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Computational Parametric Willmore Flow with Spontaneous Curvature and Area Difference Elasticity Effects

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Abstract

A new stable continuous-in-time semi-discrete parametric finite element method for Willmore flow is introduced. The approach allows for spontaneous curvature and area difference elasticity (ADE) effects, which are important for many applications, in particular, in the context of membranes. The method extends ideas from Dziuk and the present authors to obtain an approximation that allows for a tangential redistribution of mesh points, which typically leads to better mesh properties. Moreover, we consider volume and surface area preserving variants of these schemes and, in particular, we obtain stable approximations of Helfrich flow. We also discuss fully discrete variants and present several numerical computations.

Key words. Willmore flow, Helfrich flow, parametric finite elements, stability, tangential movement, spontaneous curvature, ADE model

AMS subject classifications. 65M60, 65M12, 35K55, 53C44, 74E10, 74E15

1 Introduction

The Willmore energy for hypersurfaces in the three-dimensional Euclidean space is a fundamental geometric functional, which appears in differential geometry, in optimal surface modelling, in surface restoration, and in many physical models for shells and membranes, see Willmore (1993); Welch and Witkin (1994); Clarenz *et al.* (2004); Canham (1970); Helfrich (1973); Seifert (1997). The Willmore energy is given as the integrated square of the mean curvature over the hypersurface, and hence it is a functional formulated with the help of second derivatives of a parameterization. It turns out that the first variation, which leads to the Willmore equation, is of fourth order, and is thus difficult to solve. Also evolution problems involving the Willmore functional have been studied extensively in the literature. The L^2–gradient flow of the Willmore functional leads to the so-called

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Willmore flow, which is a highly nonlinear fourth order parabolic equation. Many questions related to the Willmore energy, the Willmore equation and the Willmore flow are still open or have only been addressed recently. We refer to Simon (1993); Willmore (1993); Kuwert and Schätzle (2001); Simonett (2001); Bauer and Kuwert (2003); Droske and Rumpf (2004); Kuwert and Schätzle (2004); Bobenko and Schröder (2005); Deckelnick *et al.* (2005); Dall'Acqua *et al.* (2008); Dziuk (2008); Schygulla (2012); Marques and Neves (2014) for more information on analytical and numerical aspects in this context.

Defining $\varkappa$ as the mean curvature, i.e. the sum of the principle curvatures, of a hypersurface Γ in $\mathbb{R}^3$ the Willmore energy is given as

$$E(\Gamma) := \tfrac{1}{2} \int_\Gamma \varkappa^2 \, \mathrm{d}\mathcal{H}^2, \tag{1.1}$$

where $\mathcal{H}^2$ denotes the two-dimensional Hausdorff measure. Realistic models for biological cell membranes lead to energies more general than (1.1). 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

$$E_{\overline{\varkappa}}(\Gamma) := \tfrac{1}{2} \int_\Gamma (\varkappa - \overline{\varkappa})^2 \, \mathrm{d}\mathcal{H}^2, \tag{1.2}$$

where $\overline{\varkappa} \in \mathbb{R}$ is the given so-called spontaneous curvature. In the general model the integrated Gaussian curvature over the hypersurface also appears. However, as we will only consider closed surfaces, this contribution is constant within a fixed topological class, due to the Gauss-Bonnet theorem, and we hence will neglect this contribution.

In the context of biological membranes further aspects play a role, which we would like to take into account in this paper. Due to osmotic pressure effects between the inside and the outside of the membrane the total enclosed volume is preserved, and hence a volume constraint has to be taken into account when minimizing (1.2), or when considering the L^2–gradient flow of (1.2). Biological membranes are typically incompressible with a fixed number of molecules in the membrane. This leads to the total surface area of the membrane being fixed, which gives rise to another constraint for the functional (1.2) and for related flows. Biological membranes consist of two layers of lipids and it is difficult to exchange molecules between the two layers. In membrane theories two possibilities are considered to take this into account. Both variants use the fact, that to leading order, the actual area difference between the two layers can be described with the help of the integrated mean curvature over the hypersurface, see Seifert (1997). If one assumes that no lipid molecules swap from one layer to the other, a hard constraint on the integrated mean curvature is enforced so that the area difference in this case is fixed. Another possibility is to energetically penalize deviations from an optimal area difference. In this case we obtain the energy

$$E_{\overline{\varkappa},\beta}(\Gamma) := E_{\overline{\varkappa}}(\Gamma) + \tfrac{\beta}{2} \left(M(\Gamma) - M_0\right)^2 \tag{1.3a}$$

with

$$M(\Gamma) := \int_\Gamma \varkappa \, \mathrm{d}\mathcal{H}^2 \tag{1.3b}$$

and given constants $\beta \in \mathbb{R}_{\geq 0}$, $M_0 \in \mathbb{R}$. Models employing the energy (1.3a) are often called area difference elasticity (ADE) models, see Seifert (1997). The L^2–gradient flow of $E_{\overline{\varkappa},\beta}$ is given as

$$\mathcal{V} = -\Delta_s \, \varkappa + (\tfrac{1}{2} \, (\varkappa - \overline{\varkappa})^2 + A \, \varkappa) \, \varkappa - |\nabla_s \, \vec{\nu}|^2 \, (\varkappa - \overline{\varkappa} + A), \tag{1.4}$$

where $\mathcal{V}$ is the normal velocity of Γ, $\vec{\nu}$ is a unit normal of Γ, $A = \beta(M(\Gamma) - M_0)$ and $|\nabla_s \, \vec{\nu}|$ is the Frobenius norm of the Weingarten map. We will also look at volume preserving flows, as well as volume and surface area preserving flows. In the case $\beta = 0$, the latter is called Helfrich flow.

One of the first numerical approaches for Willmore flow was the work of Mayer and Simonett (2002), who used a finite difference scheme and numerically found an example where the Willmore flow can drive a smooth surface to a singularity in finite time. The first variational method for Willmore flow, based on a mixed method, was introduced by Rusu (2005) and has also been studied by Clarenz *et al.* (2004). Droske and Rumpf (2004) used a level set method to solve the Willmore flow equation, Deckelnick and Dziuk (2006) gave an error analysis for the Willmore flow of graphs and Deckelnick *et al.* (2015) analyzed a C^1 finite element method for Willmore flow of graphs.

There also has been considerable work on numerical aspects of more involved models like Helfrich flow or models involving spontaneous curvature and ADE effects. We only mention the work of Du *et al.* (2004); Barrett *et al.* (2008b); Bonito *et al.* (2010); Elliott and Stinner (2010).

A fundamental new approach for Willmore flow of hypersurfaces in three dimensions was a parametric finite element approach introduced by Dziuk (2008). The semi-discrete scheme of Dziuk (2008) has the property that it satisfies a stability bound. Despite the stability bound, the approach of Dziuk often leads to bad mesh properties for fully discrete variants. However, an approach of Barrett *et al.* (2008a) for geometric evolution problems uses the tangential degrees of freedom in the parameterization to obtain good mesh properties. This approach has been used for Willmore and Helfrich flow in Barrett *et al.* (2008b). However, no stability bound for this scheme seems to be possible. Hence, it would be desirable to combine the approaches of Dziuk (2008) and Barrett *et al.* (2008a,b) to obtain a stable semi-discrete parametric finite element approximation with better mesh properties. It is the goal of this paper to introduce and analyze such a method and to present several numerical computations based on this approach.

The outline of this paper is at follows. In Section 2 we state several weak formulations using the calculus of PDE constrained optimization. These weak formulations allow for stable semi-discrete finite element approximations, which are derived and analyzed in Section 3. In Section 4 we state fully discrete finite element approximations and state an existence and uniqueness result. Section 5 states how we solve the resulting algebraic equations and in Section 6 we present several numerical computations for Willmore and Helfrich flow with possibly spontaneous curvature and area difference elasticity effects.

2 Weak formulations/Calculus of PDE constrained optimization

We assume that $(\Gamma(t))_{t\in[0,T]}$ is a sufficiently smooth evolving hypersurface without boundary that is parameterized by $\vec{x}(\cdot,t):\Upsilon\to\mathbb{R}^3$, where $\Upsilon\subset\mathbb{R}^3$ is a given reference manifold, i.e. $\Gamma(t)=\vec{x}(\Upsilon,t)$. We assume also that $\Gamma(t)$ is oriented with a sufficiently smooth unit normal $\vec{\nu}(t)$. We define the velocity

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

and $\mathcal{V}:=\vec{\mathcal{V}}\,.\,\vec{\nu}$ is the normal velocity of the evolving hypersurface $\Gamma(t)$. Moreover, we define the space-time surface

$$\mathcal{G}_T:=\bigcup_{t\in[0,T]}\Gamma(t)\times\{t\}\,. \tag{2.2}$$

Let $\varkappa$ denote the mean curvature of $\Gamma(t)$, where we have adopted the sign convention given by the formula

$$\Delta_s\,\vec{\mathrm{id}}=\varkappa\,\vec{\nu}=:\vec{\varkappa}\qquad\text{on }\Gamma(t)\,, \tag{2.3}$$

where $\Delta_s=\nabla_s\,.\,\nabla_s$ is the Laplace–Beltrami operator on $\Gamma(t)$, with $\nabla_s=(\partial_{s_1},\partial_{s_2},\partial_{s_3})^T$ denoting the surface gradient on $\Gamma(t)$. In addition, we define the surface deformation tensor

$$\underline{\underline{D}}(\vec{\chi}):=\nabla_s\,\vec{\chi}+(\nabla_s\,\vec{\chi})^T\,, \tag{2.4}$$

where $\nabla_s\,\vec{\chi}=\left(\partial_{s_j}\,\chi_i\right)_{i,j=1}^3$.

We define the following time derivative that follows the parameterization $\vec{x}(\cdot,t)$ of $\Gamma(t)$. Let

$$\partial_t^\circ\,\zeta=\zeta_t+\vec{\mathcal{V}}\,.\,\nabla\,\zeta\qquad\forall\ \zeta\in H^1(\mathcal{G}_T)\,; \tag{2.5}$$

where we stress that this definition is well-defined, even though ζ_t and $\nabla\,\zeta$ do not make sense separately for a function $\zeta\in H^1(\mathcal{G}_T)$. For later use we note that

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi,\zeta\rangle_{\Gamma(t)}=\langle\partial_t^\circ\,\psi,\zeta\rangle_{\Gamma(t)}+\langle\psi,\partial_t^\circ\,\zeta\rangle_{\Gamma(t)}+\left\langle\psi\,\zeta,\nabla_s\,.\,\vec{\mathcal{V}}\right\rangle_{\Gamma(t)}\qquad\forall\ \psi,\zeta\in H^1(\mathcal{G}_T)\,, \tag{2.6}$$

see Lemma 5.2 in Dziuk and Elliott (2013). Here $\langle\cdot,\cdot\rangle_{\Gamma(t)}$ denotes the L^2–inner product on $\Gamma(t)$. It immediately follows from (2.6) that

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{H}^2(\Gamma(t))=\left\langle\nabla_s\,.\,\vec{\mathcal{V}},1\right\rangle_{\Gamma(t)}=\left\langle\nabla_s\,\vec{\mathrm{id}},\nabla_s\,\vec{\mathcal{V}}\right\rangle_{\Gamma(t)}\,. \tag{2.7}$$

Moreover, on denoting the interior of $\Gamma(t)$ by $\Omega(t)$, we recall that

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{L}^3(\Omega(t))=\left\langle\vec{\mathcal{V}},\vec{\nu}\right\rangle_{\Gamma(t)}\,, \tag{2.8}$$

where $\mathcal{L}^3$ denotes the Lebesgue measure in $\mathbb{R}^3$, and where here, and from now on, $\vec{\nu}(t)$ is the outward unit normal to $\Omega(t)$.

