a numerical method, fluid flow with an interface has to be addressed, as well as the curvature energy. In addition, these two contributions have to be coupled appropriately. For numerical aspects of fluid flow with a free boundary we refer

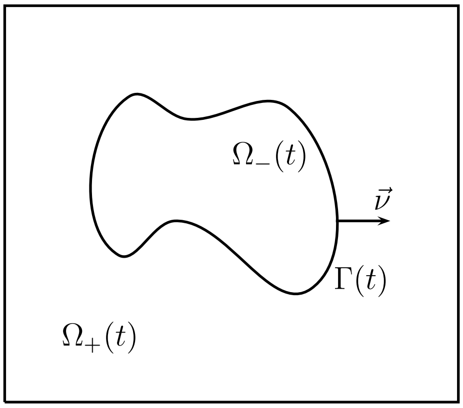

Figure 1: The domain Ω in the case $d = 2$.

the reader to the book of Groß and Reusken (2011) and to Bänsch (2001). An important contribution to the numerical approximation of evolution problems involving curvature energies of Willmore type is due to Dziuk (2008), who introduced a semi-discretization of the L^2–gradient flow of the Willmore energy, for which he was able to show a stability result.

It is the goal of this paper to introduce a discretization of the full problem, also involving energy contributions arising from the asymmetry of the membrane. Hence the equations also involve spontaneous curvature and/or area-difference elasticity contributions to the energy. Using ideas from PDE constrained optimization, we are able to derive a weak formulation (Section 3), which then allows for a semi-discretization (continuous in time, discrete in space), for which we can show a stability bound. The discretization is based on a parametric method for the interface, which is then coupled in an unfitted way to the bulk equations. The velocity and pressure in the bulk are discretized with the help of standard Taylor–Hood type elements (Section 4). For the fully discrete and fully coupled discrete system we can show unique solvability under appropriate assumptions (Section 5). After a discussion of possible solution methods for the resulting linear systems (Section 6), we present several numerical computations demonstrating the practicability of the method and the effect of the asymmetry in the membrane (Section 7).

2 Governing equations

Let $\Omega \subset \mathbb{R}^d$ be a given domain, where $d = 2$ or $d = 3$. We seek a time dependent interface $(\Gamma(t))_{t\in[0,T]}$, $\Gamma(t) \subset \Omega$, which for all $t \in [0, T]$ separates Ω into a domain $\Omega_+(t)$, occupied by the outer phase, and a domain $\Omega_-(t) := \Omega \setminus \overline{\Omega}_+(t)$, which is occupied by the inner phase, see Figure 1 for an illustration. For later use, we assume that $(\Gamma(t))_{t\in[0,T]}$ is a sufficiently smooth evolving hypersurface without boundary that is parameterized by

$\vec{x}(\cdot,t):\Upsilon\to\mathbb{R}^d$, where $\Upsilon\subset\mathbb{R}^d$ is a given reference manifold, i.e. $\Gamma(t)=\vec{x}(\Upsilon,t)$. Then

$$\vec{\mathcal{V}}(\vec{z},t):=\vec{x}_t(\vec{q},t)\qquad\forall\ \vec{z}=\vec{x}(\vec{q},t)\in\Gamma(t) \tag{2.1}$$

defines the velocity of $\Gamma(t)$, and $\mathcal{V}:=\vec{\mathcal{V}}\,.\,\vec{\nu}$ is the normal velocity of the evolving hypersurface $\Gamma(t)$, where $\vec{\nu}(t)$ is the unit normal on $\Gamma(t)$ pointing into $\Omega_+(t)$. Moreover, we define the space-time surface $\mathcal{G}_T:=\bigcup_{t\in[0,T]}\Gamma(t)\times\{t\}$.

Let $\rho(t)=\rho_+\,\mathcal{X}_{\Omega_+(t)}+\rho_-\,\mathcal{X}_{\Omega_-(t)}$, with $\rho_\pm\in\mathbb{R}_{\geq 0}$, denote the fluid densities, where here and throughout $\mathcal{X}_\mathcal{A}$ defines the characteristic function for a set $\mathcal{A}$. Denoting by $\vec{u}:\Omega\times[0,T]\to\mathbb{R}^d$ the fluid velocity, by $\underline{\underline{\sigma}}:\Omega\times[0,T]\to\mathbb{R}^{d\times d}$ the stress tensor, and by $\vec{f}:\Omega\times[0,T]\to\mathbb{R}^d$ a possible volume force, the incompressible Navier–Stokes equations in the two phases are given by

$$\rho\,(\vec{u}_t+(\vec{u}\,.\,\nabla)\,\vec{u})-\nabla\,.\,\underline{\underline{\sigma}}=\rho\,\vec{f}\qquad\text{in }\Omega_\pm(t)\,, \tag{2.2a}$$

$$\nabla\,.\,\vec{u}=0\qquad\text{in }\Omega_\pm(t)\,, \tag{2.2b}$$

$$\vec{u}=\vec{g}\qquad\text{on }\partial_1\Omega\,, \tag{2.2c}$$

$$\underline{\underline{\sigma}}\,\vec{\mathrm{n}}=\vec{0}\qquad\text{on }\partial_2\Omega\,, \tag{2.2d}$$

where $\partial\Omega=\partial_1\Omega\cup\partial_2\Omega$, with $\partial_1\Omega\cap\partial_2\Omega=\emptyset$, denotes the boundary of Ω with outer unit normal $\vec{\mathrm{n}}$. Hence (2.2c) prescribes a possibly inhomogeneous Dirichlet condition for the velocity on $\partial_1\Omega$, which collapses to the standard no-slip condition when $\vec{g}=\vec{0}$, while (2.2d) prescribes a stress-free condition on $\partial_2\Omega$. Throughout this paper we assume that $\mathcal{H}^{d-1}(\partial_1\Omega)>0$. We will also assume w.l.o.g. that $\vec{g}$ is extended so that $\vec{g}:\Omega\to\mathbb{R}^d$. In addition, the stress tensor in (2.2a) is defined by

$$\underline{\underline{\sigma}}=\mu\,(\nabla\,\vec{u}+(\nabla\,\vec{u})^T)-p\,\underline{\underline{\mathrm{Id}}}=2\,\mu\,\underline{\underline{D}}(\vec{u})-p\,\underline{\underline{\mathrm{Id}}}\,, \tag{2.3}$$

where $\underline{\underline{\mathrm{Id}}}\in\mathbb{R}^{d\times d}$ denotes the identity matrix and $\underline{\underline{D}}(\vec{u}):=\frac{1}{2}\,(\nabla\,\vec{u}+(\nabla\,\vec{u})^T)$ is the rate-of-deformation tensor, with $\nabla\,\vec{u}=\left(\partial_{x_j}\,u_i\right)_{i,j=1}^d$. Moreover, $p:\Omega\times[0,T]\to\mathbb{R}$ is the pressure and $\mu(t)=\mu_+\,\mathcal{X}_{\Omega_+(t)}+\mu_-\,\mathcal{X}_{\Omega_-(t)}$, with $\mu_\pm\in\mathbb{R}_{>0}$, denotes the dynamic viscosities in the two phases. On the free surface $\Gamma(t)$, the following conditions need to hold:

$$[\vec{u}]_-^+=\vec{0}\qquad\text{on }\Gamma(t)\,, \tag{2.4a}$$

$$\rho_\Gamma\,\partial_t^\bullet\,\vec{u}-\nabla_s\,.\,\underline{\underline{\sigma}}_\Gamma=[\underline{\underline{\sigma}}\,\vec{\nu}]_-^+ +\alpha\,\vec{f}_\Gamma\qquad\text{on }\Gamma(t)\,, \tag{2.4b}$$

$$\nabla_s\,.\,\vec{u}=0\qquad\text{on }\Gamma(t)\,, \tag{2.4c}$$

$$\vec{\mathcal{V}}\,.\,\vec{\nu}=\vec{u}\,.\,\vec{\nu}\qquad\text{on }\Gamma(t)\,, \tag{2.4d}$$

where $\rho_\Gamma\in\mathbb{R}_{\geq 0}$ denotes the surface material density, $\alpha\in\mathbb{R}_{>0}$ is the bending rigidity and $\vec{f}_\Gamma:=f_\Gamma\,\vec{\nu}$ is defined by (2.11b). In addition, $\nabla_s\,.$ denotes the surface divergence on $\Gamma(t)$, and the surface stress tensor is given by

$$\underline{\underline{\sigma}}_\Gamma=2\,\mu_\Gamma\,\underline{\underline{D}}_s(\vec{u})-p_\Gamma\,\underline{\underline{\mathcal{P}}}_\Gamma\quad\text{on }\Gamma(t)\,, \tag{2.5}$$

where $\mu_\Gamma\in\mathbb{R}_{\geq 0}$ is the interfacial shear viscosity and p_Γ denotes the surface pressure, which acts as a Lagrange multiplier for the incompressibility condition (2.4c). Here

$$\underline{\underline{\mathcal{P}}}_\Gamma=\underline{\underline{\mathrm{Id}}}-\vec{\nu}\otimes\vec{\nu}\quad\text{on }\Gamma(t) \tag{2.6a}$$

and

$$\underline{\underline{D}}_s(\vec{u}) = \tfrac{1}{2}\,\underline{\underline{\mathcal{P}}}_\Gamma\,(\nabla_s\,\vec{u} + (\nabla_s\,\vec{u})^T)\,\underline{\underline{\mathcal{P}}}_\Gamma \quad \text{on } \Gamma(t)\,, \tag{2.6b}$$

where $\nabla_s = \underline{\underline{\mathcal{P}}}_\Gamma\,\nabla = (\partial_{s_1}, \ldots, \partial_{s_d})$ denotes the surface gradient on $\Gamma(t)$, and $\nabla_s\,\vec{u} = \left(\partial_{s_j}\,u_i\right)_{i,j=1}^{d}$. Moreover, as usual, $[\vec{u}]_-^+ := \vec{u}_+ - \vec{u}_-$ and $[\underline{\underline{\sigma}}\,\vec{\nu}]_-^+ := \underline{\underline{\sigma}}_+\,\vec{\nu} - \underline{\underline{\sigma}}_-\,\vec{\nu}$ denote the jumps in velocity and normal stress across the interface $\Gamma(t)$. Here and throughout, we employ the shorthand notation $\vec{b}_\pm := \vec{b}\,|_{\Omega_\pm(t)}$ for a function $\vec{b} : \Omega \times [0,T] \to \mathbb{R}^d$; and similarly for scalar and matrix-valued functions. In addition,

$$\partial_t^\bullet\,\zeta = \zeta_t + \vec{u}\,.\,\nabla\,\zeta \qquad \forall\,\zeta \in H^1(\mathcal{G}_T) \tag{2.7}$$

denotes the material time derivative of ζ on $\Gamma(t)$. We compute $\partial_t^\bullet\,\zeta$ with the help of an extension of ζ to a neighborhood of $\mathcal{G}_T$. Here we stress that the derivative in (2.7) is well-defined, and depends only on the values of ζ on $\mathcal{G}_T$, even though ζ_t and $\nabla\,\zeta$ do not make sense separately for a function defined on $\mathcal{G}_T$; see e.g. Dziuk and Elliott (2013, p. 324). The system (2.2a–d), (2.3), (2.4a–d), (2.5) is closed with the initial conditions

$$\Gamma(0) = \Gamma_0\,, \quad \rho\,\vec{u}(\cdot,0) = \rho\,\vec{u}_0 \quad \text{in } \Omega\,, \quad \rho_\Gamma\,\vec{u}(\cdot,0) = \rho_\Gamma\,\vec{u}_0 \quad \text{on } \Gamma_0\,, \tag{2.8}$$

where $\Gamma_0 \subset \Omega$ and $\vec{u}_0 : \Omega \to \mathbb{R}^d$ are given initial data satisfying $\rho\,\nabla\,.\,\vec{u}_0 = 0$ in Ω, $\rho_\Gamma\,\nabla_s\,.\,\vec{u}_0 = 0$ on Γ_0 and $\rho_+\,\vec{u}_0 = \rho_+\,\vec{g}$ on $\partial_1\Omega$. Of course, in the case $\rho_- = \rho_+ = \rho_\Gamma = 0$ the initial data $\vec{u}_0$ is not needed. Similarly, in the case $\rho_- = \rho_+ = 0$ and $\rho_\Gamma > 0$ the initial data $\vec{u}_0$ is only needed on Γ_0. However, for ease of exposition, and in view of the unfitted nature of our numerical method, we will always assume that $\vec{u}_0$, if required, is given on all of Ω.

It is not difficult to show that the conditions (2.2b) enforce volume preservation for the phases, while (2.4c) leads to the conservation of the total surface area $\mathcal{H}^{d-1}(\Gamma(t))$, see Section 3 below for the relevant proofs. As an immediate consequence we obtain that spheres remain spheres, and that spheres with a zero bulk velocity are stationary solutions.

Furthermore, we note that

$$\nabla_s\,.\,\underline{\underline{\sigma}}_\Gamma = 2\,\mu_\Gamma\,\nabla_s\,.\,\underline{\underline{D}}_s(\vec{u}) - \nabla_s\,.\,[p_\Gamma\,\underline{\underline{\mathcal{P}}}_\Gamma] = 2\,\mu_\Gamma\,\nabla_s\,.\,\underline{\underline{D}}_s(\vec{u}) - \nabla_s\,p_\Gamma - \varkappa\,p_\Gamma\,\vec{\nu}\,.$$

Here $\varkappa$ denotes the mean curvature of $\Gamma(t)$, i.e. the sum of the principal curvatures $\varkappa_i$, $i = 1, \ldots, d-1$, of $\Gamma(t)$, where we have adopted the sign convention that $\varkappa$ is negative where $\Omega_-(t)$ is locally convex. In particular, it holds that

$$\Delta_s\,\vec{\mathrm{id}} = \varkappa\,\vec{\nu} =: \vec{\varkappa} \qquad \text{on } \Gamma(t)\,,$$

where $\Delta_s = \nabla_s\,.\,\nabla_s$ is the Laplace–Beltrami operator on $\Gamma(t)$.

Finally, the Willmore energy of $\Gamma(t)$ is given by

$$E(\Gamma(t)) = \tfrac{1}{2}\int_{\Gamma(t)} \varkappa^2 \,\mathrm{d}\mathcal{H}^{d-1} = \tfrac{1}{2}\int_{\Gamma(t)} |\vec{\varkappa}|^2 \,\mathrm{d}\mathcal{H}^{d-1}\,, \tag{2.9}$$

see e.g. Willmore (1993) for details.

Realistic models for biological cell membranes lead to energies more general than (2.9). In the original derivation of Helfrich (1973) a possible asymmetry in the membrane, originating e.g. from a different chemical environment, was taken into account. This led Helfrich to the energy

$$E_{\overline{\varkappa}}(\Gamma(t)) = \tfrac{1}{2} \int_{\Gamma(t)} (\varkappa - \overline{\varkappa})^2 \, \mathrm{d}\mathcal{H}^{d-1} = \tfrac{1}{2} \int_{\Gamma(t)} |\vec{\varkappa} - \overline{\varkappa}\, \vec{\nu}|^2 \, \mathrm{d}\mathcal{H}^{d-1} \,,$$

where $\overline{\varkappa} \in \mathbb{R}$ is the given so-called spontaneous curvature. Biological membranes consist of two layers of lipids. The number of lipid molecules is conserved and there are osmotic pressure effects, arising from the chemistry around the lipid. These both lead to constraints on the possible membrane configurations. Most models for bilayer membranes take *hard constraints on the total area and the enclosed volume* of the membrane into account. The fact that it is difficult to exchange molecules between the two layers imply that the total number of lipids in each layer is conserved and hence an area difference between the two layers will appear. The actual area difference can, to leading order, be described with the help of the total integrated mean curvature, see Seifert (1997). Now one can either incorporate this area difference by a hard constraint on the integrated mean curvature or one can penalize deviations from an optimal area difference. In the latter case, we obtain the energy

$$E_{\overline{\varkappa},\beta}(\Gamma(t)) := E_{\overline{\varkappa}}(\Gamma(t)) + \tfrac{\beta}{2} \left(M(\Gamma(t)) - M_0\right)^2 \tag{2.10a}$$

with

$$M(\Gamma(t)) = \int_{\Gamma(t)} \varkappa \, \mathrm{d}\mathcal{H}^{d-1} = \int_{\Gamma(t)} \vec{\varkappa} \,.\, \vec{\nu} \, \mathrm{d}\mathcal{H}^{d-1} \tag{2.10b}$$

and given constants $\beta \in \mathbb{R}_{\geq 0}$, $M_0 \in \mathbb{R}$. Models employing the energy (2.10a) are often called area-difference elasticity (ADE) models, see Seifert (1997).

Now the source term f_Γ in (2.4b) is given by the first variation of the energy (2.10a), i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t} E_{\overline{\varkappa},\beta}(\Gamma(t)) = - \int_{\Gamma(t)} f_\Gamma \, \mathcal{V} \, \mathrm{d}\mathcal{H}^{d-1} = - \int_{\Gamma(t)} \vec{f}_\Gamma \,.\, \vec{\mathcal{V}} \, \mathrm{d}\mathcal{H}^{d-1} \,, \tag{2.11a}$$

where $\vec{f}_\Gamma := f_\Gamma \, \vec{\nu}$ and

$$f_\Gamma = -\Delta_s \, \varkappa - (\varkappa - \overline{\varkappa}) \, |\nabla_s \, \vec{\nu}|^2 + \tfrac{1}{2} (\varkappa - \overline{\varkappa})^2 \, \varkappa + \beta \left(M(\Gamma(t)) - M_0\right) \left(|\nabla_s \, \vec{\nu}|^2 - \varkappa^2\right) \quad \text{on} \quad \Gamma(t) \,. \tag{2.11b}$$

A short derivation of (2.11a,b) can be found in Barrett *et al.* (2008b). We note that in the case $d = 2$, on account of the Gauß–Bonnet theorem, it holds that $M(\Gamma(t)) = 2\,\pi\, m(\Gamma(t))$, where $m(\Gamma(t)) \in \{\pm 1\}$ denotes the turning number of $\Gamma(t)$, which is invariant for $(\Gamma(t))_{t \in [0,T]}$. Hence f_Γ is independent of β. Moreover,

$$E_{\overline{\varkappa},0}(\Gamma(t)) = \tfrac{1}{2} \int_{\Gamma(t)} \varkappa^2 + \overline{\varkappa}^2 \, \mathrm{d}\mathcal{H}^1 - \overline{\varkappa}\, M(\Gamma(t)) = \tfrac{1}{2} \int_{\Gamma(t)} \varkappa^2 + \overline{\varkappa}^2 \, \mathrm{d}\mathcal{H}^1 - 2\,\pi\, \overline{\varkappa}\, m(\Gamma(t)) \,.$$

As the total surface length is preserved, due to the condition (2.4c), the forcing f_Γ is also independent of the spontaneous curvature in the case $d = 2$. Hence it only makes sense to consider nonzero values of $\overline{\varkappa}$ and β in the case $d = 3$. Here we note that for $\beta > 0$, as surface area is preserved, the energy (2.10a), up to a constant, is equivalent to (2.10a) with $\overline{\varkappa}$ replaced by zero and M_0 replaced by $M_0 + \frac{\overline{\varkappa}}{\beta}$. Hence it is natural to assume that $\overline{\varkappa} = 0$ if $\beta > 0$.