In this section we would like to derive a weak formulation for the L^2–gradient flow of $E_{\overline{\varkappa},\beta}(\Gamma(t))$. To this end, we need to consider variations of the energy with respect to $\Gamma(t) = \vec{x}(\Upsilon, t)$. For any given $\vec{\chi} \in [H^1(\Gamma(t))]^3$ and for any $\varepsilon \in (0, \varepsilon_0)$ for some $\varepsilon_0 \in \mathbb{R}_{>0}$, let

$$\Gamma_\varepsilon(t) := \{\vec{\Psi}(\vec{z}, \varepsilon) : \vec{z} \in \Gamma(t)\}\,, \quad \text{where} \quad \vec{\Psi}(\vec{z}, 0) = \vec{z} \text{ and } \tfrac{\partial \vec{\Psi}}{\partial \varepsilon}(\vec{z}, 0) = \vec{\chi}(\vec{z}) \quad \forall \vec{z} \in \Gamma(t)\,. \tag{2.9}$$

Then the first variation of $\mathcal{H}^2(\Gamma(t))$ with respect to $\Gamma(t)$ in the direction $\vec{\chi} \in [H^1(\Gamma(t))]^3$ is given by

$$\left[\frac{\delta}{\delta\Gamma}\,\mathcal{H}^2(\Gamma(t))\right](\vec{\chi}) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\,\mathcal{H}^2(\Gamma_\varepsilon(t))\,|_{\varepsilon=0}$$
$$= \lim_{\varepsilon\to 0} \tfrac{1}{\varepsilon}\left[\mathcal{H}^2(\Gamma_\varepsilon(t)) - \mathcal{H}^2(\Gamma(t))\right] = \left\langle \nabla_s\, \vec{\mathrm{id}}, \nabla_s\, \vec{\chi} \right\rangle_{\Gamma(t)}\,, \tag{2.10}$$

see e.g. the proof of Lemma 1 in Dziuk (2008). For later use we note that generalized variants of (2.10) also hold. Namely, we have that

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\,\langle w_\varepsilon, 1\rangle_{\Gamma_\varepsilon(t)}\,|_{\varepsilon=0} = \left\langle w\,\nabla_s\, \vec{\mathrm{id}}, \nabla_s\, \vec{\chi} \right\rangle_{\Gamma(t)} \qquad \forall\ w \in L^\infty(\Gamma(t))\,, \tag{2.11}$$

where $w_\varepsilon \in L^\infty(\Gamma_\varepsilon(t))$ is defined by $w_\varepsilon(\vec{\Psi}(\vec{z}, \varepsilon)) = w(\vec{z})$ for all $\vec{z} \in \Gamma(t)$. This definition of w_ε yields that $\partial_\varepsilon^0\, w = 0$, where

$$\partial_\varepsilon^0\, w(\vec{z}) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon} w_\varepsilon(\vec{\Psi}(\vec{z}, \varepsilon))\,|_{\varepsilon=0} \qquad \forall\ \vec{z} \in \Gamma(t). \tag{2.12}$$

Of course, (2.11) is the first variation analogue of (2.6) with $w = \psi\,\zeta$ and $\partial_t^\circ\, \psi = \partial_t^\circ\, \zeta = 0$. Similarly, it holds that

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\,\langle \vec{w}_\varepsilon, \vec{\nu}_\varepsilon\rangle_{\Gamma_\varepsilon(t)}\,|_{\varepsilon=0} = \left\langle (\vec{w}\,.\,\vec{\nu})\,\nabla_s\, \vec{\mathrm{id}}, \nabla_s\, \vec{\chi} \right\rangle_{\Gamma(t)} + \left\langle \vec{w}, \partial_\varepsilon^0\, \vec{\nu} \right\rangle_{\Gamma(t)} \quad \forall\ \vec{w} \in [L^\infty(\Gamma(t))]^3\,, \tag{2.13}$$

where $\partial_\varepsilon^0\, \vec{w} = \vec{0}$ and $\vec{\nu}_\varepsilon(t)$ denotes the unit normal on $\Gamma_\varepsilon(t)$. In this regard, we note the following result concerning the variation of $\vec{\nu}$, with respect to $\Gamma(t)$, in the direction $\vec{\chi} \in [H^1(\Gamma(t))]^3$:

$$\partial_\varepsilon^0\, \vec{\nu} = -[\nabla_s\, \vec{\chi}]^T\, \vec{\nu} \quad \text{on} \quad \Gamma(t) \quad \Rightarrow \quad \partial_t^\circ\, \vec{\nu} = -[\nabla_s\, \vec{\mathcal{V}}]^T\, \vec{\nu} \quad \text{on} \quad \Gamma(t)\,, \tag{2.14}$$

see Schmidt and Schulz (2010, Lemma 9). Finally, we note that for $\vec{\eta} \in [H^1(\Gamma(t))]^3$ it holds that

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\varepsilon} \left\langle \nabla_s\, \vec{\mathrm{id}}, \nabla_s\, \vec{\eta}_\varepsilon \right\rangle_{\Gamma_\varepsilon(t)} |_{\varepsilon=0} &= \langle \nabla_s\,.\,\vec{\eta}, \nabla_s\,.\,\vec{\chi}\rangle_{\Gamma(t)} \\
&\quad + \sum_{l,\,m=1}^{3} \left[\langle (\vec{\nu})_l\,(\vec{\nu})_m\,\nabla_s\,(\vec{\eta})_m, \nabla_s\,(\vec{\chi})_l\rangle_{\Gamma(t)} - \langle (\nabla_s)_m\,(\vec{\eta})_l, (\nabla_s)_l\,(\vec{\chi})_m\rangle_{\Gamma(t)}\right] \\
&= \langle \nabla_s\,.\,\vec{\eta}, \nabla_s\,.\,\vec{\chi}\rangle_{\Gamma(t)} + \langle \nabla_s\, \vec{\eta}, \nabla_s\, \vec{\chi}\rangle_{\Gamma(t)} - \left\langle (\nabla_s\, \vec{\eta})^T, \underline{\underline{D}}(\vec{\chi})\,(\nabla_s\, \vec{\mathrm{id}})^T \right\rangle_{\Gamma(t)}\,,
\end{aligned} \tag{2.15}$$

where $\partial_\varepsilon^0\,\vec\eta = \vec 0$, see Lemma 2 and the proof of Lemma 3 in Dziuk (2008). Here we observe that our notation is such that $\nabla_s\,\vec\chi = (\nabla_\Gamma\,\vec\chi)^T$, with $\nabla_\Gamma\,\vec\chi = (\partial_{s_i}\,\chi_j)_{i,j=1}^3$ defined as in Dziuk (2008). It follows from (2.15) that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec\eta\right\rangle_{\Gamma(t)} = \left\langle \nabla_s\,.\,\vec\eta, \nabla_s\,.\,\vec{\mathcal V}\right\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec\eta, \nabla_s\,\vec{\mathcal V}\right\rangle_{\Gamma(t)} - \left\langle (\nabla_s\,\vec\eta)^T, \underline{\underline{D}}(\vec{\mathcal V})\,(\nabla_s\,\vec{\mathrm{id}})^T\right\rangle_{\Gamma(t)} \quad \forall\ \vec\eta \in \{\vec\xi \in H^1(\mathcal G_T) : \partial_t^\circ\,\vec\xi = \vec 0\}\,. \tag{2.16}$$

In the seminal work Dziuk (2008), the author introduced a stable semi-discrete finite element approximation of Willmore flow, which is based on the discrete analogue of the identity $\frac{\mathrm{d}}{\mathrm{d}t}E(\Gamma(t)) = \frac12\,\frac{\mathrm{d}}{\mathrm{d}t}\,\langle\vec\varkappa,\vec\varkappa\rangle_{\Gamma(t)} = -\left\langle \vec f_\Gamma, \vec{\mathcal V}\right\rangle_{\Gamma(t)}$, where

$$\left\langle \vec f_\Gamma, \vec\chi\right\rangle_{\Gamma(t)} = \langle\nabla_s\,\vec\varkappa, \nabla_s\,\vec\chi\rangle_{\Gamma(t)} + \langle\nabla_s\,.\,\vec\varkappa, \nabla_s\,.\,\vec\chi\rangle_{\Gamma(t)} + \tfrac12\left\langle |\vec\varkappa|^2\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec\chi\right\rangle_{\Gamma(t)} - \left\langle (\nabla_s\,\vec\varkappa)^T, \underline{\underline{D}}(\vec\chi)\,(\nabla_s\,\vec{\mathrm{id}})^T\right\rangle_{\Gamma(t)} \qquad \forall\ \vec\chi \in [H^1(\Gamma(t))]^3\,. \tag{2.17}$$

In the recent paper Barrett *et al.* (2015a) the present authors were able to extend (2.17), and the corresponding semi-discrete approximation, to the case of nonzero β and $\overline\varkappa$ in (1.3a). The approximation is based on a suitable weak formulation, which can be obtained by considering the first variation of (1.3a) subject to the side constraint, the weak formulation of (2.3),

$$\langle\vec\varkappa,\vec\eta\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec\eta\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec\eta \in [H^1(\Gamma(t))]^3\,. \tag{2.18}$$

To this end, one defines the Lagrangian

$$L(\Gamma(t),\vec\varkappa,\vec y) = \tfrac12\,\langle\vec\varkappa - \overline\varkappa\,\vec\nu, \vec\varkappa - \overline\varkappa\,\vec\nu\rangle_{\Gamma(t)} + \tfrac{\beta}{2}\left(\langle\vec\varkappa,\vec\nu\rangle_{\Gamma(t)} - M_0\right)^2 - \langle\vec\varkappa,\vec y\rangle_{\Gamma(t)} - \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec y\right\rangle_{\Gamma(t)} \tag{2.19}$$

with $\vec y \in [H^1(\Gamma(t))]^3$ being a Lagrange multiplier for (2.18). Then, on using ideas from the adjoint approach of the calculus of PDE constrained optimization, see e.g. Hinze *et al.* (2009), one can compute the direction of steepest descent $\vec f_\Gamma$ of $E_{\overline\varkappa,\beta}(\Gamma(t))$, under the constraint (2.18). To achieve this, we consider variations $\Gamma_\varepsilon(t)$ of $\Gamma(t)$ as in (2.9). We then define $\vec\varkappa_\varepsilon$ such that

$$\langle\vec\varkappa_\varepsilon,\vec\eta\rangle_{\Gamma_\varepsilon(t)} + \left\langle \nabla_s\vec{\mathrm{id}}, \nabla_s\vec\eta\right\rangle_{\Gamma_\varepsilon(t)} = 0 \qquad \forall\ \vec\eta \in [H^1(\Gamma_\varepsilon(t))]^3, \tag{2.20}$$

and for a fixed $\vec y \in [H^1(\Gamma(t))]^3$ we define $\vec y_\varepsilon$ such that $\partial_\varepsilon^0\,\vec y = \vec 0$. It now follows from (2.19), (2.20), (1.3a,b) and (1.2) that for any $\vec y \in [H^1(\Gamma(t))]^3$

$$E_{\overline\varkappa,\beta}(\Gamma_\varepsilon(t)) = L(\Gamma_\varepsilon(t),\vec\varkappa_\varepsilon,\vec y_\varepsilon)\,. \tag{2.21}$$

We now want to compute the direction of steepest descent $\vec{f}_\Gamma$ of $E_{\overline{\varkappa},\beta}(\Gamma(t))$, where the curvature, $\vec{\varkappa} = \varkappa\,\vec{\nu}$, is given by (2.18). This means that $\vec{f}_\Gamma$ needs to fulfill

$$\left\langle \vec{f}_\Gamma, \vec{\chi} \right\rangle_{\Gamma(t)} = -\left[\frac{\delta}{\delta\Gamma}\, E_{\overline{\varkappa},\beta}(\Gamma(t))\right](\vec{\chi}) \qquad \forall\ \vec{\chi} \in [H^1(\Gamma(t))]^3\,. \tag{2.22}$$

Using (2.21) and (2.11)–(2.15) one computes

$$\begin{aligned}
-\left\langle \vec{f}_\Gamma, \vec{\chi} \right\rangle_{\Gamma(t)} = &-\langle \nabla_s\,\vec{y}, \nabla_s\,\vec{\chi}\rangle_{\Gamma(t)} - \langle \nabla_s\,.\,\vec{y}, \nabla_s\,.\,\vec{\chi}\rangle_{\Gamma(t)} + \left\langle (\nabla_s\,\vec{y})^T, \underline{\underline{D}}(\vec{\chi})\,(\nabla_s\,\vec{\mathrm{id}})^T \right\rangle_{\Gamma(t)} \\
&+ \tfrac{1}{2}\left\langle [|\vec{\varkappa} - \overline{\varkappa}\,\vec{\nu}|^2 - 2\,(\vec{y}\,.\,\vec{\varkappa})]\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\chi} \right\rangle_{\Gamma(t)} - (A - \overline{\varkappa})\,\langle \vec{\varkappa}, [\nabla_s\,\vec{\chi}]^T\,\vec{\nu}\rangle_{\Gamma(t)} \\
&+ A\left\langle (\vec{\varkappa}\,.\,\vec{\nu})\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\chi} \right\rangle_{\Gamma(t)} + \langle \vec{\varkappa} - \overline{\varkappa}\,\vec{\nu}, \partial_\varepsilon^0\,\vec{\varkappa}\rangle_{\Gamma(t)} \\
&+ A\,\langle \partial_\varepsilon^0\,\vec{\varkappa}, \vec{\nu}\rangle_{\Gamma(t)} - \langle \partial_\varepsilon^0\,\vec{\varkappa}, \vec{y}\rangle_{\Gamma(t)} \qquad \forall\ \vec{\chi} \in [H^1(\Gamma(t))]^3\,,
\end{aligned}$$

where

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

Choosing

$$\vec{y} = \vec{\varkappa} + (A - \overline{\varkappa})\,\vec{\nu} \tag{2.23}$$

leads to

$$\begin{aligned}
-\left\langle \vec{f}_\Gamma, \vec{\chi} \right\rangle_{\Gamma(t)} = &-\langle \nabla_s\,\vec{y}, \nabla_s\,\vec{\chi}\rangle_{\Gamma(t)} - \langle \nabla_s\,.\,\vec{y}, \nabla_s\,.\,\vec{\chi}\rangle_{\Gamma(t)} + \left\langle (\nabla_s\,\vec{y})^T, \underline{\underline{D}}(\vec{\chi})\,(\nabla_s\,\vec{\mathrm{id}})^T \right\rangle_{\Gamma(t)} \\
&+ \tfrac{1}{2}\left\langle [|\vec{\varkappa} - \overline{\varkappa}\,\vec{\nu}|^2 - 2\,(\vec{y}\,.\,\vec{\varkappa})]\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\chi} \right\rangle_{\Gamma(t)} - (A - \overline{\varkappa})\,\langle \vec{\varkappa}, [\nabla_s\,\vec{\chi}]^T\,\vec{\nu}\rangle_{\Gamma(t)} \\
&+ A\left\langle (\vec{\varkappa}\,.\,\vec{\nu})\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\chi} \right\rangle_{\Gamma(t)} \qquad \forall\ \vec{\chi} \in [H^1(\Gamma(t))]^3\,,
\end{aligned} \tag{2.24}$$

see Barrett *et al.* (2015a) for a similar computation.

In the context of the numerical approximation of the L^2–gradient flow of (1.3a), this gives rise to the weak formulation: Given $\Gamma(0)$, for all $t \in (0, T]$ find $\Gamma(t) = \vec{x}(\Upsilon, t)$, where $\vec{x}(t) \in [H^1(\Gamma(t))]^3$, and $\vec{y}(t) \in [H^1(\Gamma(t))]^3$ such that

$$\begin{aligned}
\left\langle \vec{\mathcal{V}}, \vec{\chi} \right\rangle_{\Gamma(t)} &- \langle \nabla_s\,\vec{y}, \nabla_s\,\vec{\chi}\rangle_{\Gamma(t)} - \langle \nabla_s\,.\,\vec{y}, \nabla_s\,.\,\vec{\chi}\rangle_{\Gamma(t)} + \left\langle (\nabla_s\,\vec{y})^T, \underline{\underline{D}}(\vec{\chi})\,(\nabla_s\,\vec{\mathrm{id}})^T \right\rangle_{\Gamma(t)} \\
&+ \tfrac{1}{2}\left\langle [|\vec{\varkappa} - \overline{\varkappa}\,\vec{\nu}|^2 - 2\,(\vec{y}\,.\,\vec{\varkappa})]\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\chi} \right\rangle_{\Gamma(t)} - (A - \overline{\varkappa})\,\langle \vec{\varkappa}, [\nabla_s\,\vec{\chi}]^T\,\vec{\nu}\rangle_{\Gamma(t)} \\
&+ A\left\langle (\vec{\varkappa}\,.\,\vec{\nu})\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\chi} \right\rangle_{\Gamma(t)} = 0 \quad \forall\ \vec{\chi} \in [H^1(\Gamma(t))]^3\,,
\end{aligned} \tag{2.25a}$$

$$\langle \vec{y}, \vec{\eta}\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\eta} \right\rangle_{\Gamma(t)} = (A - \overline{\varkappa})\,\langle \vec{\nu}, \vec{\eta}\rangle_{\Gamma(t)} \quad \forall\ \vec{\eta} \in [H^1(\Gamma(t))]^3\,, \tag{2.25b}$$

where $\vec{\varkappa} = \vec{y} - (A - \overline{\varkappa})\,\vec{\nu}$ and $A(t) = \beta\left(\langle \vec{\varkappa}, \vec{\nu}\rangle_{\Gamma(t)} - M_0\right)$.

Under discretization, (2.25a,b) does not have good mesh properties. Note that this is in contrast to the situation in Barrett *et al.* (2014), where a local incompressibility condition for the membrane leads to the constraint $\nabla_s \,.\, \vec{\mathcal{V}} = 0$ on $\Gamma(t)$. This condition arises for vesicles and membranes, as considered in Barrett *et al.* (2014), because the membrane is considered as a surface fluid. Hence, a surface (Navier-)Stokes equation has to be solved as part of the problem, which, in particular, contains an incompressibility condition for the velocity on the surface, see Barrett *et al.* (2014) for details. The position of the membrane is then advected with the fluid velocity, which leads to the incompressibility condition $\nabla_s \,.\, \vec{\mathcal{V}} = 0$ on $\Gamma(t)$. This then enforces local area preservation, and on the discrete level means that the polyhedral approximation of $\Gamma(t)$ always remains well-behaved. However, discretizations of (2.25a,b) for the gradient flow situation exhibit mesh movements that are almost exclusively in the normal direction, which in general leads to bad meshes. To see this, we note that (2.25a,b) is the weak formulation of

$$\vec{\mathcal{V}} = \left[-\Delta_s \varkappa + (\tfrac{1}{2}(\varkappa - \overline{\varkappa})^2 + A\,\varkappa)\,\varkappa - |\nabla_s \vec{\nu}|^2\,(\varkappa - \overline{\varkappa} + A)\right]\vec{\nu}\,, \tag{2.26}$$

which agrees with Barrett *et al.* (2008b, (1.12)). A derivation of (2.26), in the context of surfaces with boundary, can be found in Barrett *et al.* (2015c).

Hence, similarly to Barrett *et al.* (2012), it is natural to consider the Lagrangian

$$L(\Gamma(t), \varkappa, \vec{y}) = \tfrac{1}{2}\,\langle \varkappa - \overline{\varkappa}, \varkappa - \overline{\varkappa}\rangle_{\Gamma(t)} + \tfrac{\beta}{2}\left(\langle \varkappa, 1\rangle_{\Gamma(t)} - M_0\right)^2 - \langle \varkappa\,\vec{\nu}, \vec{y}\rangle_{\Gamma(t)} - \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{y}\right\rangle_{\Gamma(t)}\,, \tag{2.27}$$

which corresponds to minimizing (1.3a) under the side constraint

$$\langle \varkappa\,\vec{\nu}, \vec{\eta}\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\eta}\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec{\eta} \in [H^1(\Gamma(t))]^3\,. \tag{2.28}$$

A similar computation to the above leads to the following weak formulation of the L^2–gradient flow of (1.3a). Given $\Gamma(0)$, for all $t \in (0, T]$ find $\Gamma(t) = \vec{x}(\Upsilon, t)$, where $\vec{x}(t) \in [H^1(\Gamma(t))]^3$, and $\vec{y}(t) \in [H^1(\Gamma(t))]^3$ such that

$$\begin{aligned}
&\left\langle \vec{\mathcal{V}}\,.\,\vec{\nu}, \vec{\chi}\,.\,\vec{\nu}\right\rangle_{\Gamma(t)} - \langle \nabla_s\,\vec{y}, \nabla_s\,\vec{\chi}\rangle_{\Gamma(t)} - \langle \nabla_s\,.\,\vec{y}, \nabla_s\,.\,\vec{\chi}\rangle_{\Gamma(t)} + \left\langle (\nabla_s\,\vec{y})^T, \underline{\underline{D}}(\vec{\chi})\,(\nabla_s\,\vec{\mathrm{id}})^T\right\rangle_{\Gamma(t)} \\
&\quad + \tfrac{1}{2}\left\langle [(\vec{y}\,.\,\vec{\nu} - A)^2 - 2\,(\vec{y}\,.\,\vec{\nu} - A)\,(\vec{y}\,.\,\vec{\nu} - A + \overline{\varkappa})]\,\nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\chi}\right\rangle_{\Gamma(t)} \\
&\quad + \left\langle [\vec{y}\,.\,\vec{\nu} - A + \overline{\varkappa}]\,\vec{y}, [\nabla_s \chi]^T\,\vec{\nu}\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec{\chi} \in [H^1(\Gamma(t))]^3\,,
\end{aligned} \tag{2.29a}$$

$$\langle \vec{y}\,.\,\vec{\nu}, \vec{\eta}\,.\,\vec{\nu}\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\eta}\right\rangle_{\Gamma(t)} = (A - \overline{\varkappa})\,\langle \vec{\nu}, \vec{\eta}\rangle_{\Gamma(t)} \qquad \forall\ \vec{\eta} \in [H^1(\Gamma(t))]^3\,, \tag{2.29b}$$

where $A(t) = \beta\left(\langle \varkappa, 1\rangle_{\Gamma(t)} - M_0\right)$, on noting from (2.28) and (2.29b) that $\varkappa = \vec{y}\,.\,\vec{\nu} + \overline{\varkappa} - A$, can be formulated in terms of $\vec{y}$ as

$$A(t) = \frac{\beta}{1 + \beta\,\mathcal{H}^2(\Gamma(t))}\left[\langle \vec{y}\,.\,\vec{\nu} + \overline{\varkappa}, 1\rangle_{\Gamma(t)} - M_0\right]. \tag{2.29c}$$

The two-dimensional analogue of (2.29a,b), in the case $\beta = \overline{\varkappa} = 0$, has been considered in Barrett *et al.* (2012), where the corresponding semi-discrete approximation leads to equidistributed polygonal approximations of $\Gamma(t)$. This equidistribution property is a direct consequence of the discrete analogue of (2.29b), and has been exploited by the authors in a series of papers, see e.g. Barrett *et al.* (2007, 2010, 2011, 2012). In three space dimensions the discrete analogue of (2.29b) leads to so-called "conformal polyhedral surfaces", which means that meshes in general stay well-behaved, e.g. no coalescence occurs.

Surprisingly, in three space dimensions discretizations of (2.29a,b) do not work as well in practice. A common problem for numerical simulations of such discretizations is that the tangential part of the discrete variant of the Lagrange multiplier $\vec{y}$ grows unboundedly. It is for this reason that we consider a family of schemes with a relaxation parameter $\theta \in [0,1]$, where $\theta = 1$ corresponds to the discrete variants of (2.25a,b), while $\theta = 0$ corresponds to a variant with (2.29b), so that good mesh properties can be expected in practice. Hence the natural side constraint to consider is

$$\langle \theta\,\vec{\varkappa} + (1-\theta)\,(\vec{\varkappa}\,.\,\vec{\nu})\,\vec{\nu}, \vec{\eta}\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\eta}\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec{\eta} \in [H^1(\Gamma(t))]^3\,, \tag{2.30}$$

and we will present the precise details in the discrete setting below.