It does not appear possible to derive a stable discretization of the system (2.2a–d), (2.3), (2.4a–d), (2.5) based on the formulation (2.11b). Hence in the recent paper Barrett *et al.* (2014b), for the case $\overline{\varkappa} = \beta = 0$, the authors made use of the stable approximation of Willmore flow introduced in Dziuk (2008), which is based on the identity $\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\langle\vec\varkappa,\vec\varkappa\rangle_{\Gamma(t)} = -\left\langle \vec f_\Gamma, \vec{\mathcal{V}}\right\rangle_{\Gamma(t)}$, where

$$\left\langle \vec f_\Gamma, \vec\chi\right\rangle_{\Gamma(t)} = \langle\nabla_s\,\vec\varkappa, \nabla_s\,\vec\chi\rangle_{\Gamma(t)} + \langle\nabla_s\,.\,\vec\varkappa, \nabla_s\,.\,\vec\chi\rangle_{\Gamma(t)} + \tfrac{1}{2}\left\langle|\vec\varkappa|^2\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec\chi\right\rangle_{\Gamma(t)} \\ - 2\left\langle\nabla_s\,\vec\varkappa, \underline{\underline{D}}_s(\vec\chi)\,\nabla_s\,\vec{\mathrm{id}}\right\rangle_{\Gamma(t)} \qquad \forall\ \vec\chi \in [H^1(\Gamma(t))]^d\,. \tag{2.12}$$

Here $\langle\cdot,\cdot\rangle_{\Gamma(t)}$ denotes the L^2–inner product on $\Gamma(t)$. We note that the approaches in Dziuk (2008); Barrett *et al.* (2014b) rely on an approximation of the curvature vector $\vec\varkappa$, and so they cannot easily consider nonzero $\overline{\varkappa}$ or nonzero β. It is the aim of the present paper, on combining the techniques in Barrett *et al.* (2014b) and Barrett *et al.* (2012), to introduce a stable numerical approximation of fluidic biomembranes in the presence of spontaneous curvature and ADE. In particular, based on the techniques in Dziuk (2008), and using ideas from the formal calculus of PDE constrained optimization, it is possible to extend the formulation (2.12) to include nonzero $\overline{\varkappa}$ and β.

3 Weak formulations

Before introducing our finite element approximation, we will derive an appropriate weak formulation. Here the main ingredient is to find a suitable formulation of (2.11a,b), which has the property that the source term $\vec f_\Gamma$ can be written as the derivative of a suitable discrete energy. Once such a formulation is obtained, it can then be combined with the weak formulation from Barrett *et al.* (2014b) for the coupled Navier–Stokes bulk/surface equations.

3.1 Fluidic weak formulation for $\overline{\varkappa} = \beta = 0$

We begin by recalling the weak formulation of (2.2a–d), (2.3), (2.4a–d), (2.5) from Barrett *et al.* (2014b). To this end, we introduce the following function spaces for a given $\vec b \in$

$[H^1(\Omega)]^d$:

$$\mathbb{U}(\vec{b}) := \{\vec{\varphi} \in [H^1(\Omega)]^d : \vec{\varphi} = \vec{b} \text{ on } \partial_1\Omega\}\,, \quad \mathbb{V}(\vec{b}) := L^2(0,T;\mathbb{U}(\vec{b})) \cap H^1(0,T;[L^2(\Omega)]^d)\,,$$
$$\mathbb{V}_\Gamma(\vec{b}) := \{\vec{\varphi} \in \mathbb{V}(\vec{b}) : \vec{\varphi}\mid_{\mathcal{G}_T} \in [H^1(\mathcal{G}_T)]^d\}\,.$$

In addition, we let $\mathbb{P} := L^2(\Omega)$ and define

$$\widehat{\mathbb{P}} := \begin{cases} \{\eta \in \mathbb{P} : \int_\Omega \eta \,\mathrm{d}\mathcal{L}^d = 0\} & \text{if } \mathcal{H}^{d-1}(\partial_2\Omega) = 0\,, \\ \mathbb{P} & \text{if } \mathcal{H}^{d-1}(\partial_2\Omega) > 0\,. \end{cases}$$

Moreover, we let $(\cdot,\cdot)$ and $\langle\cdot,\cdot\rangle_{\partial_2\Omega}$ denote the L^2–inner products on Ω and $\partial_2\Omega$.

Similarly to (2.7) we define the following time derivative that follows the parameterization $\vec{x}(\cdot,t)$ of $\Gamma(t)$, rather than $\vec{u}$. In particular, we let

$$\partial_t^\circ\,\zeta = \zeta_t + \vec{\mathcal{V}}\,.\,\nabla\,\zeta \qquad \forall\,\zeta \in H^1(\mathcal{G}_T)\,; \tag{3.1}$$

where we stress once again that this definition is well-defined, even though ζ_t and $\nabla\,\zeta$ do not make sense separately for a function $\zeta \in H^1(\mathcal{G}_T)$. On recalling (2.7) we obtain that $\partial_t^\circ = \partial_t^\bullet$ if $\vec{\mathcal{V}} = \vec{u}$ on $\Gamma(t)$. Moreover, for later use we note that

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\chi,\zeta\rangle_{\Gamma(t)} = \langle\partial_t^\circ\,\chi,\zeta\rangle_{\Gamma(t)} + \langle\chi,\partial_t^\circ\,\zeta\rangle_{\Gamma(t)} + \left\langle\chi\,\zeta,\nabla_s\,.\,\vec{\mathcal{V}}\right\rangle_{\Gamma(t)} \qquad \forall\,\chi,\zeta \in H^1(\mathcal{G}_T)\,, \tag{3.2}$$

see Dziuk and Elliott (2013, Lem. 5.2).

Find $\Gamma(t) = \vec{x}(\Upsilon,t)$ for $t \in [0,T]$ with $\vec{\mathcal{V}} \in [L^2(\mathcal{G}_T)]^d$, and functions $\vec{u} \in \mathbb{V}_\Gamma(\vec{g})$, $p \in L^2(0,T;\widehat{\mathbb{P}})$, $p_\Gamma \in L^2(\mathcal{G}_T)$, $\vec{\varkappa} \in [H^1(\mathcal{G}_T)]^d$ and $\vec{f}_\Gamma \in [L^2(\mathcal{G}_T)]^d$ such that the initial conditions (2.8) hold and such that for almost all $t \in (0,T)$ it holds that

$$\begin{aligned}
&\tfrac12\left[\frac{\mathrm{d}}{\mathrm{d}t}(\rho\,\vec{u},\vec{\xi}) + (\rho\,\vec{u}_t,\vec{\xi}) - (\rho\,\vec{u},\vec{\xi}_t) + (\rho,[(\vec{u}\,.\,\nabla)\,\vec{u}]\,.\,\vec{\xi} - [(\vec{u}\,.\,\nabla)\,\vec{\xi}]\,.\,\vec{u}) + \rho_+\left\langle\vec{u}\,.\,\mathrm{n},\vec{u}\,.\,\vec{\xi}\right\rangle_{\partial_2\Omega}\right] \\
&\quad + 2\,(\mu\,\underline{\underline{D}}(\vec{u}),\underline{\underline{D}}(\vec{\xi})) - (p,\nabla\,.\,\vec{\xi}) + \rho_\Gamma\left\langle\partial_t^\circ\,\vec{u},\vec{\xi}\right\rangle_{\Gamma(t)} + 2\,\mu_\Gamma\left\langle\underline{\underline{D}}_s(\vec{u}),\underline{\underline{D}}_s(\vec{\xi})\right\rangle_{\Gamma(t)} \\
&\quad - \left\langle p_\Gamma,\nabla_s\,.\,\vec{\xi}\right\rangle_{\Gamma(t)} = (\rho\,\vec{f},\vec{\xi}) + \alpha\left\langle\vec{f}_\Gamma,\vec{\xi}\right\rangle_{\Gamma(t)} \qquad \forall\,\vec{\xi} \in \mathbb{V}_\Gamma(\vec{0})\,,
\end{aligned} \tag{3.3a}$$

$$(\nabla\,.\,\vec{u},\varphi) = 0 \qquad \forall\,\varphi \in \widehat{\mathbb{P}}\,, \tag{3.3b}$$

$$\langle\nabla_s\,.\,\vec{u},\eta\rangle_{\Gamma(t)} = 0 \qquad \forall\,\eta \in L^2(\Gamma(t))\,, \tag{3.3c}$$

$$\left\langle\vec{\mathcal{V}} - \vec{u},\vec{\chi}\right\rangle_{\Gamma(t)} = 0 \qquad \forall\,\vec{\chi} \in [L^2(\Gamma(t))]^d\,, \tag{3.3d}$$

$$\langle\vec{\varkappa},\vec{\eta}\rangle_{\Gamma(t)} + \left\langle\nabla_s\,\mathrm{id},\nabla_s\,\vec{\eta}\right\rangle_{\Gamma(t)} = 0 \qquad \forall\,\vec{\eta} \in [H^1(\Gamma(t))]^d\,, \tag{3.3e}$$

$$\begin{aligned}
\left\langle\vec{f}_\Gamma,\vec{\chi}\right\rangle_{\Gamma(t)} &= \langle\nabla_s\,\vec{\varkappa},\nabla_s\,\vec{\chi}\rangle_{\Gamma(t)} + \langle\nabla_s\,.\,\vec{\varkappa},\nabla_s\,.\,\vec{\chi}\rangle_{\Gamma(t)} + \tfrac12\left\langle|\vec{\varkappa}|^2\,\nabla_s\,\mathrm{id},\nabla_s\,\vec{\chi}\right\rangle_{\Gamma(t)} \\
&\quad - 2\left\langle\nabla_s\,\vec{\varkappa},\underline{\underline{D}}_s(\vec{\chi})\,\nabla_s\,\mathrm{id}\right\rangle_{\Gamma(t)} \qquad \forall\,\vec{\chi} \in [H^1(\Gamma(t))]^d\,,
\end{aligned} \tag{3.3f}$$

where in (3.3d) we have recalled (2.1). It is our aim to replace (3.3e,f) with a suitable reformulation of (2.12), where the curvature energy is replaced by (2.10a,b), recall also (2.11a,b).

It was shown in Barrett *et al.* (2014b) that choosing $\vec{\xi} = \vec{u}$ in (3.3a), $\varphi = p(\cdot, t)$ in (3.3b) and $\eta = p_\Gamma(\cdot, t)$ in (3.3c) yields that

$$\tfrac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \left(\|\rho^{\frac{1}{2}} \vec{u}\|_0^2 + \rho_\Gamma \langle \vec{u}, \vec{u} \rangle_{\Gamma(t)} \right) + 2 \|\mu^{\frac{1}{2}} \underline{\underline{D}}(\vec{u})\|_0^2 + 2 \mu_\Gamma \left\langle \underline{\underline{D}}_s(\vec{u}), \underline{\underline{D}}_s(\vec{u}) \right\rangle_{\Gamma(t)} \\ + \tfrac{1}{2} \rho_+ \left\langle \vec{u} \,.\, \mathrm{n}, |\vec{u}|^2 \right\rangle_{\partial_2\Omega} = (\rho \vec{f}, \vec{u}) + \alpha \left\langle \vec{f}_\Gamma, \vec{u} \right\rangle_{\Gamma(t)}, \tag{3.4}$$

which, on combining with $\vec{\chi} = \vec{f}_\Gamma$ in (3.3d), $\vec{\chi} = \vec{\mathcal{V}}$ in (3.3f) and (2.12), gives

$$\tfrac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \left(\|\rho^{\frac{1}{2}} \vec{u}\|_0^2 + \rho_\Gamma \langle \vec{u}, \vec{u} \rangle_{\Gamma(t)} + \alpha \langle \vec{\varkappa}, \vec{\varkappa} \rangle_{\Gamma(t)} \right) + 2 \|\mu^{\frac{1}{2}} \underline{\underline{D}}(\vec{u})\|_0^2 + 2 \mu_\Gamma \left\langle \underline{\underline{D}}_s(\vec{u}), \underline{\underline{D}}_s(\vec{u}) \right\rangle_{\Gamma(t)} \\ + \tfrac{1}{2} \rho_+ \left\langle \vec{u} \,.\, \mathrm{n}, |\vec{u}|^2 \right\rangle_{\partial_2\Omega} = (\rho \vec{f}, \vec{u}) .$$

Moreover, we recall from Barrett *et al.* (2014b) that it follows from (3.3c,d) that

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{H}^{d-1}(\Gamma(t)) = \frac{\mathrm{d}}{\mathrm{d}t} \langle 1, 1 \rangle_{\Gamma(t)} = \left\langle 1, \nabla_s \,.\, \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} = \langle 1, \nabla_s \,.\, \vec{u} \rangle_{\Gamma(t)} = 0 , \tag{3.5}$$

while (3.3b,d) imply that

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{L}^d(\Omega_-(t)) = \left\langle \vec{\mathcal{V}}, \vec{\nu} \right\rangle_{\Gamma(t)} = \langle \vec{u}, \vec{\nu} \rangle_{\Gamma(t)} = \int_{\Omega_-(t)} \nabla \,.\, \vec{u} \, \mathrm{d}\mathcal{L}^d = 0 . \tag{3.6}$$

3.2 The first variation of $E_{\overline{\varkappa},\beta}(\Gamma(t))$

In this section we would like to derive a weak formulation for the first variation of $E_{\overline{\varkappa},\beta}(\Gamma(t))$ with respect to $\Gamma(t) = \vec{x}(\Upsilon, t)$. To this end, for a given $\vec{\chi} \in [H^1(\Gamma(t))]^d$ and for $\delta \geq 0$, let $\vec{\Psi}(\cdot, \delta)$ be a family of transformations such that

$$\Gamma_\delta(t) := \{ \vec{\Psi}(\vec{z}, \delta) : \vec{z} \in \Gamma(t) \} , \quad \text{where} \quad \vec{\Psi}(\vec{z}, 0) = \vec{z} \text{ and } \tfrac{\partial \vec{\Psi}}{\partial \delta}(\vec{z}, 0) = \vec{\chi}(\vec{z}) \quad \forall \vec{z} \in \Gamma(t) .$$

Then the first variation of $\mathcal{H}^{d-1}(\Gamma(t))$ with respect to $\Gamma(t)$ in the direction $\vec{\chi} \in [H^1(\Gamma(t))]^d$ is given by

$$\left[\frac{\delta}{\delta\Gamma} \mathcal{H}^{d-1}(\Gamma(t)) \right] (\vec{\chi}) = \lim_{\delta \to 0} \tfrac{1}{\delta} \left[\mathcal{H}^{d-1}(\Gamma_\delta(t)) - \mathcal{H}^{d-1}(\Gamma(t)) \right] = \left\langle \nabla_s \, \vec{\mathrm{id}}, \nabla_s \, \vec{\chi} \right\rangle_{\Gamma(t)} , \tag{3.7}$$

see e.g. the proof of Lemma 1 in Dziuk (2008). For later use we note that generalized variants of (3.7) also hold. Namely, we have that

$$\left[\frac{\delta}{\delta\Gamma} \langle w, 1 \rangle_{\Gamma(t)} \right] (\vec{\chi}) = \lim_{\delta \to 0} \tfrac{1}{\delta} \left[\langle w_\delta, 1 \rangle_{\Gamma_\delta(t)} - \langle w, 1 \rangle_{\Gamma(t)} \right] \\ = \left\langle w \, \nabla_s \, \vec{\mathrm{id}}, \nabla_s \, \vec{\chi} \right\rangle_{\Gamma(t)} \quad \forall \, w \in L^\infty(\Gamma(t)) , \tag{3.8}$$

where $w_\delta \in L^\infty(\Gamma_\delta(t))$ is defined by $w_\delta(\vec\Psi(\vec z,\delta)) = w(\vec z)$ for all $\vec z \in \Gamma(t)$. Of course, (3.8) is the first variation analogue of (3.2) with $w = \chi\,\zeta$ and $\partial_t^\circ\,\chi = \partial_t^\circ\,\zeta = 0$. Similarly, it holds that

$$\left[\frac{\delta}{\delta\Gamma}\,\langle \vec w, \vec\nu\rangle_{\Gamma(t)}\right](\vec\chi) = \lim_{\delta\to 0}\tfrac{1}{\delta}\left[\langle \vec w_\delta, \vec\nu_\delta\rangle_{\Gamma_\delta(t)} - \langle \vec w, \vec\nu\rangle_{\Gamma(t)}\right]$$
$$= \left\langle (\vec w\,.\,\vec\nu)\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec\chi\right\rangle_{\Gamma(t)} + \left\langle \vec w, \left[\frac{\delta}{\delta\Gamma}\,\vec\nu\right](\vec\chi)\right\rangle_{\Gamma(t)} \qquad \forall\ \vec w \in [L^\infty(\Gamma(t))]^d\,,$$

where $\vec w_\delta \in [L^\infty(\Gamma_\delta(t))]^d$ is as before, and where $\vec\nu_\delta$ denotes the outward unit normal on $\Gamma_\delta(t)$. In this regard, we note the following result concerning the variation of $\vec\nu$, with respect to $\Gamma(t)$, in the direction $\vec\chi \in [H^1(\Gamma(t))]^d$:

$$\left[\frac{\delta}{\delta\Gamma}\,\vec\nu\right](\vec\chi) = -[\nabla_s\,\vec\chi]^T\,\vec\nu \quad \text{on} \quad \Gamma(t) \quad \Rightarrow \quad \partial_t^\circ\,\vec\nu = -[\nabla_s\,\vec{\mathcal{V}}]^T\,\vec\nu \quad \text{on} \quad \Gamma(t)\,, \tag{3.9}$$

see Schmidt and Schulz (2010, Lemma 9). Finally, we note that for $\vec\eta \in [H^1(\Gamma(t))]^d$ it holds that

$$\left[\frac{\delta}{\delta\Gamma}\left\langle \nabla_s\,\vec{\rm id}, \nabla_s\,\vec\eta\right\rangle_{\Gamma(t)}\right](\vec\chi) = \lim_{\delta\to 0}\tfrac{1}{\delta}\left[\left\langle \nabla_s\,\vec{\rm id}, \nabla_s\,\vec\eta_\delta\right\rangle_{\Gamma_\delta(t)} - \left\langle \nabla_s\,\vec{\rm id}, \nabla_s\,\vec\eta\right\rangle_{\Gamma(t)}\right]$$
$$= \langle \nabla_s\,.\,\vec\eta, \nabla_s\,.\,\vec\chi\rangle_{\Gamma(t)}$$
$$+ \sum_{l,\,m=1}^{d}\left[\langle (\vec\nu)_l\,(\vec\nu)_m\,\nabla_s\,(\vec\eta)_m, \nabla_s\,(\vec\chi)_l\rangle_{\Gamma(t)} - \langle (\nabla_s)_m\,(\vec\eta)_l, (\nabla_s)_l\,(\vec\chi)_m\rangle_{\Gamma(t)}\right]$$
$$= \langle \nabla_s\,.\,\vec\eta, \nabla_s\,.\,\vec\chi\rangle_{\Gamma(t)} + \langle \nabla_s\,\vec\eta, \nabla_s\,\vec\chi\rangle_{\Gamma(t)} - 2\left\langle \nabla_s\,\vec\eta, \underline{\underline{D}}_s(\vec\chi)\,\nabla_s\,\vec{\rm id}\right\rangle_{\Gamma(t)}\,, \tag{3.10}$$

where $\vec\eta_\delta \in [H^1(\Gamma_\delta(t))]^d$ is as before, see Lemma 2 and the proof of Lemma 3 in Dziuk (2008). We also refer to the remark above the proof of Lemma 3 in Dziuk (2008), which implies that our definition (2.6b) differs from Dziuk (2008, (3.14)) only by a factor of two. It follows from (3.10) that

$$\frac{\rm d}{{\rm d}t}\left\langle \nabla_s\,\vec{\rm id}, \nabla_s\,\vec\eta\right\rangle_{\Gamma(t)} = \left\langle \nabla_s\,.\,\vec\eta, \nabla_s\,.\,\vec{\mathcal{V}}\right\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec\eta, \nabla_s\,\vec{\mathcal{V}}\right\rangle_{\Gamma(t)} - 2\left\langle \nabla_s\,\vec\eta, \underline{\underline{D}}_s(\vec{\mathcal{V}})\,\nabla_s\,\vec{\rm id}\right\rangle_{\Gamma(t)}$$
$$\forall\ \vec\eta \in \{\vec\xi \in H^1(\mathcal{G}_T) : \partial_t^\circ\,\vec\xi = \vec 0\}\,. \tag{3.11}$$

We now consider the first variation of (2.10a) subject to the side constraint

$$\langle \vec\varkappa, \vec\eta\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec{\rm id}, \nabla_s\,\vec\eta\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec\eta \in [H^1(\Gamma(t))]^d\,. \tag{3.12}$$

To this end, we define the Lagrangian

$$L(\Gamma(t), \vec\varkappa, \vec y) = \tfrac12\,\langle \vec\varkappa - \overline\varkappa\,\vec\nu, \vec\varkappa - \overline\varkappa\,\vec\nu\rangle_{\Gamma(t)} + \tfrac{\beta}{2}\left(\langle \vec\varkappa, \vec\nu\rangle_{\Gamma(t)} - M_0\right)^2$$
$$- \langle \vec\varkappa, \vec y\rangle_{\Gamma(t)} - \left\langle \nabla_s\,\vec{\rm id}, \nabla_s\,\vec y\right\rangle_{\Gamma(t)}\,,$$

where $\vec{\varkappa} \in [H^1(\Gamma(t))]^d$, with $\vec{y} \in [H^1(\Gamma(t))]^d$ being a Lagrange multiplier for (3.12). In order to derive the gradient of $E_{\overline{\varkappa},\beta}(\Gamma(t))$ subject to the constraint (3.12), we set the variations of $L(\Gamma(t), \vec{\varkappa}, \vec{y})$ with respect to $\vec{\varkappa}$ and $\vec{y}$ to zero. In particular, denoting by $\vec{f}_\Gamma$ this gradient of $E_{\overline{\varkappa},\beta}(\Gamma(t))$, we obtain on using the formal calculus of PDE constrained optimization, see e.g. Tröltzsch (2010), that

$$
\begin{aligned}
\left[\frac{\delta}{\delta\Gamma} L\right](\vec{\chi}) &= \lim_{\delta\to 0} \tfrac{1}{\delta}\left[L(\Gamma_\delta(t), \vec{\varkappa}_\delta, \vec{y}_\delta) - L(\Gamma(t), \vec{\varkappa}, \vec{y})\right] = -\left\langle \vec{f}_\Gamma, \vec{\chi}\right\rangle_{\Gamma(t)}, \\
\left[\frac{\delta}{\delta\vec{\varkappa}} L\right](\vec{\xi}) &= \lim_{\delta\to 0} \tfrac{1}{\delta}\left[L(\Gamma(t), \vec{\varkappa} + \delta\,\vec{\xi}, \vec{y}) - L(\Gamma(t), \vec{\varkappa}, \vec{y})\right] = 0\,, \\
\left[\frac{\delta}{\delta\vec{y}} L\right](\vec{\eta}) &= \lim_{\delta\to 0} \tfrac{1}{\delta}\left[L(\Gamma(t), \vec{\varkappa}, \vec{y} + \delta\,\vec{\eta}) - L(\Gamma(t), \vec{\varkappa}, \vec{y})\right] = 0\,,
\end{aligned}
$$

where $\vec{\varkappa}_\delta,\ \vec{y}_\delta \in [H^1(\Gamma_\delta(t))]^d$ are as before. On recalling (3.8)–(3.10), this yields that

$$
\begin{aligned}
&\left\langle \vec{f}_\Gamma, \vec{\chi}\right\rangle_{\Gamma(t)} - \langle \nabla_s\,\vec{y}, \nabla_s\,\vec{\chi}\rangle_{\Gamma(t)} - \langle \nabla_s\,.\,\vec{y}, \nabla_s\,.\,\vec{\chi}\rangle_{\Gamma(t)} + 2\left\langle \nabla_s\,\vec{y}, \underline{\underline{D}}_s(\vec{\chi})\,\nabla_s\,\vec{\mathrm{id}}\right\rangle_{\Gamma(t)} \\
&\quad + \tfrac{1}{2}\left\langle [|\vec{\varkappa} - \overline{\varkappa}\,\vec{\nu}|^2 - 2\,(\vec{y}\,.\,\vec{\varkappa})]\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\chi}\right\rangle_{\Gamma(t)} - (A - \overline{\varkappa})\,\langle \vec{\varkappa}, [\nabla_s\,\vec{\chi}]^T\,\vec{\nu}\rangle_{\Gamma(t)} \\
&\quad + A\left\langle (\vec{\varkappa}\,.\,\vec{\nu})\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\chi}\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec{\chi} \in [H^1(\Gamma(t))]^d\,, \qquad (3.13a)
\end{aligned}
$$

$$
\left\langle \vec{\varkappa} - \overline{\varkappa}\,\vec{\nu} - \vec{y}, \vec{\xi}\right\rangle_{\Gamma(t)} + A\left\langle \vec{\nu}, \vec{\xi}\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec{\xi} \in [H^1(\Gamma(t))]^d\,, \qquad (3.13b)
$$

$$
\langle \vec{\varkappa}, \vec{\eta}\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\eta}\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec{\eta} \in [H^1(\Gamma(t))]^d\,, \qquad (3.13c)
$$

where

$$
A(t) = \beta\left(\langle \vec{\varkappa}, \vec{\nu}\rangle_{\Gamma(t)} - M_0\right). \qquad (3.13d)
$$

Clearly, (3.13b) implies that $\vec{\varkappa} + (A - \overline{\varkappa})\,\vec{\nu} = \vec{y}$. We note that (3.13a–d) collapses to (3.3e,f) in the case $\overline{\varkappa} = \beta = 0$.

The following theorem shows that $\vec{f}_\Gamma$ is indeed the gradient of $E_{\overline{\varkappa},\beta}(\Gamma(t))$ with respect to $\Gamma(t)$ subject to the constraint (3.12).

THEOREM. 3.1. *Let* $(\vec{f}_\Gamma, \vec{\varkappa}, \vec{y})$ *fulfill* (3.13a–d). *Then we have that*

$$
\frac{\mathrm{d}}{\mathrm{d}t}\,E_{\overline{\varkappa},\beta}(\Gamma(t)) = \frac{\mathrm{d}}{\mathrm{d}t}\left[\tfrac{1}{2}\,\langle |\vec{\varkappa} - \overline{\varkappa}\,\vec{\nu}|^2, 1\rangle_{\Gamma(t)} + \tfrac{\beta}{2}\left(\langle \vec{\varkappa}, \vec{\nu}\rangle_{\Gamma(t)} - M_0\right)^2\right] = -\left\langle \vec{f}_\Gamma, \vec{\mathcal{V}}\right\rangle_{\Gamma(t)}. \qquad (3.14)
$$

Proof. Taking the time derivative of (3.13c), where we choose test functions with $\partial_t^\circ\,\vec{\eta} = \vec{0}$, and noting (3.2) and (3.11), we obtain

$$
\begin{aligned}
&\langle \partial_t^\circ\,\vec{\varkappa}, \vec{\eta}\rangle_{\Gamma(t)} + \left\langle (\vec{\varkappa}\,.\,\vec{\eta})\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\mathcal{V}}\right\rangle_{\Gamma(t)} + \left\langle \nabla_s\,.\,\vec{\mathcal{V}}, \nabla_s\,.\,\vec{\eta}\right\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec{\mathcal{V}}, \nabla_s\,\vec{\eta}\right\rangle_{\Gamma(t)} \\
&\quad - 2\left\langle \underline{\underline{D}}_s(\vec{\mathcal{V}})\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\eta}\right\rangle_{\Gamma(t)} = 0\,. \qquad (3.15)
\end{aligned}
$$

Choosing $\vec{\chi} = \vec{\mathcal{V}}$ in (3.13a), $\vec{\eta} = \vec{y}$ in (3.15) and combining yields, on noting (3.9), that

$$\left\langle \vec{f}_\Gamma, \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} + \tfrac12 \left\langle [|\vec{\varkappa} - \overline{\varkappa}\,\vec{\nu}|^2 - 2\,(\vec{y} - A\,\vec{\nu})\,.\,\vec{\varkappa}]\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec{\mathcal{V}} \right\rangle_{\Gamma(t)} + \left\langle (\vec{\varkappa}\,.\,\vec{y})\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec{\mathcal{V}} \right\rangle_{\Gamma(t)}$$
$$+ (A - \overline{\varkappa})\,\langle \vec{\varkappa}, \partial_t^\circ\,\vec{\nu}\rangle_{\Gamma(t)} + \langle \partial_t^\circ\,\vec{\varkappa}, \vec{y}\rangle_{\Gamma(t)} = 0\,,$$

which implies that

$$\left\langle \vec{f}_\Gamma, \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} + \tfrac12 \left\langle [|\vec{\varkappa} - \overline{\varkappa}\,\vec{\nu}|^2 + 2\,A\,\vec{\nu}\,.\,\vec{\varkappa}]\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec{\mathcal{V}} \right\rangle_{\Gamma(t)} + (A - \overline{\varkappa})\,\langle \vec{\varkappa}, \partial_t^\circ\,\vec{\nu}\rangle_{\Gamma(t)}$$
$$+ \langle \partial_t^\circ\,\vec{\varkappa}, \vec{y}\rangle_{\Gamma(t)} = 0\,. \tag{3.16}$$

On noting that $\partial_t^\circ\,|\vec{\varkappa} - \overline{\varkappa}\,\vec{\nu}|^2 = 2\,(\vec{\varkappa} - \overline{\varkappa}\,\vec{\nu})\,.\,(\partial_t^\circ\,\vec{\varkappa} - \overline{\varkappa}\,\partial_t^\circ\,\vec{\nu}) = 2\,(\vec{\varkappa} - \overline{\varkappa}\,\vec{\nu})\,.\,\partial_t^\circ\,\vec{\varkappa} - \overline{\varkappa}\,\vec{\varkappa}\,.\,\partial_t^\circ\,\vec{\nu}$, one can immediately deduce from (3.16) that

$$\left\langle \vec{f}_\Gamma, \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} + \tfrac12\,\frac{\rm d}{{\rm d}t}\,\langle |\vec{\varkappa} - \overline{\varkappa}\,\vec{\nu}|^2, 1\rangle_{\Gamma(t)} + \tfrac{\beta}{2}\,\frac{\rm d}{{\rm d}t}\left(\langle \vec{\varkappa}, \vec{\nu}\rangle_{\Gamma(t)} - M_0\right)^2 = 0\,, \tag{3.17}$$

where, on recalling (3.13d), we have observed that

$$A\left[\left\langle (\vec{\varkappa}\,.\,\vec{\nu})\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec{\mathcal{V}} \right\rangle_{\Gamma(t)} + \langle \partial_t^\circ\,\vec{\varkappa}, \vec{\nu}\rangle_{\Gamma(t)} + \langle \vec{\varkappa}, \partial_t^\circ\,\vec{\nu}\rangle_{\Gamma(t)}\right] = \tfrac{\beta}{2}\,\frac{\rm d}{{\rm d}t}\left(\langle \vec{\varkappa}, \vec{\nu}\rangle_{\Gamma(t)} - M_0\right)^2.$$

Combining (3.17) and (3.13d), on recalling (2.10a,b), yields the desired result (3.14). □

3.3 Fluidic weak formulation for given $\overline{\varkappa} \in \mathbb{R}$ and $\beta \in \mathbb{R}_{\geq 0}$

Combining (3.3a–d) and (3.13a–d) yields the following weak formulation of the system (2.2a–d), (2.3), (2.4a–d), (2.5). Find $\Gamma(t) = \vec{x}(\Upsilon, t)$ for $t \in [0, T]$ with $\vec{\mathcal{V}} \in [L^2(\mathcal{G}_T)]^d$, and functions $\vec{u} \in \mathbb{V}_\Gamma(\vec{g})$, $p \in L^2(0, T; \widehat{\mathbb{P}})$, $p_\Gamma \in L^2(\mathcal{G}_T)$, $\vec{\varkappa}$, $\vec{y} \in [H^1(\mathcal{G}_T)]^d$ and $\vec{f}_\Gamma \in [L^2(\mathcal{G}_T)]^d$ such that the initial conditions (2.8) hold and such that (3.3a–d) and (3.13a–d) hold.

Combining (3.4) with (3.14) and (3.13a–d), i.e. choosing $\vec{\chi} = \vec{f}_\Gamma$ in (3.3d), $\vec{\eta} = \vec{y}$ in (3.13c) and $\vec{\chi} = \vec{\mathcal{V}}$ in (3.13a), yields that

$$\tfrac12\,\frac{\rm d}{{\rm d}t}\left(\|\rho^{\frac12}\,\vec{u}\|_0^2 + \rho_\Gamma\,\langle \vec{u}, \vec{u}\rangle_{\Gamma(t)} + \alpha\,\langle |\vec{\varkappa} - \overline{\varkappa}\,\vec{\nu}|^2, 1\rangle_{\Gamma(t)} + \alpha\,\beta\left(\langle \vec{\varkappa}, \vec{\nu}\rangle_{\Gamma(t)} - M_0\right)^2\right)$$
$$+ 2\,\|\mu^{\frac12}\,\underline{\underline{D}}(\vec{u})\|_0^2 + 2\,\mu_\Gamma\,\left\langle \underline{\underline{D}}_s(\vec{u}), \underline{\underline{D}}_s(\vec{u})\right\rangle_{\Gamma(t)} + \tfrac12\,\rho_+\,\left\langle \vec{u}\,.\,\vec{\rm n}, |\vec{u}|^2\right\rangle_{\partial_2\Omega} = (\rho\,\vec{f}, \vec{u})\,. \tag{3.18}$$

Of course, the conservation properties (3.5) and (3.6) still hold.

4 Semidiscrete finite element approximation

For simplicity we consider Ω to be a polyhedral domain. Then let $\mathcal{T}^h$ be a regular partitioning of Ω into disjoint open simplices o_j^h, $j = 1, \ldots, J_\Omega^h$. Associated with $\mathcal{T}^h$ are the finite element spaces

$$S^h_k := \{\chi \in C(\overline{\Omega}) : \chi\,|_o \in \mathcal{P}_k(o) \quad \forall\, o \in \mathcal{T}^h\} \subset H^1(\Omega)\,, \qquad k \in \mathbb{N}\,,$$

where $\mathcal{P}_k(o)$ denotes the space of polynomials of degree k on o. We also introduce S^h_0, the space of piecewise constant functions on $\mathcal{T}^h$. Let $\{\varphi^h_{k,j}\}_{j=1}^{K^h_k}$ be the standard basis functions for S^h_k, $k \geq 0$. We introduce $\vec{I}^h_k : [C(\overline{\Omega})]^d \to [S^h_k]^d$, $k \geq 1$, the standard interpolation operators, such that $(\vec{I}^h_k\,\vec{\eta})(\vec{p}^h_{k,j}) = \vec{\eta}(\vec{p}^h_{k,j})$ for $j = 1,\ldots,K^h_k$; where $\{\vec{p}^h_{k,j}\}_{j=1}^{K^h_k}$ denotes the coordinates of the degrees of freedom of S^h_k, $k \geq 1$. In addition we define the standard projection operator $I^h_0 : L^1(\Omega) \to S^h_0$, such that

$$(I^h_0 \eta)\,|_o = \frac{1}{\mathcal{L}^d(o)} \int_o \eta \,\mathrm{d}\mathcal{L}^d \qquad \forall\, o \in \mathcal{T}^h\,.$$

Our approximation to the velocity and pressure on $\mathcal{T}^h$ will be finite element spaces $\mathbb{U}^h(\vec{g}) \subset \mathbb{U}(\vec{I}^h_k\,\vec{g})$, for some $k \geq 2$, and $\mathbb{P}^h(t) \subset \mathbb{P}$. For the former we assume from now on that $\vec{g} \in [C(\overline{\Omega})]^d$, while for the latter we assume that $S^h_1 \subset \mathbb{P}^h(t)$. We require also the space $\widehat{\mathbb{P}}^h(t) := \mathbb{P}^h(t) \cap \widehat{\mathbb{P}}$. Based on the authors' earlier work in Barrett *et al.* (2013, 2014c), it is possible to select velocity/pressure finite element spaces that satisfy the LBB inf-sup condition, see e.g. Girault and Raviart (1986, p. 114), and augment the pressure space by the characteristic function of the inner phase. This enrichment of the pressure space is an example of an XFEM approach, and we refer to the approach from Barrett *et al.* (2013, 2014c) as XFEM$_\Gamma$. For the obtained spaces $(\mathbb{U}^h(\vec{0}), \mathbb{P}^h(t))$, because $\mathcal{T}^h$ and $\Gamma^h(t)$ are totally independent, we are unable to prove that they satisfy an LBB condition. However, the extension of the given pressure finite element space leads to exact volume conservation of the two phases within the semidiscrete finite element framework. Moreover, in extensive numerical computations for the fully discrete variant of the XFEM$_\Gamma$ approach we never encountered any difficulties. For the non-augmented spaces we may choose, for example, the lowest order Taylor-Hood element P2–P1, the P2–P0 element or the P2–(P1+P0) element on setting $\mathbb{U}^h = [S^h_2]^d \cap \mathbb{U}(\vec{I}^h_2\,\vec{g})$, and $\mathbb{P}^h = S^h_1$, S^h_0 or $S^h_1 + S^h_0$, respectively. We refer to Barrett *et al.* (2013, 2014c) for more details.