3 Semi-discrete finite element approximation

The parametric finite element spaces are defined as follows, see also Barrett *et al.* (2008a). Let $\Upsilon^h(t) \subset \mathbb{R}^3$ be a two-dimensional *polyhedral surface*, i.e. a union of non-degenerate triangles with no hanging vertices (see Deckelnick *et al.* (2005, p. 164)), approximating the reference manifold Υ. In particular, let $\Upsilon^h = \bigcup_{j=1}^J \overline{o^h_j}$, where $\{o^h_j\}_{j=1}^J$ is a family of mutually disjoint open triangles. Then let $\underline{V}^h(\Upsilon^h) := \{\vec{\chi} \in C(\Upsilon^h, \mathbb{R}^3) : \vec{\chi}\mid_{o^h_j}$ is linear $\forall\ j = 1,\ldots,J\}$. We consider a family of parameterizations $\vec{X}^h(\cdot,t) \in \underline{V}^h(\Upsilon^h)$ with $\vec{X}^h(\Upsilon^h,t) = \Gamma^h(t)$. In particular, let $\Gamma^h(t) = \bigcup_{j=1}^J \overline{\sigma^h_j(t)}$, where $\{\sigma^h_j(t)\}_{j=1}^J$ is a family of mutually disjoint open triangles with vertices $\{\vec{q}^h_k(t)\}_{k=1}^K$. Then let

$$\begin{aligned}\underline{V}^h(\Gamma^h(t)) &:= \{\vec{\chi} \in [C(\Gamma^h(t))]^3 : \vec{\chi}\,|_{\sigma^h_j} \text{ is linear } \forall\ j = 1,\ldots,J\} \\ &=: [W^h(\Gamma^h(t))]^3 \subset [H^1(\Gamma^h(t))]^3\,,\end{aligned}$$

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

$$\chi^h_k(\vec{q}^h_l(t),t) = \delta_{kl} \qquad \forall\ k,l \in \{1,\ldots,K\}\,,\ t \in [0,T]\,. \tag{3.1}$$

For later purposes, we also introduce $\pi^h(t) : C(\Gamma^h(t)) \to W^h(\Gamma^h(t))$, the standard interpolation operator at the nodes $\{\vec{q}^h_k(t)\}_{k=1}^K$, and similarly $\vec{\pi}^h(t) : [C(\Gamma^h(t))]^3 \to \underline{V}^h(\Gamma^h(t))$. In case that $\Gamma^h(t)$ encloses an open set we define $\Omega^h(t)$ to be the interior of $\Gamma^h(t)$, so that $\Gamma^h(t) = \partial\Omega^h(t)$.

We denote the L^2–inner product on $\Gamma^h(t)$ by $\langle\cdot,\cdot\rangle_{\Gamma^h(t)}$. In addition, for piecewise continuous functions, with possible jumps across the edges of $\{\sigma^h_j\}_{j=1}^J$, we also introduce the mass lumped inner product

$$\langle \eta, \zeta \rangle^h_{\Gamma^h(t)} := \tfrac{1}{3} \sum_{j=1}^{J} \mathcal{H}^2(\sigma^h_j) \sum_{k=1}^{3} (\eta \,.\, \zeta)((\vec{q}^{\,h}_{j_k})^-)\,,$$

where $\{\vec{q}^{\,h}_{j_k}\}_{k=1}^3$ are the vertices of σ^h_j, and where we define $\eta((\vec{q}^{\,h}_{j_k})^-) := \lim_{\sigma^h_j \ni \vec{p} \to \vec{q}^{\,h}_{j_k}} \eta(\vec{p})$. We naturally extend this definition to vector and tensor functions.

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

$$\vec{\mathcal{V}}^h(\vec{z}, t) := \sum_{k=1}^{K_\Gamma} \left[\frac{\mathrm{d}}{\mathrm{d}t}\, \vec{q}^{\,h}_k(t)\right] \chi^h_k(\vec{z}, t)\,. \tag{3.2}$$

Then, similarly to (2.5), we define

$$\partial_t^{\circ,h}\, \zeta = \zeta_t + \vec{\mathcal{V}}^h \,.\, \nabla\, \zeta \qquad \forall\ \zeta \in H^1(\mathcal{G}^h_T)\,, \quad \text{where} \quad \mathcal{G}^h_T := \bigcup_{t\in[0,T]} \Gamma^h(t) \times \{t\}\,. \tag{3.3}$$

For later use, we also introduce the finite element spaces

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\sigma^h_j(t)} \zeta \;\mathrm{d}\mathcal{H}^2 = \int_{\sigma^h_j(t)} \partial_t^{\circ,h}\, \zeta + \zeta\, \nabla_s \,.\, \vec{\mathcal{V}}^h \;\mathrm{d}\mathcal{H}^2 \quad \forall\ \zeta \in H^1(\sigma^h(t))\,, j \in \{1, \ldots, J_\Gamma\}\,, \tag{3.4}$$

which immediately implies that

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \eta, \zeta \rangle_{\Gamma^h(t)} = \langle \partial_t^{\circ,h}\, \eta, \zeta \rangle_{\Gamma^h(t)} + \langle \eta, \partial_t^{\circ,h}\, \zeta \rangle_{\Gamma^h(t)} + \langle \eta\, \zeta, \nabla_s \,.\, \vec{\mathcal{V}}^h \rangle_{\Gamma^h(t)} \qquad \forall\ \eta, \zeta \in W_T(\mathcal{G}^h_T)\,. \tag{3.5}$$

Similarly, we recall from Barrett *et al.* (2015b, Lem. 3.1) that

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \eta, \zeta \rangle^h_{\Gamma^h(t)} = \langle \partial_t^{\circ,h}\, \eta, \zeta \rangle^h_{\Gamma^h(t)} + \langle \eta, \partial_t^{\circ,h}\, \zeta \rangle^h_{\Gamma^h(t)} + \langle \eta\, \zeta, \nabla_s \,.\, \vec{\mathcal{V}}^h \rangle^h_{\Gamma^h(t)} \quad \forall\ \eta, \zeta \in W_T(\mathcal{G}^h_T)\,. \tag{3.6}$$

Let $\vec{\nu}^h$ denote the the outward unit normal to $\Gamma^h(t)$. For later use, we introduce the vertex normal function $\vec{\omega}^h(\cdot, t) \in \underline{V}^h(\Gamma^h(t))$ with

$$\vec{\omega}^h(\vec{q}^{\,h}_k(t), t) := \frac{1}{\mathcal{H}^2(\Lambda^h_k(t))} \sum_{j \in \Theta^h_k} \mathcal{H}^2(\sigma^h_j(t))\, \vec{\nu}^h\,|_{\sigma^h_j(t)}\,,$$

where for $k = 1, \ldots, K$ we define $\Theta^h_k := \{j : \vec{q}^{\,h}_k(t) \in \overline{\sigma^h_j(t)}\}$ and set $\Lambda^h_k(t) := \cup_{j \in \Theta^h_k} \overline{\sigma^h_j(t)}$. Here we note that

$$\left\langle \vec{z}, w\, \vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} = \left\langle \vec{z}, w\, \vec{\omega}^h \right\rangle^h_{\Gamma^h(t)} \qquad \forall\ \vec{z} \in \underline{V}^h(\Gamma^h(t))\,,\ w \in W^h(\Gamma^h(t))\,. \tag{3.7}$$

In addition, we introduce $\underline{\underline{Q}}^h_\theta$ by setting

$$\underline{\underline{Q}}^h_\theta(\vec{q}^h_k(t),t) = \theta\,\underline{\underline{\mathrm{Id}}} + (1-\theta)\,\frac{\vec{\omega}^h(\vec{q}^h_k(t),t)\otimes\vec{\omega}^h(\vec{q}^h_k(t),t)}{|\vec{\omega}^h(\vec{q}^h_k(t),t)|^2} \qquad \forall\ k\in\{1,\ldots,K\}\,, \tag{3.8}$$

where here and throughout we assume that $\vec{\omega}^h(\vec{q}^h_k(t),t)\neq\vec{0}$ for $k=1,\ldots,K$ and $t\in[0,T]$. Only in pathological cases could this assumption be violated, and in practice this never occurred. We note that

$$\left\langle \underline{\underline{Q}}^h_\theta\,\vec{z},\vec{v}\right\rangle^h_{\Gamma^h(t)} = \left\langle \vec{z},\underline{\underline{Q}}^h_\theta\,\vec{v}\right\rangle^h_{\Gamma^h(t)} \quad\text{and}\quad \left\langle \underline{\underline{Q}}^h_\theta\vec{z},\vec{\omega}^h\right\rangle^h_{\Gamma^h(t)} = \left\langle\vec{z},\vec{\omega}^h\right\rangle^h_{\Gamma^h(t)} \tag{3.9}$$

for all $\vec{z},\vec{v}\in\underline{V}^h(\Gamma^h(t))$.

Similarly to the continuous setting in (2.24,b), we consider the first variation of the discrete energy

$$E^h_{\overline{\varkappa},\beta}(\Gamma^h(t)) := \tfrac12\left\langle|\vec{\kappa}^h-\overline{\varkappa}\,\vec{\nu}^h|^2,1\right\rangle^h_{\Gamma^h(t)} + \tfrac{\beta}{2}\left(\left\langle\vec{\kappa}^h,\vec{\nu}^h\right\rangle_{\Gamma^h(t)} - M_0\right)^2 \tag{3.10}$$

subject to the side constraint

$$\left\langle\underline{\underline{Q}}^h_\theta\,\vec{\kappa}^h,\vec{\eta}\right\rangle^h_{\Gamma^h(t)} + \left\langle\nabla_s\,\vec{\mathrm{id}},\nabla_s\,\vec{\eta}\right\rangle_{\Gamma^h(t)} = 0 \qquad \forall\ \vec{\eta}\in\underline{V}^h(\Gamma^h(t))\,. \tag{3.11}$$

When taking variations of (3.11), we need to compute variations of the discrete vertex normal $\vec{\omega}^h$. To this end, for any given $\vec{\chi}\in\underline{V}^h(\Gamma^h(t))$ we introduce $\Gamma^h_\varepsilon(t)$ as in (2.9) and $\partial^{0,h}_\varepsilon$ defined by (2.12), both with $\Gamma(t)$ replaced by $\Gamma^h(t)$. We then observe that it follows from (3.7) with $w=1$ and the discrete analogue of (2.11) that

$$\left\langle\vec{z},\partial^{0,h}_\varepsilon\,\vec{\omega}^h\right\rangle^h_{\Gamma^h(t)} = \left\langle\vec{z},\partial^{0,h}_\varepsilon\,\vec{\nu}^h\right\rangle^h_{\Gamma^h(t)} + \left\langle(\vec{z}\,.\,(\vec{\nu}^h-\vec{\omega}^h))\,\nabla_s\,\vec{\mathrm{id}},\nabla_s\,\vec{\chi}\right\rangle^h_{\Gamma^h(t)} \qquad \forall\ \vec{z},\ \vec{\chi}\in\underline{V}^h(\Gamma^h(t))\,. \tag{3.12}$$

An immediate consequence is that

$$\left\langle\vec{z},\partial^{\circ,h}_t\,\vec{\omega}^h\right\rangle^h_{\Gamma^h(t)} = \left\langle\vec{z},\partial^{\circ,h}_t\,\vec{\nu}^h\right\rangle^h_{\Gamma^h(t)} + \left\langle(\vec{z}\,.\,(\vec{\nu}^h-\vec{\omega}^h))\,\nabla_s\,\vec{\mathrm{id}},\nabla_s\,\vec{\mathcal{V}}^h\right\rangle^h_{\Gamma^h(t)} \qquad \forall\ \vec{z}\in\underline{V}^h(\Gamma^h(t))\,. \tag{3.13}$$

In addition, we note that

$$\partial^{0,h}_\varepsilon\,\pi^h\left[\left(\vec{\xi}\,.\,\frac{\vec{\omega}^h}{|\vec{\omega}^h|}\right)\left(\vec{\eta}\,.\,\frac{\vec{\omega}^h}{|\vec{\omega}^h|}\right)\right] = \pi^h\left[\vec{G}^h(\vec{\xi},\vec{\eta})\,.\,\partial^{0,h}_\varepsilon\,\vec{\omega}^h\right] \quad \text{on } \Gamma^h(t) \quad \forall\ \vec{\xi},\ \vec{\eta}\in\underline{V}^h(\Gamma^h(t))\,, \tag{3.14}$$

where

$$\vec{G}^h(\vec{\xi},\vec{\eta}) = \vec{\pi}^h\left[\frac{1}{|\vec{\omega}^h|^2}\left((\vec{\xi}\,.\,\vec{\omega}^h)\,\vec{\eta} + (\vec{\eta}\,.\,\vec{\omega}^h)\,\vec{\xi} - 2\,\frac{(\vec{\eta}\,.\,\vec{\omega}^h)\,(\vec{\xi}\,.\,\vec{\omega}^h)}{|\vec{\omega}^h|^2}\,\vec{\omega}^h\right)\right]. \tag{3.15}$$