In addition to the volume conservation of the two phases, for the numerical approximation of the evolution of fluidic membranes it is also desirable to maintain the surface area of the interface, recall (3.5). Unfortunately, it does not appear possible to prove a discrete analogue of (3.5) for the above described XFEM approach from Barrett *et al.* (2013, 2014c). Hence in this paper we will modify this XFEM approach so that we obtain numerical approximations that satisfy discrete analogues of both (3.6) and (3.5). From a practical point of view, this approach is very close to the procedure in Barrett *et al.* (2013, 2014c). But the introduced modifications mean that the adjustments to the finite element approximations no longer have an interpretation within the XFEM framework. This is because the adjustments can no longer be interpreted as suitable additions to the basis of the discrete pressure spaces.

The parametric finite element spaces in order to approximate e.g. $\vec{\varkappa}$ and $\varkappa$ are defined as follows. Similarly to Barrett *et al.* (2008a), we introduce the following discrete spaces, based on the work of Dziuk (1991). Let $\Gamma^h(t) \subset \mathbb{R}^d$ be a $(d-1)$-dimensional *polyhedral surface*, i.e. a union of non-degenerate $(d-1)$-simplices with no hanging vertices (see Deckelnick *et al.* (2005, p. 164) for $d = 3$), approximating the closed surface $\Gamma(t)$. In particular, let $\Gamma^h(t) = \bigcup_{j=1}^{J_\Gamma} \overline{\sigma^h_j(t)}$, where $\{\sigma^h_j(t)\}_{j=1}^{J_\Gamma}$ is a family of mutually disjoint open $(d-1)$-simplices with vertices $\{\vec{q}^h_k(t)\}_{k=1}^{K_\Gamma}$. Then let

$$\begin{aligned}\underline{V}(\Gamma^h(t)) &:= \{\vec{\chi} \in [C(\Gamma^h(t))]^d : \vec{\chi}\,|_{\sigma^h_j} \text{ is linear } \forall\ j = 1, \ldots, J_\Gamma\} \\ &=: [W(\Gamma^h(t))]^d \subset [H^1(\Gamma^h(t))]^d\,,\end{aligned}$$

where $W(\Gamma^h(t)) \subset H^1(\Gamma^h(t))$ is the space of scalar continuous piecewise linear functions on $\Gamma^h(t)$, with $\{\chi^h_k(\cdot, t)\}_{k=1}^{K_\Gamma}$ denoting the standard basis of $W(\Gamma^h(t))$, i.e.

$$\chi^h_k(\vec{q}^h_l(t), t) = \delta_{kl} \qquad \forall\ k, l \in \{1, \ldots, K_\Gamma\}\,, t \in [0, T]\,. \tag{4.1}$$

For later purposes, we also introduce $\pi^h(t) : C(\Gamma^h(t)) \to W(\Gamma^h(t))$, the standard interpolation operator at the nodes $\{\vec{q}^h_k(t)\}_{k=1}^{K_\Gamma}$, and similarly $\vec{\pi}^h(t) : [C(\Gamma^h(t))]^d \to \underline{V}(\Gamma^h(t))$.

For scalar and vector functions η, ζ on $\Gamma^h(t)$ we introduce the L^2–inner product $\langle \cdot, \cdot \rangle_{\Gamma^h(t)}$ over the polyhedral surface $\Gamma^h(t)$ as follows

$$\langle \eta, \zeta \rangle_{\Gamma^h(t)} := \int_{\Gamma^h(t)} \eta \,.\, \zeta \;\mathrm{d}\mathcal{H}^{d-1}\,.$$

If v, w are piecewise continuous, with possible jumps across the edges of $\{\sigma^h_j\}_{j=1}^{J_\Gamma}$, we introduce the mass lumped inner product $\langle \cdot, \cdot \rangle^h_{\Gamma^h(t)}$ as

$$\langle \eta, \zeta \rangle^h_{\Gamma^h(t)} := \tfrac{1}{d} \sum_{j=1}^{J_\Gamma} \mathcal{H}^{d-1}(\sigma^h_j) \sum_{k=1}^{d} (\eta \,.\, \zeta)((\vec{q}^h_{j_k})^-),$$

where $\{\vec{q}^h_{j_k}\}_{k=1}^d$ are the vertices of σ^h_j, and where we define $\eta((\vec{q}^h_{j_k})^-) := \lim_{\sigma^h_j \ni \vec{p} \to \vec{q}^h_{j_k}} \eta(\vec{p})$.

Following Dziuk and Elliott (2013, (5.23)), we define the discrete material velocity for $\vec{z} \in \Gamma^h(t)$ by

$$\vec{\mathcal{V}}^h(\vec{z}, t) := \sum_{k=1}^{K_\Gamma} \left[\frac{\mathrm{d}}{\mathrm{d}t}\, \vec{q}^h_k(t)\right] \chi^h_k(\vec{z}, t)\,. \tag{4.2}$$

Then, similarly to (3.1), we define

$$\partial_t^{\circ,h}\, \zeta = \zeta_t + \vec{\mathcal{V}}^h \,.\, \nabla\, \zeta \qquad \forall\ \zeta \in H^1(\mathcal{G}^h_T)\,, \quad \text{where} \quad \mathcal{G}^h_T := \bigcup_{t \in [0,T]} \Gamma^h(t) \times \{t\}\,.$$

For later use, we also introduce the finite element spaces

$$\begin{aligned} W(\mathcal{G}^h_T) &:= \{\chi \in C(\mathcal{G}^h_T) : \chi(\cdot, t) \in W(\Gamma^h(t)) \quad \forall\ t \in [0, T]\}\,, \\ W_T(\mathcal{G}^h_T) &:= \{\chi \in W(\mathcal{G}^h_T) : \partial_t^{\circ,h}\, \chi \in C(\mathcal{G}^h_T)\}\,,\end{aligned}$$

as well as

$$\mathbb{V}^h_{\Gamma^h}(\vec{g}) := \{\vec{\phi} \in H^1(0,T;\mathbb{U}^h(\vec{g})) : \vec{\chi} \in [W_T(\mathcal{G}_T)]^d, \text{ where } \vec{\chi}(\cdot,t) = \vec{\pi}^h\,[\vec{\phi}|_{\Gamma^h(t)}]\ \forall\ t \in [0,T]\}\,.$$

On differentiating (4.1) with respect to t, it immediately follows that

$$\partial_t^{\circ,h}\,\chi_k^h = 0 \quad \forall\ k \in \{1,\ldots,K_\Gamma\}\,, \tag{4.3}$$

see Dziuk and Elliott (2013, Lem. 5.5). It follows directly from (4.3) that

$$\partial_t^{\circ,h}\,\zeta(\cdot,t) = \sum_{k=1}^{K_\Gamma} \chi_k^h(\cdot,t)\,\frac{\mathrm{d}}{\mathrm{d}t}\,\zeta_k(t) \quad \text{on } \Gamma^h(t)$$

for $\zeta(\cdot,t) = \sum_{k=1}^{K_\Gamma} \zeta_k(t)\,\chi_k^h(\cdot,t) \in W(\Gamma^h(t))$, and hence $\partial_t^{\circ,h}\,\vec{\mathrm{id}} = \vec{\mathcal{V}}^h$ on $\Gamma^h(t)$.

We recall from Dziuk and Elliott (2013, Lem. 5.6) that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\sigma_j^h(t)} \zeta\ \mathrm{d}\mathcal{H}^{d-1} = \int_{\sigma_j^h(t)} \partial_t^{\circ,h}\,\zeta + \zeta\,\nabla_s\,.\,\vec{\mathcal{V}}^h\ \mathrm{d}\mathcal{H}^{d-1} \quad \forall\ \zeta \in H^1(\sigma^h(t))\,, j \in \{1,\ldots,J_\Gamma\}\,,$$

which immediately implies that

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \eta,\zeta\rangle_{\Gamma^h(t)} = \langle \partial_t^{\circ,h}\,\eta,\zeta\rangle_{\Gamma^h(t)} + \langle \eta,\partial_t^{\circ,h}\,\zeta\rangle_{\Gamma^h(t)} + \langle \eta\,\zeta,\nabla_s\,.\,\vec{\mathcal{V}}^h\rangle_{\Gamma^h(t)} \qquad \forall\ \eta,\zeta \in W_T(\mathcal{G}_T^h)\,. \tag{4.4}$$

We recall from Barrett *et al.* (2014a, Lem. 2.1) that

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \eta,\zeta\rangle_{\Gamma^h(t)}^h = \langle \partial_t^{\circ,h}\,\eta,\zeta\rangle_{\Gamma^h(t)}^h + \langle \eta,\partial_t^{\circ,h}\,\zeta\rangle_{\Gamma^h(t)}^h + \langle \eta\,\zeta,\nabla_s\,.\,\vec{\mathcal{V}}^h\rangle_{\Gamma^h(t)}^h \quad \forall\ \eta,\zeta \in W_T(\mathcal{G}_T^h)\,. \tag{4.5}$$

Similarly to (2.6a,b), we introduce

$$\underline{\underline{\mathcal{P}}}_{\Gamma^h} = \underline{\underline{\mathrm{Id}}} - \vec{\nu}^h \otimes \vec{\nu}^h \quad \text{on } \Gamma^h(t)\,, \tag{4.6a}$$

and

$$\underline{\underline{D}}_s^h(\vec{\eta}) = \tfrac{1}{2}\,\underline{\underline{\mathcal{P}}}_{\Gamma^h}\,(\nabla_s\,\vec{\eta} + (\nabla_s\,\vec{\eta})^T)\,\underline{\underline{\mathcal{P}}}_{\Gamma^h} \quad \text{on } \Gamma^h(t)\,, \tag{4.6b}$$

where here $\nabla_s = \underline{\underline{\mathcal{P}}}_{\Gamma^h}\,\nabla$ denotes the surface gradient on $\Gamma^h(t)$. Moreover, we introduce the vertex normal function $\vec{\omega}^h(\cdot,t) \in \underline{V}(\Gamma^h(t))$ with

$$\vec{\omega}^h(\vec{q}_k^h(t),t) := \frac{1}{\mathcal{H}^{d-1}(\Lambda_k^h(t))} \sum_{j\in\Theta_k^h} \mathcal{H}^{d-1}(\sigma_j^h(t))\,\vec{\nu}^h\,|_{\sigma_j^h(t)}\,, \tag{4.7}$$

where for $k = 1,\ldots,K_\Gamma^h$ we define $\Theta_k^h := \{j : \vec{q}_k^h(t) \in \overline{\sigma_j^h(t)}\}$ and set

$$\Lambda_k^h(t) := \cup_{j\in\Theta_k^h}\overline{\sigma_j^h(t)}\,.$$

For later use we note that

$$\left\langle \vec{z}, w\,\vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} = \left\langle \vec{z}, w\,\vec{\omega}^h \right\rangle^h_{\Gamma^h(t)} \qquad \forall\ \vec{z} \in \underline{V}(\Gamma^h(t))\,,\ w \in W(\Gamma^h(t))\,. \tag{4.8}$$

Given $\Gamma^h(t)$, we let $\Omega^h_+(t)$ denote the exterior of $\Gamma^h(t)$ and let $\Omega^h_-(t)$ denote the interior of $\Gamma^h(t)$, so that $\Gamma^h(t) = \partial\Omega^h_-(t) = \overline{\Omega^h_-(t)} \cap \overline{\Omega^h_+(t)}$. We then partition the elements of the bulk mesh $\mathcal{T}^h$ into interior, exterior and interfacial elements as follows. Let

$$\begin{aligned}
\mathcal{T}^h_-(t) &:= \{o \in \mathcal{T}^h : o \subset \Omega^h_-(t)\}\,,\\
\mathcal{T}^h_+(t) &:= \{o \in \mathcal{T}^h : o \subset \Omega^h_+(t)\}\,,\\
\mathcal{T}^h_{\Gamma^h}(t) &:= \{o \in \mathcal{T}^h : o \cap \Gamma^h(t) \neq \emptyset\}\,.
\end{aligned}$$

Clearly $\mathcal{T}^h = \mathcal{T}^h_-(t) \cup \mathcal{T}^h_+(t) \cup \mathcal{T}^h_\Gamma(t)$ is a disjoint partition. In addition, we define the piecewise constant unit normal $\vec{\nu}^h(t)$ to $\Gamma^h(t)$ such that $\vec{\nu}^h(t)$ points into $\Omega^h_+(t)$. Moreover, we introduce the discrete density $\rho^h(t) \in S^h_0$ and the discrete viscosity $\mu^h(t) \in S^h_0$ as

$$\rho^h(t)\,|_o = \begin{cases} \rho_- & o \in \mathcal{T}^h_-(t)\,,\\ \rho_+ & o \in \mathcal{T}^h_+(t)\,,\\ \tfrac12\,(\rho_- + \rho_+) & o \in \mathcal{T}^h_{\Gamma^h}(t)\,, \end{cases} \quad \text{and} \quad \mu^h(t)\,|_o = \begin{cases} \mu_- & o \in \mathcal{T}^h_-(t)\,,\\ \mu_+ & o \in \mathcal{T}^h_+(t)\,,\\ \tfrac12\,(\mu_- + \mu_+) & o \in \mathcal{T}^h_{\Gamma^h}(t)\,. \end{cases}$$

In what follows we will introduce a finite element approximation for the free boundary problem (2.2a–d), (2.3), (2.4a–d), (2.5), which is based on the weak formulation (3.3a–d), (3.13a–d). The discretization of the former is the same as in Barrett *et al.* (2014b). By repeating on the discrete level the steps in §3.2, we will now derive a discrete analogue of (3.13a–d).

Similarly to the continuous setting in (3.13a–c), we consider the first variation of the discrete energy

$$E^h_{\overline{\varkappa},\beta}(\Gamma^h(t)) := \tfrac12 \left\langle |\vec{\kappa}^h - \overline{\varkappa}\,\vec{\nu}^h|^2, 1\right\rangle^h_{\Gamma^h(t)} + \tfrac{\beta}{2}\left(\left\langle \vec{\kappa}^h, \vec{\nu}^h\right\rangle_{\Gamma^h(t)} - M_0\right)^2$$

subject to the side constraint

$$\left\langle \vec{\kappa}^h, \vec{\eta}\right\rangle^h_{\Gamma(t)} + \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\eta}\right\rangle_{\Gamma^h(t)} = 0 \qquad \forall\ \vec{\eta} \in \underline{V}(\Gamma^h(t))\,. \tag{4.9}$$

We define the Lagrangian

$$\begin{aligned}
L^h(\Gamma^h(t), \vec{\kappa}^h, \vec{Y}^h) = \tfrac12 \left\langle |\vec{\kappa}^h - \overline{\varkappa}\,\vec{\nu}^h|^2, 1\right\rangle^h_{\Gamma^h(t)} + \tfrac{\beta}{2}\left(\left\langle \vec{\kappa}^h, \vec{\nu}^h\right\rangle^h_{\Gamma^h(t)} - M_0\right)^2 - \left\langle \vec{\kappa}^h, \vec{Y}^h\right\rangle^h_{\Gamma^h(t)}\\
- \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{Y}^h\right\rangle_{\Gamma^h(t)}\,,
\end{aligned}$$

where $\vec{\kappa}^h \in \underline{V}(\Gamma^h(t))$, with $\vec{Y}^h \in \underline{V}(\Gamma^h(t))$ being a Lagrange multiplier for (4.9). Similarly to (3.13a–d), on recalling the formal calculus of PDE constrained optimization, we obtain the gradient of $E^h_{\overline{\varkappa},\beta}(\Gamma^h(t))$ with respect to $\Gamma^h(t)$ subject to the side constraint (4.9) by setting $[\frac{\delta}{\delta\Gamma^h}\, L^h](\vec\chi) = -\left\langle \vec F^h_\Gamma, \vec\chi\right\rangle^h_{\Gamma^h(t)}$ for $\vec\chi \in \underline{V}(\Gamma^h(t))$, $[\frac{\delta}{\delta\vec\kappa^h}\, L^h](\vec\xi) = 0$ for $\vec\xi \in \underline{V}(\Gamma^h(t))$ and $[\frac{\delta}{\delta\vec Y^h}\, L^h](\vec\eta) = 0$ for $\vec\eta \in \underline{V}(\Gamma^h(t))$. On noting that the obvious discrete variants of (3.8)–(3.10) hold, we then obtain that

$$
\begin{aligned}
&\left\langle \vec F^h_\Gamma, \vec\chi\right\rangle^h_{\Gamma^h(t)} - \left\langle \nabla_s\, \vec Y^h, \nabla_s\, \vec\chi\right\rangle_{\Gamma^h(t)} - \left\langle \nabla_s\,.\,\vec Y^h, \nabla_s\,.\,\vec\chi\right\rangle_{\Gamma^h(t)} + 2\left\langle \nabla_s\,\vec Y^h, \underline{\underline{D}}^h_s(\vec\chi)\,\nabla_s\,\vec{\rm id}\right\rangle_{\Gamma^h(t)} \\
&\quad + \tfrac12\left\langle [|\vec\kappa^h - \overline{\varkappa}\,\vec\nu^h|^2 - 2\,(\vec Y^h\,.\,\vec\kappa^h)]\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec\chi\right\rangle^h_{\Gamma^h(t)} - (A^h - \overline{\varkappa})\left\langle \vec\kappa^h, [\nabla_s\,\vec\chi]^T\,\vec\nu^h\right\rangle^h_{\Gamma^h(t)} \\
&\quad + A^h\left\langle (\vec\kappa^h\,.\,\vec\nu^h)\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec\chi\right\rangle_{\Gamma^h(t)} = 0 \qquad \forall\ \vec\chi \in \underline{V}(\Gamma^h(t))\,, \qquad (4.10a)
\end{aligned}
$$

$$
\left\langle \vec\kappa^h - \overline{\varkappa}\,\vec\nu^h - \vec Y^h, \vec\xi\right\rangle^h_{\Gamma^h(t)} + A^h\left\langle \vec\nu^h, \vec\xi\right\rangle^h_{\Gamma^h(t)} = 0 \qquad \forall\ \vec\xi \in \underline{V}(\Gamma^h(t))\,, \qquad (4.10b)
$$

$$
\left\langle \vec\kappa^h, \vec\eta\right\rangle^h_{\Gamma^h(t)} + \left\langle \nabla_s\,\vec{\rm id}, \nabla_s\,\vec\eta\right\rangle_{\Gamma^h(t)} = 0 \qquad \forall\ \vec\eta \in \underline{V}(\Gamma^h(t))\,, \qquad (4.10c)
$$

where

$$
A^h(t) = \beta\left(\left\langle \vec\kappa^h, \vec\nu^h\right\rangle^h_{\Gamma^h(t)} - M_0\right). \qquad (4.10d)
$$

We note that (4.10b) and (4.8) imply that $\vec\kappa^h = \vec Y^h - (A^h - \overline{\varkappa})\,\vec\omega^h$.