It follows that

$$\vec{G}^h(\vec{\xi},\vec{\eta})\,.\,\vec{\omega}^h = 0 \quad \forall\, \vec{\xi},\ \vec{\eta} \in \underline{V}^h(\Gamma^h(t))\,. \tag{3.16}$$

Now we define the Lagrangian

$$L^h(\Gamma^h(t),\vec{\kappa}^h,\vec{Y}^h) = \tfrac12 \left\langle |\vec{\kappa}^h - \overline{\varkappa}\,\vec{\nu}^h|^2, 1\right\rangle^h_{\Gamma^h(t)} + \tfrac{\beta}{2}\left(\left\langle \vec{\kappa}^h,\vec{\nu}^h\right\rangle_{\Gamma^h(t)} - M_0\right)^2 - \left\langle \underline{\underline{Q}}^h_\theta\,\vec{\kappa}^h,\vec{Y}^h\right\rangle^h_{\Gamma^h(t)}$$
$$- \left\langle \nabla_s\,\vec{\rm id}, \nabla_s\,\vec{Y}^h\right\rangle_{\Gamma^h(t)} \tag{3.17}$$

with $\vec{Y}^h \in \underline{V}^h(\Gamma^h(t))$ being a Lagrange multiplier for (3.11). Similarly to (2.22), (2.24) and (2.25a,b), we obtain the L^2–gradient flow of $E^h_{\overline{\varkappa},\beta}(\Gamma^h(t))$ subject to the side constraint (3.11) by setting $[\frac{\delta}{\delta\Gamma^h}\,E^h_{\overline{\varkappa},\beta}](\vec{\chi}) = -\left\langle \underline{\underline{Q}}^h_\theta\,\vec{\mathcal{V}}^h,\vec{\chi}\right\rangle^h_{\Gamma^h(t)}$ for all $\vec{\chi} \in \underline{V}^h(\Gamma^h(t))$, where $\vec{\kappa}^h$ is given by (3.11). Once again, on recalling the calculus of PDE constrained optimization, we want to compute the first variation of $E^h_{\overline{\varkappa},\beta}$ with the help of the Lagrangian L^h. For fixed $\varepsilon \in (0,\varepsilon_0)$, we now choose $\vec{\kappa}^h_\varepsilon \in \underline{V}^h(\Gamma^h_\varepsilon(t))$ solving

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

where $\underline{\underline{Q}}^h_{\theta,\varepsilon}$ is now based on $\vec{\omega}^h_\varepsilon$ which satisfies (3.7) with $\Gamma^h(t)$ replaced by $\Gamma^h_\varepsilon(t)$. Then with $\vec{Y}^h_\varepsilon \in \underline{V}^h(\Gamma^h_\varepsilon(t))$ satisfying $\partial^{0,h}_\varepsilon\,\vec{Y}^h = \vec{0}$ for any $\vec{Y}^h \in \underline{V}^h(\Gamma^h(t))$, we obtain that

$$E^h_{\overline{\varkappa},\beta}(\Gamma^h_\varepsilon(t)) = L^h(\Gamma^h_\varepsilon(t),\vec{\kappa}^h_\varepsilon,\vec{Y}^h_\varepsilon),$$

and we compute the first variation of the left hand side by differentiating the right hand side, see e.g. Hinze *et al.* (2009). Choosing $\vec{Y}^h \in \underline{V}^h(\Gamma^h(t))$ such that

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

which is the analogue of (2.23), we obtain similarly as in the continuous case the following semi-discrete finite element approximation of Willmore flow with spontaneous curvature and ADE effects. Given $\Gamma^h(0)$, for all $t \in (0,T]$ find $\Gamma^h(t)$ and $\vec{\kappa}^h(t),\vec{Y}^h(t) \in \underline{V}^h(\Gamma^h(t))$ such that

$$\left\langle \underline{\underline{Q}}^h_\theta\,\vec{\mathcal{V}}^h,\vec{\chi}\right\rangle^h_{\Gamma^h(t)} - \left\langle \nabla_s\,\vec{Y}^h,\nabla_s\,\vec{\chi}\right\rangle_{\Gamma^h(t)} - \left\langle \nabla_s\,.\,\vec{Y}^h,\nabla_s\,.\,\vec{\chi}\right\rangle_{\Gamma^h(t)}$$
$$+ \left\langle (\nabla_s\,\vec{Y}^h)^T, \underline{\underline{D}}(\vec{\chi})\,(\nabla_s\,\vec{\rm id})^T\right\rangle_{\Gamma^h(t)} + \tfrac12 \left\langle \left[|\vec{\kappa}^h - \overline{\varkappa}\,\vec{\nu}^h|^2 - 2\,\vec{Y}^h\,.\,\underline{\underline{Q}}^h_\theta\,\vec{\kappa}^h\right]\nabla_s\,\vec{\rm id},\nabla_s\,\vec{\chi}\right\rangle^h_{\Gamma^h(t)}$$
$$- (A^h - \overline{\varkappa})\left\langle \vec{\kappa}^h, [\nabla_s\,\vec{\chi}]^T\,\vec{\nu}^h\right\rangle^h_{\Gamma^h(t)} + A^h\left\langle (\vec{\kappa}^h\,.\,\vec{\nu}^h)\,\nabla_s\,\vec{\rm id},\nabla_s\,\vec{\chi}\right\rangle_{\Gamma^h(t)}$$
$$- (1-\theta)\left\langle (\vec{G}^h(\vec{Y}^h,\vec{\kappa}^h)\,.\,\vec{\nu}^h)\,\nabla_s\,\vec{\rm id},\nabla_s\,\vec{\chi}\right\rangle^h_{\Gamma^h(t)}$$
$$+ (1-\theta)\left\langle \vec{G}^h(\vec{Y}^h,\vec{\kappa}^h), [\nabla_s\,\vec{\chi}]^T\,\vec{\nu}^h\right\rangle^h_{\Gamma^h(t)} = 0 \qquad \forall\, \vec{\chi} \in \underline{V}^h(\Gamma^h(t))\,, \tag{3.18a}$$

$$\left\langle \vec{\kappa}^h + (A^h - \overline{\varkappa})\,\vec{\nu}^h - \underline{\underline{Q}}^h_\theta\,\vec{Y}^h,\vec{\xi}\right\rangle^h_{\Gamma^h(t)} = 0 \qquad \forall\, \vec{\xi} \in \underline{V}^h(\Gamma^h(t))\,, \tag{3.18b}$$

$$\left\langle \underline{\underline{Q}}^h_\theta\,\vec{\kappa}^h,\vec{\eta}\right\rangle^h_{\Gamma^h(t)} + \left\langle \nabla_s\,\vec{\rm id},\nabla_s\,\vec{\eta}\right\rangle_{\Gamma^h(t)} = 0 \qquad \forall\, \vec{\eta} \in \underline{V}^h(\Gamma^h(t))\,, \tag{3.18c}$$

where $\vec{G}^h(\vec{Y}^h, \vec{\kappa}^h) \in \underline{V}^h(\Gamma^h(t))$ is defined as in (3.15), and

$$A^h(t) = \beta\left(\left\langle \vec{\kappa}^h, \vec{\nu}^h\right\rangle_{\Gamma^h(t)} - M_0\right). \tag{3.18d}$$

In deriving (3.18a–d) from the variation of L^h mentioned above, we have made use of the obvious discrete variants of (2.11)–(2.15), and recalled (3.12), (3.14) and (3.16). We note that (3.18b) and (3.7) imply that

$$\vec{\kappa}^h = \vec{\pi}^h\,[\underline{\underline{Q}}^h_\theta\,\vec{Y}^h] - (A^h - \overline{\varkappa})\,\vec{\omega}^h\,. \tag{3.19}$$

In addition, we note that the last two terms on the left hand side of (3.18a) vanishes on the continuous level, since there

$$\vec{G}(\vec{\xi}, \vec{\eta}) = (\vec{\xi}\,.\,\vec{\nu})\,\vec{\eta} + (\vec{\eta}\,.\,\vec{\nu})\,\vec{\xi} - 2\,(\vec{\eta}\,.\,\vec{\nu})\,(\vec{\xi}\,.\,\vec{\nu})\,\vec{\nu}\,, \tag{3.20}$$

and so $\vec{G}(\vec{y}, \vec{\varkappa}) = \vec{0}$.

In order to be able to consider area and volume preserving variants of (3.18a–d), we introduce Lagrange multipliers $\lambda^h(t), \mu^h(t) \in \mathbb{R}$ for the constraints

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{H}^2(\Gamma^h(t)) = \left\langle \nabla_s\,.\,\vec{\mathcal{V}}^h, 1\right\rangle_{\Gamma^h(t)} = 0 \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{L}^3(\Omega^h(t)) = \left\langle \vec{\mathcal{V}}^h, \vec{\nu}^h\right\rangle_{\Gamma^h(t)} = 0\,, \tag{3.21}$$

where we recall (2.7) and (2.8), and where $\Omega^h(t)$ denotes the interior of $\Gamma^h(t)$. Hence, on writing (3.18a) as

$$\left\langle \underline{\underline{Q}}^h_\theta\,\vec{\mathcal{V}}^h, \vec{\chi}\right\rangle^h_{\Gamma^h(t)} = \left\langle \nabla_s\,\vec{Y}^h, \nabla_s\,\vec{\chi}\right\rangle_{\Gamma^h(t)} + \left\langle \vec{f}^h, \vec{\chi}\right\rangle^h_{\Gamma^h(t)} \qquad \forall\ \vec{\chi} \in \underline{V}^h(\Gamma^h(t))\,,$$

we consider

$$\left\langle \underline{\underline{Q}}^h_\theta\,\vec{\mathcal{V}}^h, \vec{\chi}\right\rangle^h_{\Gamma^h(t)} = \left\langle \nabla_s\,\vec{Y}^h, \nabla_s\,\vec{\chi}\right\rangle_{\Gamma^h(t)} + \left\langle \vec{f}^h, \vec{\chi}\right\rangle^h_{\Gamma^h(t)} + \lambda^h\left\langle \underline{\underline{Q}}^h_\theta\,\vec{\kappa}^h, \vec{\chi}\right\rangle^h_{\Gamma^h(t)} + \mu^h\left\langle \vec{\omega}^h, \vec{\chi}\right\rangle^h_{\Gamma^h(t)} \tag{3.22}$$

for all $\vec{\chi} \in \underline{V}^h(\Gamma^h(t))$, where $(\lambda^h(t), \mu^h(t))^T \in \mathbb{R}^2$ solve the symmetric linear system

$$\begin{pmatrix} \left\langle \underline{\underline{Q}}^h_\theta\,\vec{\kappa}^h, \vec{\kappa}^h\right\rangle^h_{\Gamma^h(t)} & \left\langle \vec{\kappa}^h, \vec{\omega}^h\right\rangle^h_{\Gamma^h(t)} \\ \left\langle \vec{\kappa}^h, \vec{\omega}^h\right\rangle^h_{\Gamma^h(t)} & \left\langle \vec{\omega}^h, \vec{\omega}^h\right\rangle^h_{\Gamma^h(t)} \end{pmatrix} \begin{pmatrix} \lambda^h \\ \mu^h \end{pmatrix} = \begin{pmatrix} -\left\langle \nabla_s\,\vec{Y}^h, \nabla_s\,\vec{\kappa}^h\right\rangle_{\Gamma^h(t)} - \left\langle \vec{f}^h, \vec{\kappa}^h\right\rangle^h_{\Gamma^h(t)} \\ -\left\langle \nabla_s\,\vec{Y}^h, \nabla_s\,\vec{\omega}^h\right\rangle_{\Gamma^h(t)} - \left\langle \vec{f}^h, \vec{\omega}^h\right\rangle^h_{\Gamma^h(t)} \end{pmatrix}. \tag{3.23}$$

In order to motivate (3.23) we firstly note, on recalling (3.9) and (3.18c), that

$$\left\langle \underline{\underline{Q}}^h_\theta\,\vec{\mathcal{V}}^h, \vec{\kappa}^h\right\rangle^h_{\Gamma^h(t)} = \left\langle \underline{\underline{Q}}^h_\theta\,\vec{\kappa}^h, \vec{\mathcal{V}}^h\right\rangle^h_{\Gamma^h(t)} = -\left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec{\mathcal{V}}^h\right\rangle_{\Gamma^h(t)} = -\left\langle \nabla_s\,.\,\vec{\mathcal{V}}^h, 1\right\rangle_{\Gamma^h(t)}. \tag{3.24}$$

Secondly, it follows from (3.9) and (3.7) that

$$\left\langle \underline{\underline{Q}}^h_\theta\,\vec{\mathcal{V}}^h, \vec{\omega}^h\right\rangle^h_{\Gamma^h(t)} = \left\langle \vec{\mathcal{V}}^h, \vec{\omega}^h\right\rangle^h_{\Gamma^h(t)} = \left\langle \vec{\mathcal{V}}^h, \vec{\nu}^h\right\rangle_{\Gamma^h(t)}. \tag{3.25}$$

Hence the solution to (3.23) is such that (3.21) is satisfied, on noting (3.9). Clearly, the determinant of the matrix in (3.23), on recalling (3.9) and that $\theta \in [0,1]$, is equal to

$$
\begin{aligned}
&\left\langle \underline{\underline{Q}}^h_\theta\,\vec\kappa^h, \vec\kappa^h \right\rangle^h_{\Gamma^h(t)} \left\langle \vec\omega^h, \vec\omega^h \right\rangle^h_{\Gamma^h(t)} - \left(\left\langle \underline{\underline{Q}}^h_\theta\,\vec\kappa^h, \vec\omega^h \right\rangle^h_{\Gamma^h(t)} \right)^2 \\
&\quad \geq \left\langle \vec\omega^h, \vec\omega^h \right\rangle^h_{\Gamma^h(t)} \left(\left\langle \underline{\underline{Q}}^h_\theta\,\vec\kappa^h, \vec\kappa^h \right\rangle^h_{\Gamma^h(t)} - \left\langle \underline{\underline{Q}}^h_\theta\,\vec\kappa^h, \underline{\underline{Q}}^h_\theta\,\vec\kappa^h \right\rangle^h_{\Gamma^h(t)} \right) \\
&\quad = \left\langle \vec\omega^h, \vec\omega^h \right\rangle^h_{\Gamma^h(t)} \theta\,(1-\theta) \left(\left\langle \vec\kappa^h, \vec\kappa^h \right\rangle^h_{\Gamma^h(t)} - \left\langle \frac{\vec\kappa^h\,.\,\vec\omega^h}{|\vec\omega^h|}, \frac{\vec\kappa^h\,.\,\vec\omega^h}{|\vec\omega^h|} \right\rangle^h_{\Gamma^h(t)} \right) \geq 0\,, \qquad (3.26)
\end{aligned}
$$

with equality in the first inequality if and only if $\underline{\underline{Q}}^h_\theta\,\vec\kappa^h$ and $\vec\omega^h$ are linearly dependent, i.e. if and only if $\vec\kappa^h$ and $\vec\omega^h$ are linearly dependent. Hence the linear system (3.23) has a unique solution unless $\vec\kappa^h$ is a scalar multiple of $\vec\omega^h$. Of course, the natural discretization of volume preserving Willmore flow is given by (3.22) with $\mu^h = -\left(\left\langle \nabla_s\,\vec Y^h, \nabla_s\,\vec\omega^h \right\rangle_{\Gamma^h(t)} + \left\langle \vec f^h, \vec\omega^h \right\rangle^h_{\Gamma^h(t)} \right) / \left\langle \vec\omega^h, \vec\omega^h \right\rangle^h_{\Gamma^h(t)}$ and $\lambda^h = 0$, together with (3.18b–d). Similarly, the natural discretization of surface area preserving Willmore flow is given by (3.22) with $\lambda^h = -\left(\left\langle \nabla_s\,\vec Y^h, \nabla_s\,\vec\kappa^h \right\rangle_{\Gamma^h(t)} + \left\langle \vec f^h, \vec\kappa^h \right\rangle^h_{\Gamma^h(t)} \right) / \left\langle \underline{\underline{Q}}^h_\theta\,\vec\kappa^h, \vec\kappa^h \right\rangle^h_{\Gamma^h(t)}$ and $\mu^h = 0$, together with (3.18b–d).

The following theorem establishes that (3.18a–d) is indeed a weak formulation for the L^2–gradient flow of $E^h_{\overline{\varkappa},\beta}(\Gamma^h(t))$ subject to the side constraint (3.11). We will also show that for $\theta = 0$ the scheme produces *conformal polyhedral surfaces*. Here we recall from Barrett *et al.* (2008a, §4.1) that the surface $\Gamma^h(t)$ is a conformal polyhedral surfaces if

$$
\left\langle \nabla_s\,\vec{\rm id}, \nabla_s\,\vec\eta \right\rangle_{\Gamma^h(t)} = 0 \quad \forall\ \vec\eta \in \left\{ \vec\xi \in \underline{V}^h(\Gamma^h(t)) : \vec\xi(\vec q^h_k(t))\,.\,\vec\omega^h(\vec q^h_k(t), t) = 0, k = 1,\ldots,K \right\}. \tag{3.27}
$$

We recall from Barrett *et al.* (2008a) that conformal polyhedral surfaces exhibit good meshes. In particular, coalescence of vertices in practice never occurred. Moreover, we recall that the two-dimensional analogue of conformal polyhedral surfaces are equidistributed polygonal curves, see Barrett *et al.* (2007, 2011).

THEOREM. 3.1. *Let $\theta \in [0,1]$ and let $\{(\Gamma^h, \vec\kappa^h, \vec Y^h)(t)\}_{t\in[0,T]}$ be a solution to (3.18a–d). Then*

$$
\frac{\rm d}{{\rm d}t}\,E^h_{\overline{\varkappa},\beta}(\Gamma^h(t)) = -\left\langle \underline{\underline{Q}}^h_\theta\,\vec{\mathcal V}^h, \vec{\mathcal V}^h \right\rangle^h_{\Gamma^h(t)} \leq 0\,. \tag{3.28}
$$

Moreover, if $\theta = 0$ then $\Gamma^h(t)$ is a conformal polyhedral surface for all $t \in (0,T]$.

Proof. Taking the time derivative of (3.18c) with $\partial_t^{\circ,h}\,\vec\eta = \vec 0$, yields that

$$
\begin{aligned}
&\left\langle \partial_t^{\circ,h}\,(\underline{\underline{Q}}^h_\theta\,\vec\kappa^h), \vec\eta \right\rangle^h_{\Gamma^h(t)} + \left\langle (\underline{\underline{Q}}^h_\theta\,\vec\kappa^h\,.\,\vec\eta)\,\nabla_s\,\vec{\rm id}, \nabla_s\,\vec{\mathcal V}^h \right\rangle^h_{\Gamma^h(t)} + \left\langle \nabla_s\,.\,\vec{\mathcal V}^h, \nabla_s\,.\,\vec\eta \right\rangle_{\Gamma^h(t)} \\
&\qquad + \left\langle \nabla_s\,\vec{\mathcal V}^h, \nabla_s\,\vec\eta \right\rangle_{\Gamma^h(t)} - \left\langle \underline{\underline{D}}(\vec{\mathcal V}^h)\,(\nabla_s\,\vec{\rm id})^T, (\nabla_s\,\vec\eta)^T \right\rangle_{\Gamma^h(t)} = 0\,, \qquad (3.29)
\end{aligned}
$$

where we have noted (3.6) and the discrete version of (2.16). Choosing $\vec{\chi} = \vec{\mathcal{V}}^h$ in (3.18a), $\vec{\eta} = \vec{Y}^h$ in (3.29) and combining yields, on noting the discrete variant of (2.14), that

$$\begin{aligned}
&\left\langle \underline{\underline{Q}}^h_\theta\, \vec{\mathcal{V}}^h, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} + \tfrac{1}{2} \left\langle [|\vec{\kappa}^h - \overline{\varkappa}\, \vec{\nu}^h|^2 - 2\, \vec{Y}^h \,.\, \underline{\underline{Q}}^h_\theta\, \vec{\kappa}^h + 2\, A^h\, (\vec{\kappa}^h \,.\, \vec{\nu}^h)]\, \nabla_s\, \vec{\mathrm{id}}, \nabla_s\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} \\
&\quad + (A^h - \overline{\varkappa}) \left\langle \vec{\kappa}^h, \partial_t^{\circ,h}\, \vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} + \left\langle \partial_t^{\circ,h}\, (\underline{\underline{Q}}^h_\theta\, \vec{\kappa}^h), \vec{Y}^h \right\rangle^h_{\Gamma^h(t)} + \left\langle (\underline{\underline{Q}}^h_\theta\, \vec{\kappa}^h \,.\, \vec{Y}^h)\, \nabla_s\, \vec{\mathrm{id}}, \nabla_s\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} \\
&\quad - (1-\theta) \left(\left\langle (\vec{G}^h(\vec{Y}^h, \vec{\kappa}^h) \,.\, \vec{\nu}^h)\, \nabla_s\, \vec{\mathrm{id}}, \nabla_s\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} - \left\langle \vec{G}^h(\vec{Y}^h, \vec{\kappa}^h), [\nabla_s\, \vec{\mathcal{V}}^h]^T\, \vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} \right) = 0\,,
\end{aligned} \tag{3.30}$$

which implies, on recalling (3.7), that

$$\begin{aligned}
&\left\langle \underline{\underline{Q}}^h_\theta\, \vec{\mathcal{V}}^h, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} + \tfrac{1}{2} \left\langle |\vec{\kappa}^h - \overline{\varkappa}\, \vec{\nu}^h|^2\, \nabla_s\, \vec{\mathrm{id}}, \nabla_s\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} - \overline{\varkappa} \left\langle \vec{\kappa}^h, \partial_t^{\circ,h}\, \vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} \\
&\quad + \left\langle \partial_t^{\circ,h}\, \vec{\kappa}^h, \underline{\underline{Q}}^h_\theta\, \vec{Y}^h - A^h\, \vec{\omega}^h \right\rangle^h_{\Gamma^h(t)} + \left\langle \partial_t^{\circ,h}\, (\underline{\underline{Q}}^h_\theta\, \vec{\kappa}^h), \vec{Y}^h \right\rangle^h_{\Gamma^h(t)} - \left\langle \partial_t^{\circ,h}\, \vec{\kappa}^h, \underline{\underline{Q}}^h_\theta\, \vec{Y}^h \right\rangle^h_{\Gamma^h(t)} \\
&\quad + A^h \left[\left\langle (\vec{\kappa}^h \,.\, \vec{\nu}^h)\, \nabla_s\, \vec{\mathrm{id}}, \nabla_s\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} + \left\langle \partial_t^{\circ,h}\, \vec{\kappa}^h, \vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} + \left\langle \vec{\kappa}^h, \partial_t^{\circ,h}\, \vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} \right] \\
&\quad - (1-\theta) \left(\left\langle (\vec{G}^h(\vec{Y}^h, \vec{\kappa}^h) \,.\, \vec{\nu}^h)\, \nabla_s\, \vec{\mathrm{id}}, \nabla_s\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} - \left\langle \vec{G}^h(\vec{Y}^h, \vec{\kappa}^h), [\nabla_s\, \vec{\mathcal{V}}^h]^T\, \vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} \right) = 0\,.
\end{aligned} \tag{3.31}$$

On recalling (3.18d) and (3.6), we observe that

$$\begin{aligned}
&A^h \left[\left\langle (\vec{\kappa}^h \,.\, \vec{\nu}^h)\, \nabla_s\, \vec{\mathrm{id}}, \nabla_s\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} + \left\langle \partial_t^{\circ,h}\, \vec{\kappa}^h, \vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} + \left\langle \vec{\kappa}^h, \partial_t^{\circ,h}\, \vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} \right] \\
&\qquad = \tfrac{\beta}{2}\, \frac{\mathrm{d}}{\mathrm{d}t} \left(\left\langle \vec{\kappa}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)} - M_0 \right)^2 .
\end{aligned} \tag{3.32}$$