The following theorem establishes that $\vec F^h_\Gamma$ is indeed the gradient of $E^h_{\overline{\varkappa},\beta}(\Gamma^h(t))$ with respect to $\Gamma^h(t)$ subject to the side constraint (4.9). It is the direct discrete analogue of Theorem 3.1.

THEOREM. 4.1. *Let* $(\vec F^h_\Gamma, \vec\kappa^h, \vec Y^h)$ *fulfill* (4.10a–d). *Then*

$$
\frac{\rm d}{{\rm d}t}\left[\tfrac12\left\langle |\vec\kappa^h - \overline{\varkappa}\,\vec\nu^h|^2, 1\right\rangle^h_{\Gamma^h(t)} + \tfrac{\beta}{2}\left(\left\langle \vec\kappa^h, \vec\nu^h\right\rangle^h_{\Gamma^h(t)} - M_0\right)^2\right] = -\left\langle \vec F^h_\Gamma, \vec{\mathcal V}^h\right\rangle^h_{\Gamma^h(t)}. \qquad (4.11)
$$

Proof. Taking the time derivative of (4.10c), where we choose discrete test functions $\vec\eta$ such that $\partial_t^{\circ,h}\,\vec\eta = \vec 0$, yields that

$$
\begin{aligned}
&\left\langle \partial_t^{\circ,h}\,\vec\kappa^h, \vec\eta\right\rangle^h_{\Gamma^h(t)} + \left\langle (\vec\kappa^h\,.\,\vec\eta)\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec{\mathcal V}^h\right\rangle^h_{\Gamma^h(t)} + \left\langle \nabla_s\,.\,\vec{\mathcal V}^h, \nabla_s\,.\,\vec\eta\right\rangle_{\Gamma^h(t)} + \left\langle \nabla_s\,\vec{\mathcal V}^h, \nabla_s\,\vec\eta\right\rangle_{\Gamma^h(t)} \\
&\quad - 2\left\langle \underline{\underline{D}}^h_s(\vec{\mathcal V}^h)\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec\eta\right\rangle_{\Gamma^h(t)} = 0\,, \qquad (4.12)
\end{aligned}
$$

where we have noted (4.5) and the discrete version of (3.11). Choosing $\vec\chi = \vec{\mathcal V}^h$ in (4.10a), $\vec\eta = \vec Y^h$ in (4.12) and combining yields, on noting the discrete variant of (3.9), that

$$
\begin{aligned}
&\left\langle \vec F^h_\Gamma, \vec{\mathcal V}^h\right\rangle^h_{\Gamma^h(t)} + \tfrac12\left\langle [|\vec\kappa^h - \overline{\varkappa}\,\vec\nu^h|^2 - 2\,(\vec Y^h - A^h\,\vec\nu^h)\,.\,\vec\kappa^h]\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec{\mathcal V}^h\right\rangle^h_{\Gamma^h(t)} \\
&\quad + (A^h - \overline{\varkappa})\left\langle \vec\kappa^h, \partial_t^{\circ,h}\,\vec\nu^h\right\rangle^h_{\Gamma^h(t)} + \left\langle \partial_t^{\circ,h}\,\vec\kappa^h, \vec Y^h\right\rangle^h_{\Gamma^h(t)} + \left\langle (\vec\kappa^h\,.\,\vec Y^h)\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec{\mathcal V}^h\right\rangle^h_{\Gamma^h(t)} = 0\,,
\end{aligned}
$$

which implies, on recalling (4.8), that

$$\left\langle \vec{F}^h_\Gamma, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} + \tfrac12 \left\langle [|\vec\kappa^h - \overline{\varkappa}\,\vec\nu^h|^2 + 2\,A^h\,\vec\nu^h\,.\,\vec\kappa^h]\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} \\ + (A^h - \overline{\varkappa}) \left\langle \vec\kappa^h, \partial_t^{\circ,h}\,\vec\nu^h \right\rangle^h_{\Gamma^h(t)} + \left\langle \partial_t^{\circ,h}\,\vec\kappa^h, \vec\kappa^h + (A^h - \overline{\varkappa})\,\vec\nu^h \right\rangle^h_{\Gamma^h(t)} = 0\,. \tag{4.13}$$

Similarly to (3.17), one can immediately deduce from (4.13) that the desired result (4.11) holds, where, on recalling (4.10d) and (4.8), we have observed that

$$A^h \left[\left\langle (\vec\kappa^h\,.\,\vec\nu^h)\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} + \left\langle \partial_t^{\circ,h}\,\vec\kappa^h, \vec\nu^h \right\rangle^h_{\Gamma^h(t)} + \left\langle \vec\kappa^h, \partial_t^{\circ,h}\,\vec\nu^h \right\rangle^h_{\Gamma^h(t)} \right] \\ = \tfrac{\beta}{2}\,\frac{\rm d}{{\rm d}t} \left(\langle \vec\kappa^h, \vec\nu^h \rangle^h_{\Gamma^h(t)} - M_0 \right)^2.$$

□

Overall, we then obtain the following semidiscrete continuous-in-time finite element approximation, which is the semidiscrete analogue of the weak formulation (3.3a–d), (3.13a–d). Given $\Gamma^h(0)$ and $\vec U^h(\cdot,0) \in \mathbb{U}^h(\vec g)$, find $\Gamma^h(t)$ such that $\vec{\rm id}\,|_{\Gamma^h(t)} \in \underline{V}(\Gamma^h(t))$ for $t \in [0,T]$, and functions $\vec U^h \in \mathbb{V}^h_{\Gamma^h}(\vec g)$, $P^h \in \mathbb{P}^h_T := \{\varphi \in L^2(0,T;\widehat{\mathbb{P}}) : \varphi(t) \in \widehat{\mathbb{P}}^h(t)$ for a.e. $t \in (0,T)\}$, $P^h_\Gamma \in W(\mathcal{G}^h_T)$, $\vec\kappa^h$, $\vec Y^h \in [W(\mathcal{G}^h_T)]^d$ and $\vec F^h_\Gamma \in [W(\mathcal{G}^h_T)]^d$ such that for almost all $t \in (0,T)$ it holds that

$$\tfrac12 \left[\frac{\rm d}{{\rm d}t} \left(\rho^h\,\vec U^h, \vec\xi \right) + \left(\rho^h\,\vec U^h_t, \vec\xi \right) - (\rho^h\,\vec U^h, \vec\xi_t) + \rho_+ \left\langle \vec U^h\,.\,\vec{\rm n}, \vec U^h\,.\,\vec\xi \right\rangle_{\partial_2\Omega} \right] \\ + 2 \left(\mu^h\,\underline{\underline{D}}(\vec U^h), \underline{\underline{D}}(\vec\xi) \right) + \tfrac12 \left(\rho^h, [(\vec U^h\,.\,\nabla)\,\vec U^h]\,.\,\vec\xi - [(\vec U^h\,.\,\nabla)\,\vec\xi]\,.\,\vec U^h \right) - \left(P^h, \nabla\,.\,\vec\xi \right) \\ + \rho_\Gamma \left\langle \partial_t^{\circ,h}\,\vec\pi^h\,\vec U^h, \vec\xi \right\rangle^h_{\Gamma^h(t)} + 2\,\mu_\Gamma \left\langle \underline{\underline{D}}^h_s(\vec\pi^h\,\vec U^h), \underline{\underline{D}}^h_s(\vec\pi^h\,\vec\xi) \right\rangle_{\Gamma^h(t)} \\ - \left\langle P^h_\Gamma, \nabla_s\,.\,(\vec\pi^h\,\vec\xi) \right\rangle_{\Gamma^h(t)} = \left(\rho^h\,\vec f^h, \vec\xi \right) + \alpha \left\langle \vec F^h_\Gamma, \vec\xi \right\rangle^h_{\Gamma^h(t)} \qquad \forall\ \vec\xi \in H^1(0,T;\mathbb{U}^h(\vec 0))\,, \tag{4.14a}$$

$$\left(\nabla\,.\,\vec U^h, \varphi \right) = 0 \qquad \forall\ \varphi \in \widehat{\mathbb{P}}^h(t)\,, \tag{4.14b}$$

$$\left\langle \nabla_s\,.\,(\vec\pi^h\,\vec U^h), \eta \right\rangle_{\Gamma^h(t)} = 0 \qquad \forall\ \eta \in W(\Gamma^h(t))\,, \tag{4.14c}$$

$$\left\langle \vec{\mathcal{V}}^h, \vec\chi \right\rangle^h_{\Gamma^h(t)} = \left\langle \vec U^h, \vec\chi \right\rangle^h_{\Gamma^h(t)} \qquad \forall\ \vec\chi \in \underline{V}(\Gamma^h(t))\,, \tag{4.14d}$$

$$\left\langle \vec Y^h, \vec\eta \right\rangle^h_{\Gamma^h(t)} + \left\langle \nabla_s\,\vec{\rm id}, \nabla_s\,\vec\eta \right\rangle_{\Gamma^h(t)} = (A^h - \overline{\varkappa})\,\langle \vec\omega^h, \vec\eta \rangle^h_{\Gamma^h(t)} \qquad \forall\ \vec\eta \in \underline{V}(\Gamma^h(t))\,, \tag{4.14e}$$

$$\left\langle \vec F^h_\Gamma, \vec\chi \right\rangle^h_{\Gamma^h(t)} = \left\langle \nabla_s\,\vec Y^h, \nabla_s\,\vec\chi \right\rangle_{\Gamma^h(t)} + \left\langle \nabla_s\,.\,\vec Y^h, \nabla_s\,.\,\vec\chi \right\rangle_{\Gamma^h(t)} - 2 \left\langle \nabla_s\,\vec Y^h, \underline{\underline{D}}^h_s(\vec\chi)\,\nabla_s\,\vec{\rm id} \right\rangle_{\Gamma^h(t)} \\ - \tfrac12 \left\langle [|\vec\kappa^h - \overline{\varkappa}\,\vec\nu^h|^2 - 2\,(\vec Y^h - A^h\,\vec\nu^h)\,.\,\vec\kappa^h]\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec\chi \right\rangle^h_{\Gamma^h(t)} \\ + (A^h - \overline{\varkappa})\,\langle \vec\kappa^h, [\nabla_s\,\vec\chi]^T\,\vec\nu^h \rangle^h_{\Gamma^h(t)} \qquad \forall\ \vec\chi \in \underline{V}(\Gamma^h(t))\,, \tag{4.14f}$$

$$A^h = \beta\left(\left\langle \vec\kappa^h, \vec\nu^h \right\rangle^h_{\Gamma^h(t)} - M_0\right), \quad \vec\kappa^h = \vec Y^h - (A^h - \overline{\varkappa})\,\vec\omega^h, \tag{4.14g}$$

where we recall (4.2). Here we have defined $\vec f^h(\cdot,t) := \vec I^h_2\,\vec f(\cdot,t)$, where here and throughout we assume that $\vec f \in L^2(0,T;[C(\overline\Omega)]^d)$. We note that in the special case $\overline{\varkappa} = \beta = 0$, the scheme (4.14a–g) collapses to the semidiscrete approximation from Barrett *et al.* (2014b).

In the following theorem we derive discrete analogues of (3.18) and (3.5) for the scheme (4.14a–g).

THEOREM. 4.2. *Let* $\{(\Gamma^h, \vec U^h, P^h, P^h_\Gamma, \vec\kappa^h, \vec Y^h, \vec F^h_\Gamma)(t)\}_{t\in[0,T]}$ *be a solution to* (4.14a–g). *Then, in the case* $\vec g = \vec 0$, *it holds that*

$$\begin{aligned}
&\tfrac12 \frac{\mathrm d}{\mathrm dt}\left(\|[\rho^h]^{\frac12}\,\vec U^h\|_0^2 + \rho_\Gamma\left\langle \vec U^h, \vec U^h\right\rangle^h_{\Gamma^h(t)} + \alpha\left\langle |\vec\kappa^h - \overline{\varkappa}\,\vec\nu^h|^2, 1\right\rangle^h_{\Gamma^h(t)}\right) \\
&\quad + \tfrac12 \frac{\mathrm d}{\mathrm dt}\alpha\,\beta\left(\left\langle \vec\kappa^h, \vec\nu^h\right\rangle^h_{\Gamma^h(t)} - M_0\right)^2 + 2\,\|[\mu^h]^{\frac12}\,\underline{\underline{D}}(\vec U^h)\|_0^2 \\
&\quad + 2\,\mu_\Gamma\left\langle \underline{\underline{D}}{}^h_s(\vec\pi^h\,\vec U^h), \underline{\underline{D}}{}^h_s(\vec\pi^h\,\vec U^h)\right\rangle_{\Gamma^h(t)} + \tfrac12\,\rho_+\left\langle \vec U^h\,.\,\mathrm{n}, |\vec U^h|^2\right\rangle_{\partial_2\Omega} = (\rho^h\,\vec f^h, \vec U^h)\,.
\end{aligned} \tag{4.15}$$

Moreover, it holds that

$$\frac{\mathrm d}{\mathrm dt}\left\langle \chi^h_k, 1\right\rangle_{\Gamma^h(t)} = 0 \quad \forall\ k \in \{1,\ldots,K_\Gamma\} \tag{4.16}$$

and hence that

$$\frac{\mathrm d}{\mathrm dt}\,\mathcal H^{d-1}(\Gamma^h(t)) = 0\,. \tag{4.17}$$

Proof. Choosing $\vec\xi = \vec U^h$ in (4.14a), recall that $\vec g = \vec 0$, $\varphi = P^h$ in (4.14b) and $\eta = P^h_\Gamma$ in (4.14c) yields that

$$\begin{aligned}
&\tfrac12 \frac{\mathrm d}{\mathrm dt}\|[\rho^h]^{\frac12}\,\vec U^h\|_0^2 + 2\,\|[\mu^h]^{\frac12}\,\underline{\underline{D}}(\vec U^h)\|_0^2 + \rho_\Gamma\left\langle \partial_t^{\circ,h}\,\vec\pi^h\,\vec U^h, \vec U^h\right\rangle^h_{\Gamma^h(t)} + \tfrac12\,\rho_+\left\langle \vec U^h\,.\,\mathrm{n}, |\vec U^h|^2\right\rangle_{\partial_2\Omega} \\
&\quad + 2\,\mu_\Gamma\left\langle \underline{\underline{D}}{}^h_s(\vec\pi^h\,\vec U^h), \underline{\underline{D}}{}^h_s(\vec\pi^h\,\vec U^h)\right\rangle_{\Gamma^h(t)} = (\rho^h\,\vec f^h, \vec U^h) + \alpha\left\langle \vec F^h_\Gamma, \vec U^h\right\rangle^h_{\Gamma^h(t)}\,.
\end{aligned} \tag{4.18}$$

Moreover, we note that (4.5), (4.14d) and (4.14c) with $\eta = \pi^h\,[|\vec U^h\,|_{\Gamma^h(t)}\,|^2]$ imply that

$$\begin{aligned}
\tfrac12\,\rho_\Gamma \frac{\mathrm d}{\mathrm dt}\left\langle \vec U^h, \vec U^h\right\rangle^h_{\Gamma^h(t)} &= \tfrac12\,\rho_\Gamma\left\langle \partial_t^{\circ,h}\,\pi^h\,[|\vec U^h|^2], 1\right\rangle^h_{\Gamma^h(t)} + \tfrac12\,\rho_\Gamma\left\langle \nabla_s\,.\,\vec{\mathcal V}^h, |\vec U^h|^2\right\rangle^h_{\Gamma^h(t)} \\
&= \rho_\Gamma\left\langle \partial_t^{\circ,h}\,\vec\pi^h\,\vec U^h, \vec U^h\right\rangle^h_{\Gamma^h(t)} + \tfrac12\,\rho_\Gamma\left\langle \nabla_s\,.\,(\vec\pi^h\,\vec U^h), |\vec U^h|^2\right\rangle^h_{\Gamma^h(t)} \\
&= \rho_\Gamma\left\langle \partial_t^{\circ,h}\,\vec\pi^h\,\vec U^h, \vec U^h\right\rangle^h_{\Gamma^h(t)}\,.
\end{aligned} \tag{4.19}$$

Choosing $\vec\chi = \vec F^h_\Gamma$ in (4.14d) and $\vec\chi = \vec{\mathcal V}^h$ in (4.14f), and combining with (4.11), yields that

$$\begin{aligned}
\left\langle \vec F^h_\Gamma, \vec U^h\right\rangle^h_{\Gamma^h(t)} &= \left\langle \vec F^h_\Gamma, \vec{\mathcal V}^h\right\rangle^h_{\Gamma^h(t)} \\
&= -\frac{\mathrm d}{\mathrm dt}\left(\tfrac12\left\langle |\vec\kappa^h - \overline{\varkappa}\,\vec\nu^h|^2, 1\right\rangle^h_{\Gamma^h(t)} + \tfrac{\beta}{2}\left(\left\langle \vec\kappa^h, \vec\nu^h\right\rangle^h_{\Gamma^h(t)} - M_0\right)^2\right).
\end{aligned} \tag{4.20}$$

The desired result (4.15) now directly follows from combining (4.18), (4.19) and (4.20), on recalling (4.5).

Similarly to (3.5), it immediately follows from (4.4) and (4.3), on choosing $\eta = \chi_k^h$ in (4.14c), and on recalling from (4.14d) that $\vec{\mathcal{V}}^h = \vec{\pi}^h\,\vec{U}^h$, that

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\langle \chi_k^h, 1\rangle_{\Gamma^h(t)} = \left\langle \chi_k^h, \nabla_s\,.\,\vec{\mathcal{V}}^h\right\rangle_{\Gamma^h(t)} = 0\,, \tag{4.21}$$

which proves the desired result (4.16). Summing (4.16) for all $k = 1,\ldots,K_\Gamma$ then yields the desired result (4.17). □

We note that on replacing the space of continuous piecewise linear finite elements $W(\Gamma^h(t))$ for the surface pressure functions P_Γ^h, and for the test functions in (4.14c), with the space of discontinuous piecewise constant functions, it is possible to obtain a scheme that satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{H}^{d-1}(\sigma_j^h(t)) = 0 \qquad \forall\ j \in \{1,\ldots,J_\Gamma\} \tag{4.22}$$

in place of (4.21). However, the fully discrete variant of this modified (4.14a–g) for $d = 3$ does not perform very well in practice, as the constraint (4.22) is too severe, see Remark 4.2 in Barrett *et al.* (2014b) for more details.

We observe that it does not appear possible to prove a discrete analogue of (3.6) for the scheme (4.14a–g). The reason is that $\vec{\chi} = \vec{\nu}^h$ is not a valid test function in (4.14d). However, a procedure similarly to the XFEM approach introduced by the authors in Barrett *et al.* (2013, 2014c) ensures that a modified variant of (4.14a–g) conserves the enclosed volumes. We are now in a position to propose the following adaptation of (4.14a–g).

Given $\Gamma^h(0)$ and $\vec{U}^h(\cdot,0) \in \mathbb{U}^h(\vec{g})$, find $\Gamma^h(t)$ such that $\vec{\mathrm{id}}\,|_{\Gamma^h(t)} \in \underline{V}(\Gamma^h(t))$ for $t \in [0,T]$, and functions $\vec{U}^h \in \mathbb{V}^h_{\Gamma^h}(\vec{g})$, $P^h \in \mathbb{P}^h_T$, $P^h_{\rm sing} \in L^2(0,T;\mathbb{R})$, $P^h_\Gamma \in W(\mathcal{G}^h_T)$, $\vec{Y}^h \in [W(\mathcal{G}^h_T)]^d$ and $\vec{F}^h_\Gamma \in [W(\mathcal{G}^h_T)]^d$ such that for almost all $t \in (0,T)$ it holds that

$$\begin{aligned}
&\tfrac12\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\rho^h\,\vec{U}^h,\vec{\xi}\right) + \left(\rho^h\,\vec{U}^h_t,\vec{\xi}\right) - (\rho^h\,\vec{U}^h,\vec{\xi}_t) + \rho_+\left\langle \vec{U}^h\,.\,\vec{\rm n}, \vec{U}^h\,.\,\vec{\xi}\right\rangle_{\partial_2\Omega}\right] \\
&\quad + 2\left(\mu^h\,\underline{\underline{D}}(\vec{U}^h),\underline{\underline{D}}(\vec{\xi})\right) + \tfrac12\left(\rho^h,[(\vec{U}^h\,.\,\nabla)\,\vec{U}^h]\,.\,\vec{\xi} - [(\vec{U}^h\,.\,\nabla)\,\vec{\xi}]\,.\,\vec{U}^h\right) - \left(P^h,\nabla\,.\,\vec{\xi}\right) \\
&\quad - P^h_{\rm sing}\left\langle \vec{\omega}^h,\vec{\xi}\right\rangle^h_{\Gamma^h(t)} + \rho_\Gamma\left\langle \partial_t^{\circ,h}\,\vec{\pi}^h\,\vec{U}^h,\vec{\xi}\right\rangle^h_{\Gamma^h(t)} + 2\,\mu_\Gamma\left\langle \underline{\underline{D}}^h_s(\vec{\pi}^h\,\vec{U}^h),\underline{\underline{D}}^h_s(\vec{\pi}^h\,\vec{\xi})\right\rangle_{\Gamma^h(t)} \\
&\quad - \left\langle P^h_\Gamma,\nabla_s\,.\,(\vec{\pi}^h\,\vec{\xi})\right\rangle_{\Gamma^h(t)} = \left(\rho^h\,\vec{f}^h,\vec{\xi}\right) + \alpha\left\langle \vec{F}^h_\Gamma,\vec{\xi}\right\rangle^h_{\Gamma^h(t)} \qquad \forall\ \vec{\xi} \in H^1(0,T;\mathbb{U}^h(\vec{0}))\,,
\end{aligned} \tag{4.23a}$$

$$\left(\nabla\,.\,\vec{U}^h,\varphi\right) = 0 \qquad \forall\ \varphi \in \widehat{\mathbb{P}}^h(t) \qquad \text{and} \qquad \left\langle \vec{U}^h,\vec{\omega}^h\right\rangle^h_{\Gamma^h(t)} = 0 \tag{4.23b}$$

and (4.14c–g) hold. Of course, $\vec{\chi} = \vec{\omega}^h$ is a valid test function in (4.14d), and so combining with (4.14b) yields a discrete volume preservation property, as is shown in the following theorem.

THEOREM. 4.3. *Let* $\{(\Gamma^h, \vec{U}^h, P^h, P^h_{\rm sing}, P^h_\Gamma, \vec\kappa^h, \vec{Y}^h, \vec{F}^h_\Gamma)(t)\}_{t\in[0,T]}$ *be a solution to* (4.23a,b), (4.14c–g). *Then* (4.15) *holds if* $\vec{g} = \vec{0}$. *In addition,* (4.17) *and*

$$\frac{\rm d}{{\rm d}t}\,\mathcal{L}^d(\Omega^h_-(t)) = 0 \tag{4.24}$$

hold.

Proof. The proofs for (4.15) and (4.17) are analogous to the proofs in Theorem 4.2. In order to prove (4.24) we choose $\vec\chi = \vec\omega^h \in \underline{V}(\Gamma^h(t))$ in (4.14d) to yield that

$$\frac{\rm d}{{\rm d}t}\mathcal{L}^d(\Omega^h_-(t)) = \left\langle \vec{\mathcal{V}}^h, \vec\nu^h \right\rangle_{\Gamma^h(t)} = \left\langle \vec{\mathcal{V}}^h, \vec\nu^h \right\rangle^h_{\Gamma^h(t)} = \left\langle \vec{\mathcal{V}}^h, \vec\omega^h \right\rangle^h_{\Gamma^h(t)} = \left\langle \vec{U}^h, \vec\omega^h \right\rangle^h_{\Gamma^h(t)} = 0\,,$$

where we have used (4.8) and (4.23b). □

We remark that the approach in (4.23a,b) can be viewed as an example of the recently proposed framework of virtual element methods, see Beirão da Veiga *et al.* (2013). We refer to Barrett *et al.* (2014b) for more details.

5 Fully discrete finite element approximation

We consider the partitioning $t_m = m\,\tau$, $m = 0,\ldots,M$, of $[0,T]$ into uniform time steps $\tau = T/M$. The time discrete spatial discretizations then directly follow from the finite element spaces introduced in §3, where in order to allow for adaptivity in space we consider bulk finite element spaces that change in time.

For all $m \geq 0$, let $\mathcal{T}^m$ be a regular partitioning of Ω into disjoint open simplices o^m_j, $j = 1,\ldots,J^m_\Omega$. Associated with $\mathcal{T}^m$ are the finite element spaces S^m_k for $k \geq 0$. We introduce also $\vec{I}^m_k : [C(\overline{\Omega})]^d \to [S^m_k]^d$, $k \geq 1$, the standard interpolation operators, and the standard projection operator $I^m_0 : L^1(\Omega) \to S^m_0$.

Similarly, the parametric finite element spaces are given by

$$\underline{V}(\Gamma^m) := \{\vec\chi \in [C(\Gamma^m)]^d : \vec\chi|_{\sigma^m_j} \text{ is linear } \forall\ j = 1,\ldots,J_\Gamma\} =: [W(\Gamma^m)]^d \subset [H^1(\Gamma^m)]^d\,,$$

for $m = 0,\ldots,M-1$. Here $\Gamma^m = \bigcup_{j=1}^{J_\Gamma} \overline{\sigma^m_j}$, where $\{\sigma^m_j\}_{j=1}^{J_\Gamma}$ is a family of mutually disjoint open $(d-1)$-simplices with vertices $\{\vec{q}^m_k\}_{k=1}^{K_\Gamma}$. We denote the standard basis of $W(\Gamma^m)$ by $\{\chi^m_k(\cdot,t)\}_{k=1}^{K_\Gamma}$. We also introduce $\pi^m : C(\Gamma^m) \to W(\Gamma^m)$, the standard interpolation operator at the nodes $\{\vec{q}^m_k\}_{k=1}^{K_\Gamma}$, and similarly $\vec\pi^m : [C(\Gamma^m)]^d \to \underline{V}(\Gamma^m)$. Throughout this paper, we will parameterize the new closed surface Γ^{m+1} over Γ^m, with the help of a parameterization $\vec{X}^{m+1} \in \underline{V}(\Gamma^m)$, i.e. $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$.

We also introduce the L^2–inner product $\langle\cdot,\cdot\rangle_{\Gamma^m}$ over the current polyhedral surface Γ^m, as well as the the mass lumped inner product $\langle\cdot,\cdot\rangle^h_{\Gamma^m}$. Similarly to (4.6a,b), we introduce

$$\underline{\underline{\mathcal{P}}}_{\Gamma^m} = \underline{\underline{\rm Id}} - \vec\nu^m \otimes \vec\nu^m \quad \text{on } \Gamma^m\,,$$

and

$$\underline{\underline{D}}_s^m(\vec{\eta}) = \tfrac{1}{2}\,\underline{\underline{\mathcal{P}}}_{\Gamma^m}\,(\nabla_s\,\vec{\eta} + (\nabla_s\,\vec{\eta})^T)\,\underline{\underline{\mathcal{P}}}_{\Gamma^m} \quad \text{on } \Gamma^m\,,$$

where here $\nabla_s = \underline{\underline{\mathcal{P}}}_{\Gamma^m}\,\nabla$ denotes the surface gradient on Γ^m.

Given Γ^m, we let Ω^m_+ denote the exterior of Γ^m and let Ω^m_- denote the interior of Γ^m, so that $\Gamma^m = \partial\Omega^m_- = \overline{\Omega^m_-}\cap\overline{\Omega^m_+}$. We then partition the elements of the bulk mesh $\mathcal{T}^m$ into interior, exterior and interfacial elements as before, and we introduce ρ^m, $\mu^m \in S^m_0$, for $m \geq 0$, as

$$\rho^m\,|_{o^m} = \begin{cases} \rho_- & o^m \in \mathcal{T}^m_-\,,\\ \rho_+ & o^m \in \mathcal{T}^m_+\,,\\ \tfrac{1}{2}\,(\rho_- + \rho_+) & o^m \in \mathcal{T}^m_{\Gamma^m}\,,\end{cases} \quad \text{and} \quad \mu^m\,|_{o^m} = \begin{cases} \mu_- & o^m \in \mathcal{T}^m_-\,,\\ \mu_+ & o^m \in \mathcal{T}^m_+\,,\\ \tfrac{1}{2}\,(\mu_- + \mu_+) & o^m \in \mathcal{T}^m_{\Gamma^m}\,.\end{cases}$$

We introduce the following pushforward operator for the discrete interfaces Γ^m and Γ^{m-1}, for $m = 0,\ldots,M$. Here we set $\Gamma^{-1} := \Gamma^0$. Let $\vec{\Pi}^m_{m-1} : [C(\Gamma^{m-1})]^d \to \underline{V}(\Gamma^m)$ such that

$$(\vec{\Pi}^m_{m-1}\,\vec{z})(\vec{q}^m_k) = \vec{z}(\vec{q}^{m-1}_k)\,, \qquad k = 1,\ldots,K_\Gamma\,, \qquad \forall\ \vec{z} \in [C(\Gamma^{m-1})]^d\,, \tag{5.1}$$

for $m = 1,\ldots,M$, and set $\vec{\Pi}^0_{-1} := \vec{\pi}^0$. Analogously to (5.1) we also introduce $\Pi^m_{m-1} : C(\Gamma^{m-1}) \to W(\Gamma^m)$.

Similarly to (4.7), we let

$$\vec{\omega}^m := \sum_{k=1}^{K_\Gamma} \chi^m_k\,\vec{\omega}^m_k \in \underline{V}(\Gamma^m)\,,$$

where for $k = 1,\ldots,K_\Gamma$ we let $\Theta^m_k := \{j : \vec{q}^m_k \in \overline{\sigma^m_j}\}$ and set

$$\Lambda^m_k := \cup_{j\in\Theta^m_k}\overline{\sigma^m_j} \qquad \text{and} \qquad \vec{\omega}^m_k := \frac{1}{\mathcal{H}^{d-1}(\Lambda^m_k)}\sum_{j\in\Theta^m_k}\mathcal{H}^{d-1}(\sigma^m_j)\,\vec{\nu}^m_j\,.$$

For the approximation to the velocity and pressure on $\mathcal{T}^m$ we use the finite element spaces $\mathbb{U}^m(\vec{g})$ and $\mathbb{P}^m$, which are the direct time discrete analogues of $\mathbb{U}^h(\vec{g})$ and $\mathbb{P}^h(t_m)$, as well as $\widehat{\mathbb{P}}^m \subset \widehat{\mathbb{P}}$. We also say that $(\mathbb{U}^m(\vec{0}),\mathbb{P}^m,W(\Gamma^m))$ satisfy the LBB$_\Gamma$ inf-sup condition if there exists a constant $C_0 \in \mathbb{R}_{>0}$ independent of h^m such that

$$\inf_{(\varphi,\lambda,\eta)\in\widehat{\mathbb{P}}^m\times\mathbb{R}\times W(\Gamma^m)}\ \sup_{\vec{\xi}\in\mathbb{U}^m(\vec{0})} \frac{(\varphi,\nabla\,.\,\vec{\xi}) + \lambda\left\langle\vec{\omega}^m,\vec{\xi}\right\rangle^h_{\Gamma^m} + \left\langle\eta,\nabla_s\,.\,(\vec{\pi}^m\,\vec{\xi}|_{\Gamma^m})\right\rangle_{\Gamma^m}}{(\|\varphi\|_0 + |\lambda| + \|\eta\|_{0,\Gamma^m})\,(\|\vec{\xi}\|_1 + \|\vec{\pi}^m\,\underline{\underline{\mathcal{P}}}_{\Gamma^m}\,\vec{\xi}|_{\Gamma^m}\,\|_{1,\Gamma^m})} \geq C_0\,, \tag{5.2}$$

where $\|\eta\|^2_{0,\Gamma^m} := \langle\eta,\eta\rangle_{\Gamma^m}$ and $\|\vec{\eta}\|^2_{1,\Gamma^m} := \langle\vec{\eta},\vec{\eta}\rangle_{\Gamma^m} + \langle\nabla_s\,\vec{\eta},\nabla_s\,\vec{\eta}\rangle_{\Gamma^m}$ for $\vec{\eta} \in \underline{V}(\Gamma^m)$. Unfortunately, it does not appear possible to prove that (5.2) holds for e.g. $(\mathbb{U}^m(\vec{0}),\mathbb{P}^m) = ([S^m_2]^d \cap \mathbb{U}(\vec{0}), S^m_1)$, because $\mathcal{T}^m$ and Γ^m are totally independent. Recall that also in the much simpler situation of the XFEM$_\Gamma$ approach from Barrett *et al.* (2013, 2014c), which corresponds to setting $\eta = 0$ in (5.2) and replacing $\left\langle \vec\omega^m, \vec\xi \right\rangle^h_{\Gamma^m}$ with $\left\langle \vec\nu^m, \vec\xi \right\rangle^h_{\Gamma^m}$, the authors were unable to show that an LBB condition holds.

Our proposed fully discrete equivalent of (4.23a,b), (4.14c–g) is then given as follows. Let Γ^0, an approximation to $\Gamma(0)$, as well as $\vec\kappa^0, \vec Y^0 \in \underline{V}(\Gamma^0)$, $A^0 \in \mathbb{R}$ and $\vec U^0 \in \mathbb{U}^0(\vec g)$ be given. For $m = 0, \ldots, M-1$, find $\vec U^{m+1} \in \mathbb{U}^m(\vec g)$, $P^{m+1} \in \widehat{\mathbb{P}}^m$, $P^{m+1}_{\rm sing} \in \mathbb{R}$, $P^{m+1}_\Gamma \in W(\Gamma^m)$, $\vec X^{m+1} \in \underline{V}(\Gamma^m)$, $\vec Y^{m+1} \in \underline{V}(\Gamma^m)$ and $\vec F^{m+1}_\Gamma \in \underline{V}(\Gamma^m)$ such that

$$
\begin{aligned}
&\tfrac12 \left(\frac{\rho^m\,\vec U^{m+1} - (I^m_0\,\rho^{m-1})\,\vec I^m_2\,\vec U^m}{\tau} + (I^m_0\,\rho^{m-1})\,\frac{\vec U^{m+1} - \vec I^m_2\,\vec U^m}{\tau}, \vec\xi \right) \\
&\quad + 2\left(\mu^m\,\underline{\underline{D}}(\vec U^{m+1}), \underline{\underline{D}}(\vec\xi)\right) + \tfrac12 \left(\rho^m, [(\vec I^m_2\,\vec U^m\,.\,\nabla)\,\vec U^{m+1}]\,.\,\vec\xi - [(\vec I^m_2\,\vec U^m\,.\,\nabla)\,\vec\xi]\,.\,\vec U^{m+1}\right) \\
&\quad - \left(P^{m+1}, \nabla\,.\,\vec\xi\right) - P^{m+1}_{\rm sing}\left\langle \vec\omega^m, \vec\xi\right\rangle^h_{\Gamma^m} + \rho_\Gamma \left\langle \frac{\vec U^{m+1} - \vec\Pi^m_{m-1}\,(\vec I^m_2\,\vec U^m)\,|_{\Gamma^{m-1}}}{\tau}, \vec\xi \right\rangle^h_{\Gamma^m} \\
&\quad + 2\,\mu_\Gamma \left\langle \underline{\underline{D}}^m_s(\vec\pi^m\,\vec U^{m+1}), \underline{\underline{D}}^m_s(\vec\pi^m\,\vec\xi)\right\rangle_{\Gamma^m} - \left\langle P^{m+1}_\Gamma, \nabla_s\,.\,(\vec\pi^m\,\vec\xi)\right\rangle_{\Gamma^m} \\
&\qquad = \left(\rho^m\,\vec f^{m+1}, \vec\xi\right) + \alpha \left\langle \vec F^{m+1}_\Gamma, \vec\xi\right\rangle^h_{\Gamma^m} - \tfrac12\,\rho_+ \left\langle \vec U^m\,.\,\vec{\rm n}, \vec U^m\,.\,\vec\xi\right\rangle_{\partial_2\Omega} \qquad \forall\ \vec\xi \in \mathbb{U}^m(\vec 0)\,,
\end{aligned}
\tag{5.3a}
$$

$$
\left(\nabla\,.\,\vec U^{m+1}, \varphi\right) = 0 \quad \forall\ \varphi \in \widehat{\mathbb{P}}^m \quad \text{and} \quad \left\langle \vec U^{m+1}, \vec\omega^m\right\rangle^h_{\Gamma^m} = 0\,, \tag{5.3b}
$$

$$
\left\langle \nabla_s\,.\,(\vec\pi^m\,\vec U^{m+1}), \eta\right\rangle_{\Gamma^m} = 0 \quad \forall\ \eta \in W(\Gamma^m)\,, \tag{5.3c}
$$

$$
\left\langle \frac{\vec X^{m+1} - \vec{\rm id}}{\tau}, \vec\chi \right\rangle^h_{\Gamma^m} = \left\langle \vec U^{m+1}, \vec\chi\right\rangle^h_{\Gamma^m} \quad \forall\ \vec\chi \in \underline{V}(\Gamma^m)\,, \tag{5.3d}
$$

$$
\left\langle \vec Y^{m+1}, \vec\eta\right\rangle^h_{\Gamma^m} + \left\langle \nabla_s\,\vec X^{m+1}, \nabla_s\,\vec\eta\right\rangle_{\Gamma^m} = (A^m - \overline\varkappa)\,\langle \vec\omega^m, \vec\eta\rangle^h_{\Gamma^m} \quad \forall\ \vec\eta \in \underline{V}(\Gamma^m)\,, \tag{5.3e}
$$

$$
\begin{aligned}
&\left\langle \vec F^{m+1}_\Gamma, \vec\chi\right\rangle^h_{\Gamma^m} = \left\langle \nabla_s\,\vec Y^{m+1}, \nabla_s\,\vec\chi\right\rangle_{\Gamma^m} + \left\langle \nabla_s\,.\,(\vec\Pi^m_{m-1}\,\vec Y^m), \nabla_s\,.\,\vec\chi\right\rangle_{\Gamma^m} \\
&\quad - 2\left\langle \nabla_s\,(\vec\Pi^m_{m-1}\,\vec Y^m), \underline{\underline{D}}^m_s(\vec\chi)\,\nabla_s\,\vec{\rm id}\right\rangle_{\Gamma^m} + (A^m - \overline\varkappa)\left\langle \vec\Pi^m_{m-1}\,\vec\kappa^m, [\nabla_s\,\vec\chi]^T\,\vec\nu^m\right\rangle^h_{\Gamma^m} \\
&\quad - \tfrac12 \left\langle [|\vec\Pi^m_{m-1}\,\vec\kappa^m - \overline\varkappa\,\vec\nu^m|^2 - 2\,(\vec\Pi^m_{m-1}\,\vec Y^m - A^m\,\vec\nu^m)\,.\,(\vec\Pi^m_{m-1}\,\vec\kappa^m)]\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec\chi\right\rangle^h_{\Gamma^m} \\
&\qquad\qquad \forall\ \vec\chi \in \underline{V}(\Gamma^m)
\end{aligned}
\tag{5.3f}
$$

and set $\Gamma^{m+1} = \vec X^{m+1}(\Gamma^m)$. Moreover, set

$$
\vec\kappa^{m+1} = \vec Y^{m+1} - (A^m - \overline\varkappa)\,\vec\omega^m \in \underline{V}(\Gamma^m) \quad \text{and} \quad A^{m+1} = \beta\left(\langle \vec\kappa^{m+1}, \vec\nu^m\rangle^h_{\Gamma^m} - M_0\right). \tag{5.4}
$$

Here we have defined $\vec f^{m+1} := \vec I^m_2\,\vec f(\cdot, t_{m+1})$. We observe that (5.3a–f) is a linear scheme in that it leads to a linear system of equations for the unknowns $(\vec U^{m+1}, P^{m+1}, P^{m+1}_{\rm sing}, P^{m+1}_\Gamma, \vec X^{m+1}, \vec Y^{m+1}, \vec F^{m+1}_\Gamma)$ at each time level.