Combining (3.31), (3.32) and (3.19), on noting (3.7) and (3.10), yields that

$$\left\langle \underline{\underline{Q}}^h_\theta\, \vec{\mathcal{V}}^h, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} + \frac{\mathrm{d}}{\mathrm{d}t}\, E^h_{\overline{\varkappa},\beta}(\Gamma^h(t)) + (1-\theta)\, \Pi = 0\,,$$

where

$$\begin{aligned}
\Pi :=& \left\langle \vec{\kappa}^h \,.\, \partial_t^{\circ,h}\, \vec{\omega}^h, \frac{\vec{Y}^h \,.\, \vec{\omega}^h}{|\vec{\omega}^h|^2} \right\rangle^h_{\Gamma^h(t)} + \left\langle \vec{Y}^h \,.\, \partial_t^{\circ,h}\, \vec{\omega}^h, \frac{\vec{\kappa}^h \,.\, \vec{\omega}^h}{|\vec{\omega}^h|^2} \right\rangle^h_{\Gamma^h(t)} \\
&- 2 \left\langle (\vec{\kappa}^h \,.\, \vec{\omega}^h)\, (\vec{Y}^h \,.\, \vec{\omega}^h), \frac{\vec{\omega}^h \,.\, \partial_t^{\circ,h}\, \vec{\omega}^h}{|\vec{\omega}^h|^4} \right\rangle^h_{\Gamma^h(t)} - \left\langle (\vec{G}^h(\vec{Y}^h, \vec{\kappa}^h) \,.\, \vec{\nu}^h)\, \nabla_s\, \vec{\mathrm{id}}, \nabla_s\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} \\
&+ \left\langle \vec{G}^h(\vec{Y}^h, \vec{\kappa}^h), [\nabla_s\, \vec{\mathcal{V}}^h]^T\, \vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} .
\end{aligned} \tag{3.33}$$

It remains to show that Π as defined in (3.33) vanishes. To see this, we observe that it follows from (3.16), (3.15) and (3.13) that

$$\Pi = \left\langle (\vec{G}^h(\vec{Y}^h, \vec{\kappa}^h), \partial_t^{\circ,h} \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h + \left\langle (\vec{G}^h(\vec{Y}^h, \vec{\kappa}^h) \,.\, (\vec{\omega}^h - \vec{\nu}^h) \nabla_s \vec{\mathrm{id}}, \nabla_s \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h$$
$$- \left\langle (\vec{G}^h(\vec{Y}^h, \vec{\kappa}^h), \partial_t^{\circ,h} \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h = 0\,. \tag{3.34}$$

This proves the desired result (3.28).

If $\theta = 0$ then it immediately follows from (3.18c) that (3.27) holds. Hence $\Gamma^h(t)$ is a conformal polyhedral surface. □

REMARK. 3.1. *It is clear from the above proof that on replacing* $\langle \underline{\underline{Q}}_\theta^h \vec{\mathcal{V}}^h, \vec{\chi}\rangle_{\Gamma^h(t)}^h$ *in* (3.18a) *with* $\langle \vec{\mathcal{V}}^h, \vec{\chi}\rangle_{\Gamma^h(t)}^h$ *we obtain a slightly different family of schemes that is also stable. I.e. solutions to this scheme satisfy* $\frac{\mathrm{d}}{\mathrm{d}t} E_{\overline{\varkappa},\beta}^h(\Gamma^h(t)) = -\langle \vec{\mathcal{V}}^h, \vec{\mathcal{V}}^h\rangle_{\Gamma^h(t)}^h$ *in place of* (3.28)*. However, the proof of the following theorem demonstrates that in order to satisfy the first conservation property in* (3.21)*, it is crucial to keep the left hand side of* (3.22) *as stated.*

THEOREM. 3.2. *Let* $\theta \in [0,1]$ *and let* $\{(\Gamma^h, \vec{\kappa}^h, \vec{Y}^h, \lambda^h, \mu^h)(t)\}_{t\in[0,T]}$ *be a solution to* (3.22)*,* (3.18b–d) *and* (3.23)*. Then it holds that*

$$\frac{\mathrm{d}}{\mathrm{d}t} E_{\overline{\varkappa},\beta}^h(\Gamma^h(t)) = -\left\langle \underline{\underline{Q}}_\theta^h \vec{\mathcal{V}}^h, \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h \leq 0, \tag{3.35}$$

as well as

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{H}^2(\Gamma^h(t)) = 0 \quad \textit{and} \quad \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{L}^3(\Omega^h(t)) = 0\,, \tag{3.36}$$

where $\Omega^h(t)$ *denotes the region bounded by* $\Gamma^h(t)$*. Moreover, if* $\theta = 0$ *then* $\Gamma^h(t)$ *is a conformal polyhedral surface for all* $t \in (0,T]$.

Proof. Choosing $\vec{\chi} = \vec{\omega}^h$ in (3.22) yields, on recalling (3.9), that

$$\left\langle \vec{\mathcal{V}}^h, \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h = \left\langle \nabla_s \vec{Y}^h, \nabla_s \vec{\omega}^h \right\rangle_{\Gamma^h(t)} + \left\langle \vec{f}^h, \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h + \lambda^h \langle \vec{\kappa}^h, \vec{\omega}^h\rangle_{\Gamma^h(t)}^h + \mu^h \langle \vec{\omega}^h, \vec{\omega}^h\rangle_{\Gamma^h(t)}^h$$
$$= 0\,, \tag{3.37}$$

where we have observed (3.23) in deducing the second equality. Similarly, choosing $\vec{\chi} = \vec{\kappa}^h$ in (3.22) yields that

$$\left\langle \underline{\underline{Q}}_\theta^h \vec{\mathcal{V}}^h, \vec{\kappa}^h \right\rangle_{\Gamma^h(t)}^h = \left\langle \nabla_s \vec{Y}^h, \nabla_s \vec{\kappa}^h \right\rangle_{\Gamma^h(t)} + \left\langle \vec{f}^h, \vec{\kappa}^h \right\rangle_{\Gamma^h(t)}^h + \lambda^h \left\langle \underline{\underline{Q}}_\theta^h \vec{\kappa}^h, \vec{\kappa}^h \right\rangle_{\Gamma^h(t)}^h$$
$$+ \mu^h \langle \vec{\omega}^h, \vec{\kappa}^h\rangle_{\Gamma^h(t)}^h = 0\,. \tag{3.38}$$

It follows from (3.24), (3.25), (3.38) and (3.37), that (3.21) holds, which yields the desired results (3.36). The stability result (3.35) directly follows from the proof of Theorem 3.1. In particular, choosing $\vec{\chi} = \vec{\mathcal{V}}^h$ in (3.22), on noting (3.37) and (3.38), yields that

$$\left\langle \underline{\underline{Q}}_\theta^h \vec{\mathcal{V}}^h, \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h = \left\langle \nabla_s \vec{Y}^h, \nabla_s \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)} + \left\langle \vec{f}^h, \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h.$$

Combining this with (3.29) yields that (3.30) holds, and the rest of the proof proceeds as that of Theorem 3.1. Finally, as in the proof of Theorem 3.1, for $\theta = 0$ it follows from (3.18c) that $\Gamma^h(t)$ is a conformal polyhedral surface. □

REMARK. 3.2. *We recall the following semi-discrete scheme from Dziuk (2008) for the case $\overline{\varkappa} = \beta = 0$. Given $\Gamma^h(0)$, for all $t \in (0,T]$ find $\Gamma^h(t)$ and $\vec\kappa^h(t) \in \underline{V}^h(\Gamma^h(t))$ such that*

$$\left\langle \vec{\mathcal{V}}^h, \vec\chi \right\rangle_{\Gamma^h(t)} - \left\langle \nabla_s \vec\kappa^h, \nabla_s \vec\chi \right\rangle_{\Gamma^h(t)} - \left\langle \nabla_s \,.\, \vec\kappa^h, \nabla_s \,.\, \vec\chi \right\rangle_{\Gamma^h(t)} - \tfrac12 \left\langle |\vec\kappa^h|^2 \, \nabla_s \, \vec{\rm id}, \nabla_s \, \vec\chi \right\rangle_{\Gamma^h(t)}$$
$$= - \left\langle (\nabla_s \, \vec\kappa^h)^T, \underline{\underline{D}}(\vec\chi) \, (\nabla_s \, \vec X^h)^T \right\rangle_{\Gamma^h(t)} \qquad \forall \ \vec\chi \in \underline{V}^h(\Gamma^h(t)) \,, \tag{3.39a}$$

$$\left\langle \vec\kappa^h, \vec\eta \right\rangle_{\Gamma^h(t)} + \left\langle \nabla_s \, \vec{\rm id}, \nabla_s \, \vec\eta \right\rangle_{\Gamma^h(t)} = 0 \qquad \forall \ \vec\eta \in \underline{V}^h(\Gamma^h(t)) \,. \tag{3.39b}$$

Clearly, the scheme (3.18a–d) *for $\theta = 1$, in the case $\overline{\varkappa} = \beta = 0$, collapses to a variant of* (3.39a,b) *with mass-lumping. In particular, we obtain* (3.39a,b) *with $\langle \cdot, \cdot \rangle_{\Gamma^h(t)}$ replaced by $\langle \cdot, \cdot \rangle^h_{\Gamma^h(t)}$ in the first and fourth term in* (3.39a)*, as well as in the first term in* (3.39b)*.*

REMARK. 3.3. *A natural alternative to the scheme* (3.18a–d)*, which does not use the normalization of the discrete vertex normal $\vec\omega^h$ as in* (3.8)*, is given as follows. Let*

$$\underline{\underline{\mathcal{Q}}}^h_\theta(\vec q^h_k(t), t) = \theta \, \underline{\underline{\rm Id}} + (1-\theta) \, \vec\omega^h(\vec q^h_k(t), t) \otimes \vec\omega^h(\vec q^h_k(t), t) \qquad \forall \ k \in \{1, \ldots, K\} \,. \tag{3.40}$$

Given $\Gamma^h(0)$, for all $t \in (0,T]$ find $\Gamma^h(t)$ and $\vec\kappa^h(t), \vec Y^h(t) \in \underline{V}^h(\Gamma^h(t))$ such that

$$\left\langle \underline{\underline{\mathcal{Q}}}^h_\theta \, \vec{\mathcal{V}}^h, \vec\chi \right\rangle^h_{\Gamma^h(t)} - \left\langle \nabla_s \, \vec Y^h, \nabla_s \, \vec\chi \right\rangle_{\Gamma^h(t)} - \left\langle \nabla_s \,.\, \vec Y^h, \nabla_s \,.\, \vec\chi \right\rangle_{\Gamma^h(t)}$$
$$+ \left\langle (\nabla_s \, \vec Y^h)^T, \underline{\underline{D}}(\vec\chi) \, (\nabla_s \, \vec{\rm id})^T \right\rangle_{\Gamma^h(t)} + (A^h - \overline{\varkappa}) \left\langle \vec\kappa^h, [\nabla_s \, \vec\chi]^T \, \vec\nu^h \right\rangle^h_{\Gamma^h(t)}$$
$$+ \tfrac12 \left\langle \left[|\vec\kappa^h - \overline{\varkappa} \, \vec\nu^h|^2 - 2 \, (\theta \, \vec\kappa^h + (1-\theta) \, (\vec\kappa^h \,.\, \vec\omega^h) \, \vec\omega^h) \,.\, \vec Y^h + 2 \, A^h \, \vec\kappa^h \,.\, \vec\nu^h \right] \nabla_s \, \vec{\rm id}, \nabla_s \, \vec\chi \right\rangle^h_{\Gamma^h(t)}$$
$$- (1-\theta) \left\langle (\vec\nu^h - \vec\omega^h) \,.\, \left[(\vec Y^h \,.\, \vec\omega^h) \, \vec\kappa^h + (\vec\kappa^h \,.\, \vec\omega^h) \, \vec Y^h \right] \nabla_s \, \vec{\rm id}, \nabla_s \, \vec\chi \right\rangle^h_{\Gamma^h(t)}$$
$$+ (1-\theta) \left\langle (\vec Y^h \,.\, \vec\omega^h) \, \vec\kappa^h + (\vec\kappa^h \,.\, \vec\omega^h) \, \vec Y^h, [\nabla_s \, \vec\chi]^T \, \vec\nu^h \right\rangle^h_{\Gamma^h(t)} = 0 \quad \forall \ \vec\chi \in \underline{V}^h(\Gamma^h(t)) \,, \tag{3.41a}$$

$$\left\langle \vec\kappa^h - (\overline{\varkappa} - A^h) \, \vec\nu^h - \underline{\underline{\mathcal{Q}}}^h_\theta \, \vec Y^h, \vec\xi \right\rangle^h_{\Gamma^h(t)} = 0 \quad \forall \ \vec\xi \in \underline{V}^h(\Gamma^h(t)) \,, \tag{3.41b}$$

$$\left\langle \underline{\underline{\mathcal{Q}}}^h_\theta \, \vec\kappa^h, \vec\eta \right\rangle^h_{\Gamma^h(t)} + \left\langle \nabla_s \, \vec{\rm id}, \nabla_s \, \vec\eta \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \ \vec\eta \in \underline{V}^h(\Gamma^h(t)) \,, \tag{3.41c}$$

where

$$A^h(t) = \beta \left(\left\langle \vec\kappa^h, \vec\nu^h \right\rangle_{\Gamma^h(t)} - M_0 \right) . \tag{3.41d}$$