In the absence of the LBB$_\Gamma$ condition (5.2) we need to consider the reduced system (5.3a,d–f), where $\mathbb{U}^m(\vec 0)$ in (5.3a) is replaced by $\mathbb{U}^m_0(\vec 0)$. Here we define

$$\mathbb{U}^m_0(\vec b) := \left\{\vec U \in \mathbb{U}^m(\vec b) : (\nabla\,.\,\vec U, \varphi) = 0 \quad \forall\, \varphi \in \widehat{\mathbb{P}}^m\,, \left\langle \nabla_s\,.\,(\vec\pi^m\,\vec U), \eta\right\rangle_{\Gamma^m} = 0 \quad \forall\, \eta \in W(\Gamma^m) \right.$$
$$\left. \text{and } \left\langle \vec U, \vec\omega^m\right\rangle^h_{\Gamma^m} = 0 \right\},$$

for given data $\vec b \in [C(\overline\Omega)]^d$.

In order to prove the existence of a unique solution to (5.3a–f) we make the following very mild well-posedness assumption.

($\mathcal{A}$) We assume for $m = 0, \ldots, M-1$ that $\mathcal{H}^{d-1}(\sigma^m_j) > 0$ for all $j = 1, \ldots, J_\Gamma$, and that $\Gamma^m \subset \Omega$.

Theorem. 5.1. *Let the assumption* ($\mathcal{A}$) *hold. If the LBB$_\Gamma$ condition* (5.2) *holds, then there exists a unique solution* $(\vec U^{m+1}, P^{m+1}, P^{m+1}_{\rm sing}, P^{m+1}_\Gamma, \vec X^{m+1}, \vec Y^{m+1}, \vec F^{m+1}_\Gamma) \in \mathbb{U}^m(\vec g) \times \widehat{\mathbb{P}}^m \times \mathbb{R} \times W(\Gamma^m) \times [\underline{V}(\Gamma^m)]^3$ *to* (5.3a–f). *In all other cases, on assuming that* $\mathbb{U}^m_0(\vec g)$ *is nonempty, there exists a unique solution* $(\vec U^{m+1}, \vec X^{m+1}, \vec Y^{m+1}, \vec F^{m+1}_\Gamma) \in \mathbb{U}^m_0(\vec g) \times [\underline{V}(\Gamma^m)]^3$ *to the reduced system* (5.3a,d–f) *with* $\mathbb{U}^m(\vec 0)$ *replaced by* $\mathbb{U}^m_0(\vec 0)$.

Proof. As the system (5.3a–f) is linear, existence follows from uniqueness. In order to establish the latter, we consider the homogeneous system. Find $(\vec U, P, P_{\rm sing}, P_\Gamma, \vec X, \vec Y, \vec F_\Gamma) \in \mathbb{U}^m(\vec 0) \times \widehat{\mathbb{P}}^m \times \mathbb{R} \times W(\Gamma^m) \times [\underline{V}(\Gamma^m)]^3$ such that

$$\begin{aligned}
&\tfrac{1}{2\,\tau}\left((\rho^m + I^m_0\,\rho^{m-1})\,\vec U, \vec\xi\right) + 2\left(\mu^m\,\underline{\underline{D}}(\vec U), \underline{\underline{D}}(\vec\xi)\right) - \left(P, \nabla\,.\,\vec\xi\right) - P_{\rm sing}\left\langle \vec\omega^m, \vec\xi\right\rangle^h_{\Gamma^m} \\
&\quad + \tfrac12\left(\rho^m, [(\vec I^m_2\,\vec U^m\,.\,\nabla)\,\vec U]\,.\,\vec\xi - [(\vec I^m_2\,\vec U^m\,.\,\nabla)\,\vec\xi]\,.\,\vec U\right) \\
&\quad + \tfrac{1}{\tau}\,\rho_\Gamma\left\langle \vec U, \vec\xi\right\rangle^h_{\Gamma^m} + 2\,\mu_\Gamma\left\langle \underline{\underline{D}}^m_s(\vec\pi^m\,\vec U), \underline{\underline{D}}^m_s(\vec\pi^m\,\vec\xi)\right\rangle_{\Gamma^m} \\
&\quad - \left\langle P_\Gamma, \nabla_s\,.\,(\vec\pi^m\,\vec\xi)\right\rangle_{\Gamma^m} - \alpha\left\langle \vec F_\Gamma, \vec\xi\right\rangle^h_{\Gamma^m} = 0 \qquad \forall\, \vec\xi \in \mathbb{U}^m(\vec 0)\,, && \text{(5.5a)}\\
&\left(\nabla\,.\,\vec U, \varphi\right) = 0 \qquad \forall\, \varphi \in \widehat{\mathbb{P}}^m \qquad \text{and} \qquad \left\langle \vec U, \vec\omega^m\right\rangle^h_{\Gamma^m} = 0\,, && \text{(5.5b)}\\
&\left\langle \nabla_s\,.\,(\vec\pi^m\,\vec U), \eta\right\rangle_{\Gamma^m} = 0 \qquad \forall\, \eta \in W(\Gamma^m)\,, && \text{(5.5c)}\\
&\tfrac{1}{\tau}\left\langle \vec X, \vec\chi\right\rangle^h_{\Gamma^m} = \left\langle \vec U, \vec\chi\right\rangle^h_{\Gamma^m} \qquad \forall\, \vec\chi \in \underline{V}(\Gamma^m)\,, && \text{(5.5d)}\\
&\left\langle \vec Y, \vec\eta\right\rangle^h_{\Gamma^m} + \left\langle \nabla_s\,\vec X, \nabla_s\,\vec\eta\right\rangle_{\Gamma^m} = 0 \qquad \forall\, \vec\eta \in \underline{V}(\Gamma^m)\,, && \text{(5.5e)}\\
&\left\langle \vec F_\Gamma, \vec\chi\right\rangle^h_{\Gamma^m} - \left\langle \nabla_s\,\vec Y, \nabla_s\,\vec\chi\right\rangle_{\Gamma^m} = 0 \qquad \forall\, \vec\chi \in \underline{V}(\Gamma^m)\,. && \text{(5.5f)}
\end{aligned}$$

Choosing $\vec{\xi} = \vec{U}$ in (5.5a), $\varphi = P$ in (5.5b), $\eta = P_\Gamma$ in (5.5c), $\vec{\chi} = \vec{F}_\Gamma$ in (5.5d), $\vec{\eta} = \vec{Y}$ in (5.5e) and $\vec{\chi} = \vec{X}$ in (5.5f) yields that

$$\tfrac{1}{2}\left((\rho^m + I_0^m\,\rho^{m-1})\,\vec{U},\vec{U}\right) + 2\,\tau\left(\mu^m\,\underline{\underline{D}}(\vec{U}),\underline{\underline{D}}(\vec{U})\right) + \rho_\Gamma\left\langle \vec{U},\vec{U}\right\rangle_{\Gamma^m}^h$$
$$+ 2\,\tau\,\mu_\Gamma\left\langle \underline{\underline{D}}_s^m(\vec{\pi}^m\,\vec{U}), \underline{\underline{D}}_s^m(\vec{\pi}^m\,\vec{U})\right\rangle_{\Gamma^m} + \alpha\left\langle \vec{Y},\vec{Y}\right\rangle_{\Gamma^m}^h = 0\,. \tag{5.6}$$

It immediately follows from (5.6), Korn's inequality and $\alpha > 0$, that $\vec{U} = \vec{0} \in \mathbb{U}^m(\vec{0})$ and $\vec{Y} = \vec{0}$. (For the application of Korn's inequality we recall that $\mathcal{H}^{d-1}(\partial_1\Omega) > 0$.) Hence (5.5d,f) yield that $\vec{X} = \vec{0}$ and $\vec{F}_\Gamma = \vec{0}$, respectively. Finally, if (5.2) holds then (5.5a) with $\vec{U} = \vec{0}$ and $\vec{F}_\Gamma = \vec{0}$ implies that $P = 0 \in \widehat{\mathbb{P}}^m$, $P_{\text{sing}} = 0$ and $P_\Gamma = 0 \in W(\Gamma^m)$. This shows existence and uniqueness of $(\vec{U}^{m+1}, P^{m+1}, P_\Gamma^{m+1}, \vec{X}^{m+1}, \vec{Y}^{m+1}, \vec{F}_\Gamma^{m+1}) \in \mathbb{U}^m(\vec{g}) \times \widehat{\mathbb{P}}^m \times W(\Gamma^m) \times [\underline{V}(\Gamma^m)]^3$ to (5.3a–f). The proof for the reduced system is very similar. The homogeneous system to consider is (5.5a,d–f) with $\mathbb{U}^m(\vec{0})$ replaced by $\mathbb{U}_0^m(\vec{0})$. As before, we infer that (5.6) holds, which yields that $\vec{U} = \vec{0} \in \mathbb{U}_0^m(\vec{0})$, $\vec{Y} = \vec{0}$, and hence $\vec{X} = \vec{0}$ and $\vec{F}_\Gamma = \vec{0}$. □

6 Solution methods

Using the notation introduced in Barrett *et al.* (2014b), the linear system (5.3a–f) can be written as

$$\begin{pmatrix} \vec{B}_\Omega & \vec{\mathcal{C}} & 0 & 0 & -\alpha\,\vec{M}_{\Gamma,\Omega} \\ \vec{\mathcal{C}}^T & 0 & 0 & 0 & 0 \\ (\vec{M}_{\Gamma,\Omega})^T & 0 & 0 & -\frac{1}{\tau}\,\vec{M}_\Gamma & 0 \\ 0 & 0 & \vec{M}_\Gamma & \vec{A}_\Gamma & 0 \\ 0 & 0 & -\vec{A}_\Gamma & 0 & \vec{M}_\Gamma \end{pmatrix} \begin{pmatrix} \vec{U}^{m+1} \\ \widetilde{P}^{m+1} \\ \vec{Y}^{m+1} \\ \delta\vec{X}^{m+1} \\ \vec{F}_\Gamma^{m+1} \end{pmatrix}$$
$$= (\vec{b}, 0, 0, -\vec{A}_\Gamma\,\vec{X}^m + (A^m - \overline{\varkappa})\,\vec{M}_\Gamma\,\vec{\omega}^m, \vec{\mathcal{Z}}_\Gamma\,\vec{Y}^m + \vec{A}_{\Gamma,\vec{Y}}\,\vec{X}^m - \vec{c})^T\,, \tag{6.1}$$

where in addition to the matrices, and $\vec{b}$, from Barrett *et al.* (2014b) we define

$$[\vec{A}_{\Gamma,\vec{Y}}]_{kl} := -\tfrac{1}{2}\left\langle |\vec{\Pi}_{m-1}^m\,\vec{\kappa}^m - \overline{\varkappa}\,\vec{\nu}^m|^2\,\nabla_s\,\chi_l^m, \nabla_s\,\chi_k^m\right\rangle_{\Gamma^m}^h \underline{\underline{\rm Id}}$$
$$+ \left\langle (\vec{\Pi}_{m-1}^m\,\vec{Y}^m - A^m\,\vec{\nu}^m)\,.\,(\vec{\Pi}_{m-1}^m\,\vec{\kappa}^m)\,\nabla_s\,\chi_l^m, \nabla_s\,\chi_k^m\right\rangle_{\Gamma^m}^h \underline{\underline{\rm Id}}\,,$$
$$[\vec{\mathcal{M}}_\Gamma]_{kl} := \langle \chi_l^m, \chi_k^m\,\vec{\omega}^m \otimes \vec{\omega}^m\rangle_{\Gamma^m}^h\ ,$$

for $k, l = 1, \ldots, K_\Gamma$, as well as $\vec{c} \in (\mathbb{R}^d)^{K_\Gamma}$ with

$$\vec{c}_k = \left\langle \overline{\varkappa} - A^m, (\vec{\Pi}_{m-1}^m\,\vec{\kappa}^m\,.\,\nabla_s\,\chi_k^m)\,\vec{\nu}^m\right\rangle_{\Gamma^m}^h\,.$$

As the linear operator on the left hand side of (6.1) is exactly the same as in Barrett *et al.* (2014b), the system (6.1) can be solved with the Schur complement approach introduced in Barrett *et al.* (2014b).

7 Numerical results

We implemented the scheme (5.3a–f) with the help of the finite element toolbox ALBERTA, see Schmidt and Siebert (2005). In what follows we present numerical simulations for the scheme (5.3a–f) in the case $d = 3$. We recall that, on account of the Gauß–Bonnet theorem, in two space dimensions the fluidic biomembrane problem (3.3a–d) and (3.13a–d) is independent of the values of $\overline{\varkappa}$ and β. Hence for the case $d = 2$ we can refer to our numerical simulations in Barrett *et al.* (2014b) for the case $\overline{\varkappa} = \beta = 0$.

For the bulk mesh adaptation in our numerical computations we use the strategy from Barrett *et al.* (2014c), which results in a fine mesh size h_f around Γ^m and a coarse mesh size h_c further away from it. Here $h_f = \frac{2\,\min\{H_1,H_2\}}{N_f}$ and $h_c = \frac{2\,\min\{H_1,H_2\}}{N_c}$ are given by two integer numbers $N_f > N_c$, where we assume from now on that the convex hull of Ω is given by $\times_{i=1}^{3}(-H_i, H_i)$.

Given the initial triangulation Γ^0, the initial data $\vec{Y}^0 \in \underline{V}(\Gamma^0)$, $A^0 \in \mathbb{R}$ and $\vec{\kappa}^0 \in \underline{V}(\Gamma^0)$ are always computed as

$$\vec{Y}^0 = \vec{\kappa}^0 + (A^0 - \overline{\varkappa})\,\vec{\omega}^0\,, \quad A^0 = \beta\left(\left\langle \vec{\kappa}^0, \vec{\nu}^0\right\rangle_{\Gamma^0}^h - M_0\right),$$

where $\vec{\kappa}^0 \in \underline{V}(\Gamma^0)$ is the solution to

$$\left\langle \vec{\kappa}^0, \vec{\eta}\right\rangle_{\Gamma^0}^h + \left\langle \nabla_s\, \mathrm{i\vec{d}}, \nabla_s\, \vec{\eta}\right\rangle_{\Gamma^0} = 0 \qquad \forall\ \vec{\eta} \in \underline{V}(\Gamma^0)\,.$$

In addition, in all computations we set $(\mathbb{U}^m(\vec{0}), \mathbb{P}^m) = ([S_2^m]^d \cap \mathbb{U}(\vec{0}), S_1^m)$, i.e. the lowest order Taylor–Hood element P2–P1, and let $\vec{U}^0 = \vec{I}_2^0\,\vec{u}_0$. Unless stated otherwise we fix $\partial_1\Omega = \partial\Omega$, $\vec{g} = \vec{0}$ and $\vec{u}_0 = \vec{0}$. The volume force is always set to $\vec{f} = \vec{0}$. Moreover, unless otherwise stated, we set the physical parameters to $\rho_\pm = \mu_\pm = \mu_\Gamma = \alpha = 1$ and $\rho_\Gamma = 0$. Similarly, we set $\overline{\varkappa} = \beta = 0$ unless stated otherwise.

At times we will discuss the discrete energy of the numerical solutions. On recalling Theorem 4.1 and (5.4) the discrete energy is defined by

$$\mathcal{E}^h(\Gamma^m, \vec{Y}^{m+1}) := \mathcal{E}^h_{kin}(\Gamma^m, \rho^m, \vec{U}^{m+1}) + \tfrac{1}{2}\,\alpha\left[\left\langle |\vec{\kappa}^{m+1} - \overline{\varkappa}\,\vec{\nu}^m|^2, 1\right\rangle_{\Gamma^m}^h + \tfrac{1}{\beta}(A^m)^2\right],$$

where

$$\mathcal{E}^h_{kin}(\Gamma^m, \rho^m, \vec{U}^{m+1}) := \tfrac{1}{2}\,\|[\rho^m]^{\frac{1}{2}}\,\vec{U}^{m+1}\|_0^2 + \tfrac{1}{2}\,\rho_\Gamma\left\langle \vec{U}^{m+1}, \vec{U}^{m+1}\right\rangle_{\Gamma^m}^h$$

represents the kinetic part of the discrete energy. For the simulation of vesicles the reduced volume is often mentioned as a characteristic number. In the case $d = 3$, and for the initial discrete interface Γ^0, this is defined as

$$v_r = \frac{3\,\mathcal{L}^3(\Omega_-^0)}{4\,\pi\,(\frac{\mathcal{H}^2(\Gamma^0)}{4\,\pi})^{\frac{3}{2}}} = \frac{6\,\pi^{\frac{1}{2}}\,\mathcal{L}^3(\Omega_-^0)}{(\mathcal{H}^2(\Gamma^0))^{\frac{3}{2}}}\,,$$

see e.g. Wintz *et al.* (1996).

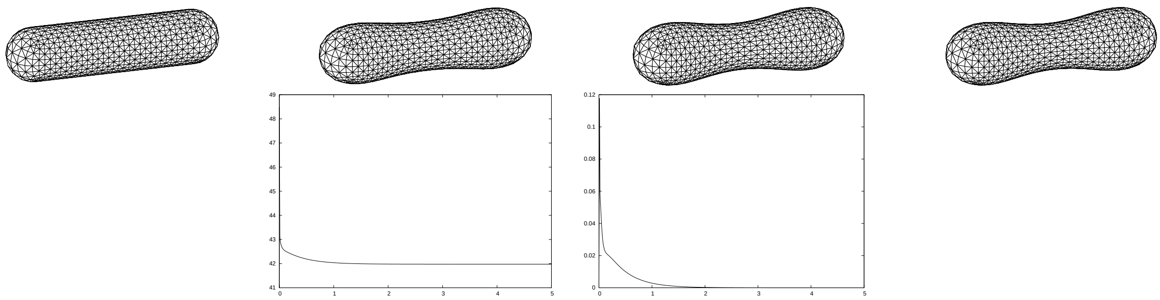

Figure 2: Flow for an elongated tube of dimensions $4 \times 1 \times 1$ for the scheme (5.3a–f). The triangulations of Γ^m at times $t = 0,\ 1,\ 3,\ 5$. The lower row shows plots of the discrete energy and the discrete kinetic energy. We note that $\mathcal{H}^2(\Gamma^0) = 12.5$ and $\mathcal{L}^3(\Omega_-^0) = 2.84$.

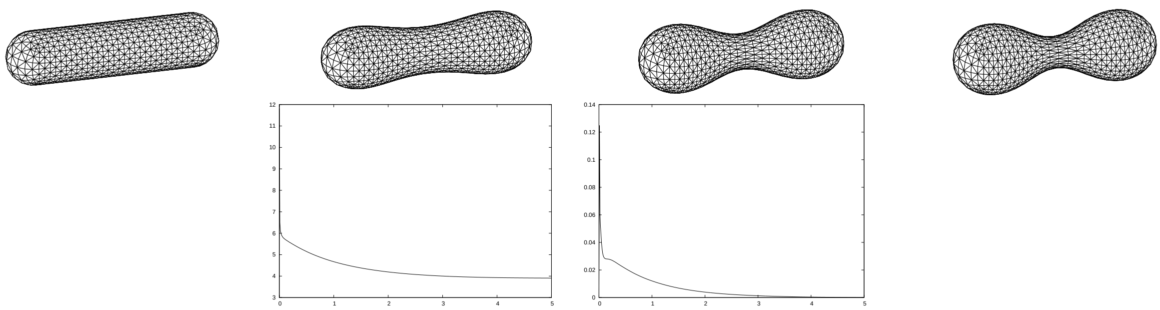

Figure 3: Same as Figure 2, but with $\overline{\varkappa} = -2$.

We consider evolutions for an initially elongated tube of total dimensions $4 \times 1 \times 1$. The initial shape has a reduced volume of $v_r = 0.6853$. Here we consider the effect of spontaneous curvature. As the computational domain we choose $\Omega = (-2.5, 2.5)^3$. In Figure 2 we show the evolution of the discrete interface when $\overline{\varkappa} = 0$, while in Figure 3 we repeat the simulation with $\overline{\varkappa} = -2$. The final forms are typical prolate-like dumbbell shapes, which have axisymmetry and reflective symmetry, as discussed in Seifert (1997), and they are in accordance with the phase diagrams in Figures 14 and 18 of that paper.

In what follows, we numerically investigate some of the regions in the other shape diagrams in Seifert (1997, Fig. 16, 17); see also Ziherl and Svetina (2005, Fig. 1). Note that the parameters m_0 and α in Seifert (1997, Fig. 16, 17) are such that $m_0 = -M_0 \left(\frac{\pi}{\mathcal{H}^2(\Gamma^0)}\right)^{\frac{1}{2}}$ and $\beta = 1.4\,\frac{\pi}{\mathcal{H}^2(\Gamma^0)}$ in our notation.

We begin with a cup-like (also called stomatocyte) initial shape with reduced volume $v_r = 0.65$ and $\mathcal{H}^2(\Gamma^0) = 82.31$. We would like to investigate the flow towards the minimizer for the choice $m_0/(4\,\pi) = 0.75$, which means that we need to set $M_0 = -3\,(\pi\,\mathcal{H}^2(\Gamma^0))^{\frac{1}{2}} \approx -48.24$ and $\beta = 1.4\,\frac{\pi}{\mathcal{H}^2(\Gamma^0)} \approx 0.053$. A simulation for this initial data can be seen in

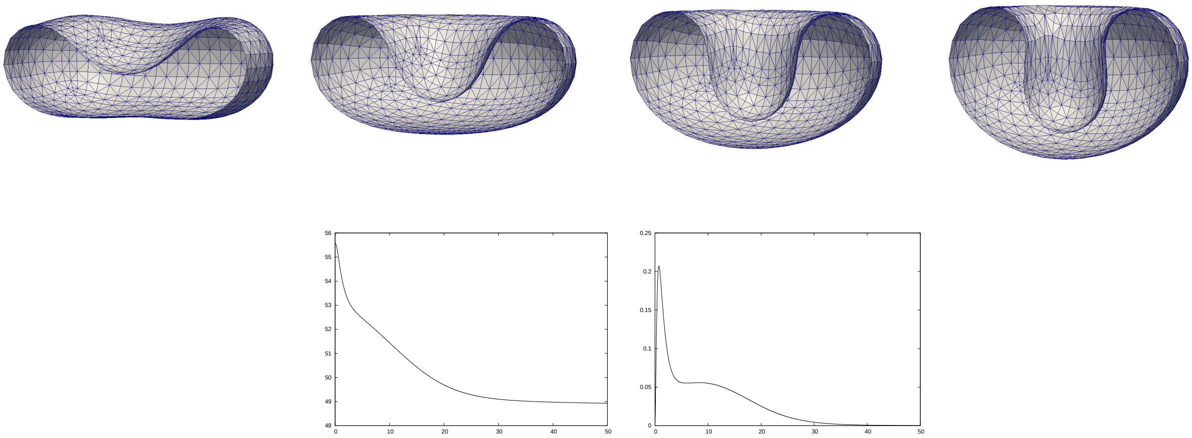

Figure 4: ($\rho_\Gamma = 1$) Flow for a cup-like shape with $v_r = 0.65$ the scheme (5.3a–f). Cuts of the triangulations of Γ^m at times $t = 0,\ 10,\ 20,\ 50$. The lower row shows plots of the discrete energy and the discrete kinetic energy. We note that $\mathcal{H}^2(\Gamma^0) = 82.31$ and $\mathcal{L}^3(\Omega^0_-) = 45.63$. $M_0 = -48.24$ and $\beta = 0.053$.

Figure 4. Here we set $\rho_\Gamma = 1$. As a comparison, we show the same simulation with $\beta = 0$ in Figure 5. Both evolutions appear to have reached a numerical steady state, with the latter evolution having reached a typical biconcave shape with axisymmetry and reflective symmetry, i.e. a discocyte. The stomatocyte shape, which only has axisymmetry, is in accordance with the phase diagram in Seifert (1997, Fig. 16), and the discocyte shape can be found in Seifert (1997, Figs. 3, 14).

Next we use a varying-diameter cigar-like shape with reduced volume $v_r = 0.75$ and $\mathcal{H}^2(\Gamma^0) = 9.65$. We would like to investigate the flow towards the minimizer for the choice $m_0/(4\,\pi) = 1.52$, which means that we need to set $M_0 = -33.5$ and $\beta = 0.46$. The results from our numerical simulation can be seen in Figure 6. As a comparison, we show a simulation with $\beta = 0$ in Figure 7. The pear shaped final membrane in Figure 6 appears in the shape diagram of Seifert (1997, Fig. 16) for high m_0. It is also typical that the reflective asymmetry does not appear without the ADE contribution, see Figure 7.

Finally, we consider a flat pear-like initial shape with reduced volume $v_r = 0.5$ and $\mathcal{H}^2(\Gamma^0) = 38.58$. We would like to investigate the flow towards the minimizer for the choice $m_0/(4\,\pi) = 1.3$, which means that we need to set $M_0 = -\frac{26}{5}\,(\pi\,\mathcal{H}^2(\Gamma^0))^{\frac{1}{2}} \approx -57.25$ and $\beta = 1.4\,\frac{\pi}{\mathcal{H}^2(\Gamma^0)} \approx 0.114$. A simulation for this initial data can be seen in Figure 8. As a comparison, we show a simulation with $\beta = 0$ in Figure 9. Also in these two figures one observes that in the case $\beta = 0$ the evolution leads to a discocyte shape, whereas in the case $\beta > 0$ the shape maintains reflective symmetry but does not gain axisymmetry.

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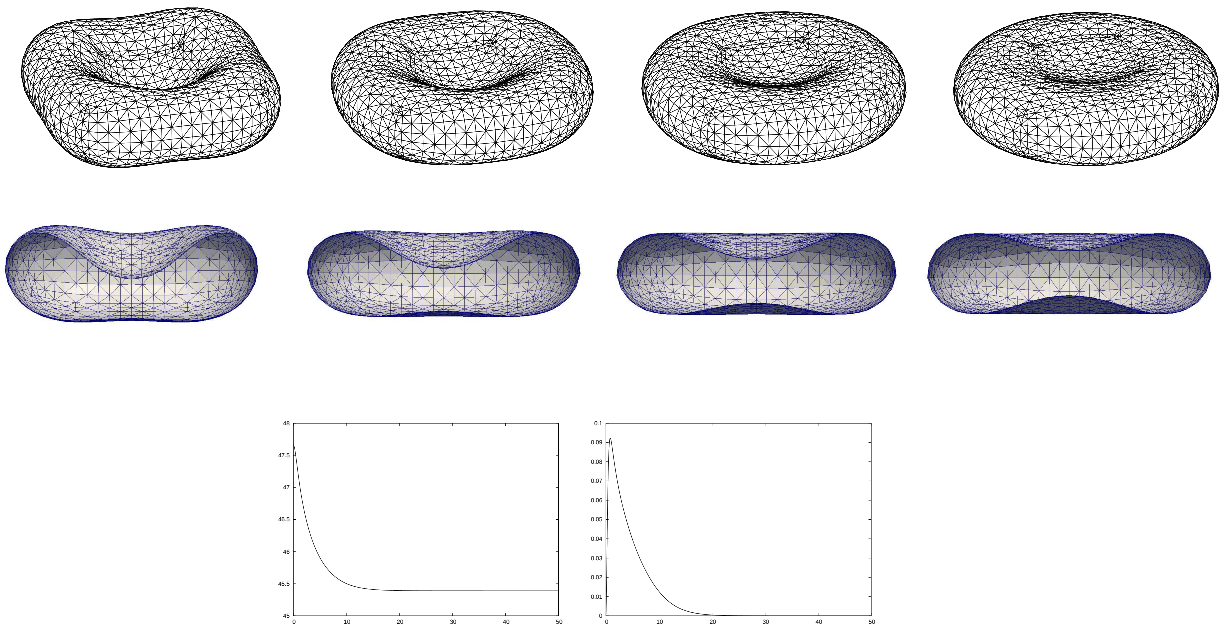

Figure 5: Same as Figure 4, but with $\beta = 0$. Here we show the triangulations Γ^m, and their cuts, at times $t = 0,\ 10,\ 20,\ 50$.

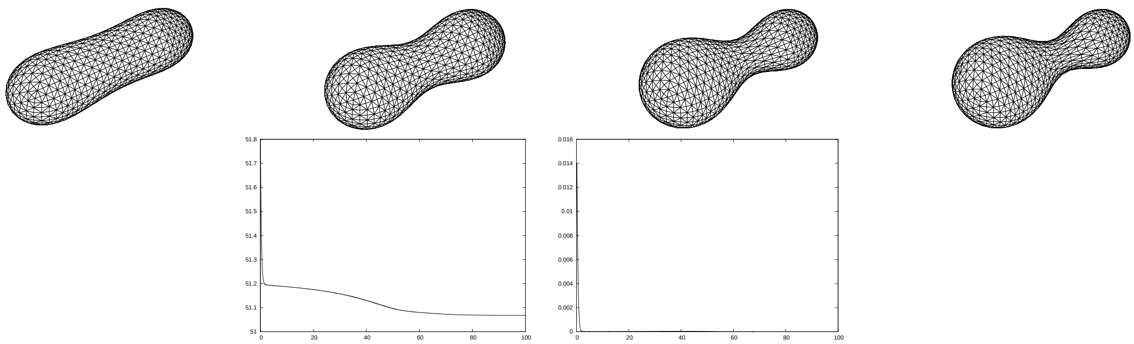

Figure 6: Flow for a varying-diameter cigar-like shape with $v_r = 0.75$ for the scheme (5.3a–f). The triangulations of Γ^m at times $t = 0,\ 5,\ 50,\ 100$. The lower row shows plots of the discrete energy and the discrete kinetic energy. We note that $\mathcal{H}^2(\Gamma^0) = 9.65$ and $\mathcal{L}^3(\Omega^0_-) = 2.11$. $M_0 = -33.5$ and $\beta = 0.46$.

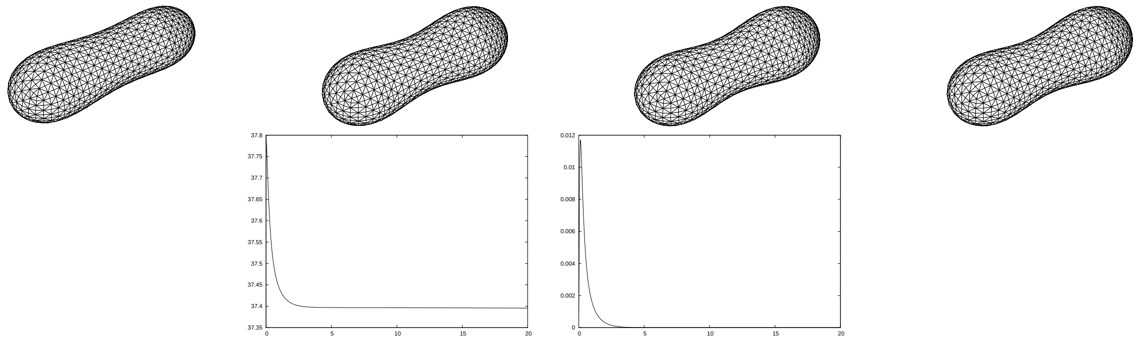

Figure 7: Same as Figure 6, but with $\beta = 0$.

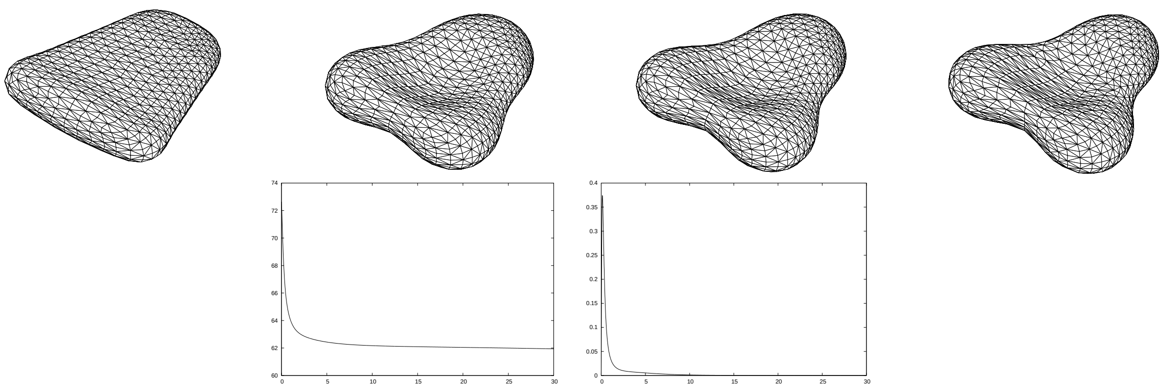

Figure 8: Flow for a flat pear-shape for the scheme (5.3a–f). The triangulations of Γ^m at times $t = 0,\ 5,\ 10,\ 30$. The lower row shows plots of the discrete energy and the discrete kinetic energy. We note that $\mathcal{H}^2(\Gamma^0) = 38.58$ and $\mathcal{L}^3(\Omega^0_-) = 11.26$. $M_0 = -57.25$ and $\beta = 0.114$.

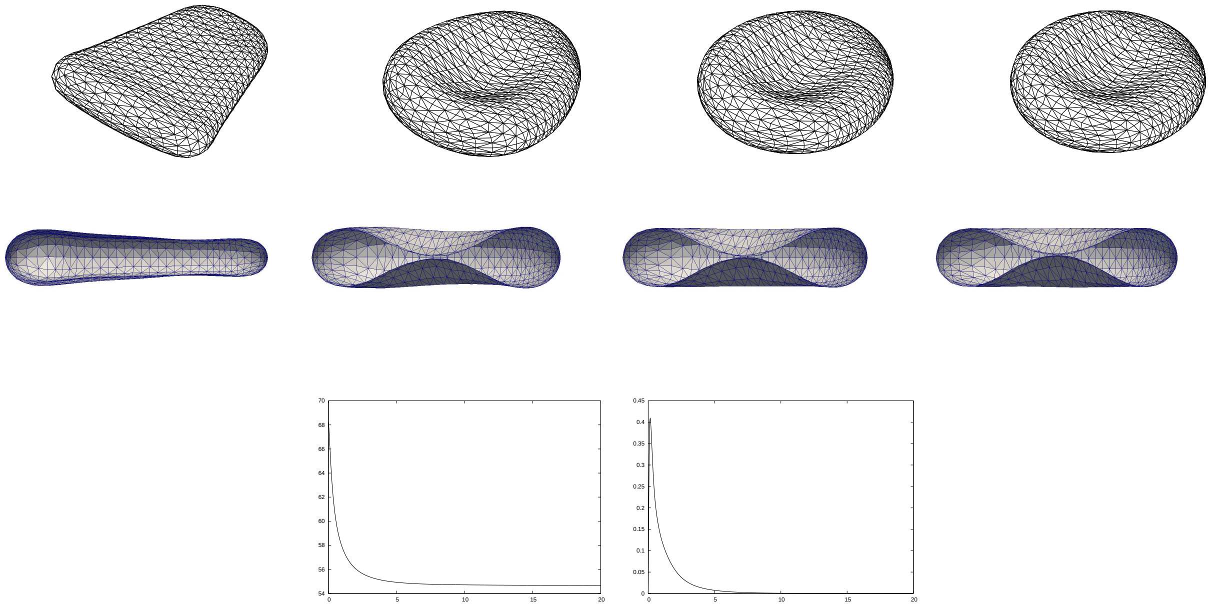

Figure 9: Same as Figure 8, but with $\beta = 0$.

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