This is a slightly simpler scheme, whose two-dimensional analogue in the case $\theta = \overline{\varkappa} = \beta = 0$ has similarities with the scheme (3.40a,b) *in Barrett* et al. *(2012) in the isotropic* *case. In addition, with a simple adaptation of the proof of* Theorem 3.1, *it is possible to show that* (3.41a–d) *is stable, i.e. that* $\frac{\mathrm{d}}{\mathrm{d}t} E^h_{\varkappa,\beta}(\Gamma^h(t)) = -\left\langle \underline{\underline{\mathcal{Q}}}^h_\theta \vec{\mathcal{V}}^h, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} \leq 0$ *for a solution of* (3.41a–d)*. The same remains valid if* $\underline{\underline{\mathcal{Q}}}^h_\theta$ *in* (3.41a)*, and in the energy bound, is replaced by* $\underline{\underline{\mathrm{Id}}}$.

However, it does not appear possible to introduce Lagrange multipliers λ^h *and* μ^h *for* (3.41a–d)*, even as stated with* $\underline{\underline{\mathcal{Q}}}^h_\theta$*, such that the two conservation properties in* (3.36) *hold, and such that the approximation remains stable. In particular, while it is still possible to find a* λ^h *such that the surface area* $\mathcal{H}^2(\Gamma^h(t))$ *is maintained, it does not appear possible to define a* μ^h *to ensure volume preservation. It is for this reason that we do not pursue the scheme* (3.41a–d) *further in this paper.*

4 Fully discrete finite element approximation

In this section we consider a fully discrete variant of the scheme (3.22), (3.18b–d) from Section 3. To this end, let $0 = t_0 < t_1 < \ldots < t_{M-1} < t_M = T$ be a partitioning of $[0, T]$ into possibly variable time steps $\tau_m := t_{m+1} - t_m$, $m = 0, \ldots, M-1$. Let Γ^m be a polyhedral surface, approximating the $\Gamma^h(t_m)$, $m = 0, \ldots, M$. Following Dziuk (1991), we now parameterize the new closed surface Γ^{m+1} over Γ^m. Hence, we introduce the following finite element spaces. Let $\Gamma^m = \bigcup_{j=1}^J \overline{\sigma^m_j}$, where $\{\sigma^m_j\}_{j=1}^J$ is a family of mutually disjoint open triangles with vertices $\{\vec{q}^m_k\}_{k=1}^K$. Then for $m = 0, \ldots, M-1$, let

$$\underline{V}^h(\Gamma^m) := \{\vec{\chi} \in [C(\Gamma^m)]^3 : \vec{\chi}|_{\sigma^m_j} \text{ is linear } \forall\ j = 1, \ldots, J_\Gamma\} =: [W^h(\Gamma^m)]^3 \subset [H^1(\Gamma^m)]^3\,,$$

for $m = 0, \ldots, M-1$. We denote the standard basis of $W^h(\Gamma^m)$ by $\{\chi^m_k\}_{k=1}^K$. We also introduce $\pi^m : C(\Gamma^m) \to W^h(\Gamma^m)$, the standard interpolation operator at the nodes $\{\vec{q}^m_k\}_{k=1}^K$, and similarly $\vec{\pi}^m : [C(\Gamma^m)]^3 \to \underline{V}^h(\Gamma^m)$. Throughout this paper, we will parameterize the new closed surface Γ^{m+1} over Γ^m, with the help of a parameterization $\vec{X}^{m+1} \in \underline{V}^h(\Gamma^m)$, 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, the the mass lumped inner product $\langle \cdot, \cdot \rangle^h_{\Gamma^m}$, as well as the outer unit normal $\vec{\nu}^m$ to Γ^m. Similarly to (3.7), we note that

$$\langle \vec{z}, w\, \vec{\nu}^m \rangle^h_{\Gamma^m} = \langle \vec{z}, w\, \vec{\omega}^m \rangle^h_{\Gamma^m} \qquad \forall\ \vec{z} \in \underline{V}^h(\Gamma^m)\,,\ w \in W^h(\Gamma^m)\,,$$

where $\vec{\omega}^m := \sum_{k=1}^{K_\Gamma} \chi^m_k\, \vec{\omega}^m_k \in \underline{V}^h(\Gamma^m)$, and where for $k = 1, \ldots, K_\Gamma$ we let $\Theta^m_k := \{j : \vec{q}^m_k \in \overline{\sigma^m_j}\}$ and set $\Lambda^m_k := \cup_{j \in \Theta^m_k} \overline{\sigma^m_j}$ and $\vec{\omega}^m_k := \frac{1}{\mathcal{H}^2(\Lambda^m_k)} \sum_{j \in \Theta^m_k} \mathcal{H}^2(\sigma^m_j)\, \vec{\nu}^m_j$.

We make the following very mild assumption.

($\mathcal{A}$) We assume for $m = 0, \ldots, M-1$ that $\mathcal{H}^2(\sigma^m_j) > 0$ for all $j = 1, \ldots, J$ and that $\vec{0} \notin \{\vec{\omega}^m_k\}_{k=1}^K$, for all $m = 0, \ldots, M-1$. If $\theta = 0$ we also assume that $\dim \operatorname{span}\{\vec{\omega}^m_k\}_{k=1}^K = 3$, for all $m = 0, \ldots, M-1$.

In addition, we introduce $\underline{\underline{Q}}_\theta^m \in [W^h(\Gamma^m)]^{3\times 3}$ by setting $\underline{\underline{Q}}_\theta^m(\vec{q}_k^m) = \theta\,\vec{\mathrm{Id}} + (1-\theta)\,|\vec{\omega}_k^m|^{-2}\,\vec{\omega}_k^m \otimes \vec{\omega}_k^m$ for $k = 1,\ldots,K$. Similarly to (3.15), we let

$$\vec{G}^m(\vec{\xi},\vec{\eta}) = \vec{\pi}^m\left[\frac{1}{|\vec{\omega}^m|^2}\left((\vec{\xi}\,.\,\vec{\omega}^m)\,\vec{\eta} + (\vec{\eta}\,.\,\vec{\omega}^m)\,\vec{\xi} - 2\,\frac{(\vec{\eta}\,.\,\vec{\omega}^m)\,(\vec{\xi}\,.\,\vec{\omega}^m)}{|\vec{\omega}^m|^2}\,\vec{\omega}^m\right)\right]. \tag{4.1}$$

On recalling (3.7), we consider the following fully discrete approximation of (3.22), (3.18b–d). Given Γ^0, $A^0 \in \mathbb{R}$ and $\vec{\kappa}^0$, $\vec{Y}^0 \in \underline{V}^h(\Gamma^0)$, for $m = 0,\ldots,M-1$ find $(\vec{X}^{m+1},\vec{\kappa}^{m+1},\vec{Y}^{m+1}) \in [\underline{V}^h(\Gamma^m)]^3$ such that

$$\begin{aligned}
&\left\langle \underline{\underline{Q}}_\theta^m\,\frac{\vec{X}^{m+1}-\vec{\mathrm{id}}}{\tau_m},\vec{\chi}\right\rangle_{\Gamma^m}^h - \left\langle \nabla_s\,\vec{Y}^{m+1},\nabla_s\,\vec{\chi}\right\rangle_{\Gamma^m} = \left\langle \nabla_s\,.\,\vec{Y}^m,\nabla_s\,.\,\vec{\chi}\right\rangle_{\Gamma^m} \\
&\quad - \left\langle (\nabla_s\,\vec{Y}^m)^T,\underline{\underline{D}}(\vec{\chi})\,(\nabla_s\,\vec{\mathrm{id}})^T\right\rangle_{\Gamma^m} + (A^m - \overline{\varkappa})\,\langle\vec{\kappa}^m,[\nabla_s\,\vec{\chi}]^T\,\vec{\nu}^m\rangle_{\Gamma^m}^h \\
&\quad - \tfrac12\left\langle\left[|\vec{\kappa}^m - \overline{\varkappa}\,\vec{\nu}^m|^2 - 2\,\vec{Y}^m\,.\,\underline{\underline{Q}}_\theta^m\,\vec{\kappa}^m + 2\,A^m\,\vec{\kappa}^m\,.\,\vec{\nu}^m\right]\nabla_s\,\vec{\mathrm{id}},\nabla_s\,\vec{\chi}\right\rangle_{\Gamma^m}^h \\
&\quad + (1-\theta)\left(\left\langle(\vec{G}^m(\vec{Y}^m,\vec{\kappa}^m)\,.\,\vec{\nu}^m)\,\nabla_s\,\vec{\mathrm{id}},\nabla_s\,\vec{\chi}\right\rangle_{\Gamma^m}^h - \left\langle\vec{G}^m(\vec{Y}^m,\vec{\kappa}^m),[\nabla_s\,\vec{\chi}]^T\,\vec{\nu}^m\right\rangle_{\Gamma^m}^h\right) \\
&\quad + \left\langle\lambda^m\,\underline{\underline{Q}}_\theta^m\,\vec{\kappa}^m + \mu^m\,\vec{\omega}^m,\vec{\chi}\right\rangle_{\Gamma^m}^h \qquad \forall\ \vec{\chi} \in \underline{V}^h(\Gamma^m)\,,
\end{aligned} \tag{4.2a}$$

$$\left\langle\vec{\kappa}^{m+1} + (A^m - \overline{\varkappa})\,\vec{\omega}^m - \underline{\underline{Q}}_\theta^m\,\vec{Y}^{m+1},\vec{\xi}\right\rangle_{\Gamma^m}^h = 0 \quad \forall\ \vec{\xi} \in \underline{V}^h(\Gamma^m)\,, \tag{4.2b}$$

$$\left\langle\underline{\underline{Q}}_\theta^m\,\vec{\kappa}^{m+1},\vec{\eta}\right\rangle_{\Gamma^m}^h + \left\langle\nabla_s\,\vec{X}^{m+1},\nabla_s\,\vec{\eta}\right\rangle_{\Gamma^m} = 0 \quad \forall\ \vec{\eta} \in \underline{V}^h(\Gamma^m)\,, \tag{4.2c}$$

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

$$A^{m+1} = \beta\left(\langle\vec{\kappa}^{m+1},\vec{\omega}^m\rangle_{\Gamma^m}^h - M_0\right). \tag{4.2d}$$

Of course, (4.2a–d) with $\lambda^m = \mu^m = 0$ corresponds to a fully discrete approximation of (3.18a–d). For a fully discrete approximation of Helfrich flow we let $(\lambda^m,\mu^m)^T \in \mathbb{R}^2$ be the solution to the symmetric linear system

$$\begin{pmatrix} \left\langle\underline{\underline{Q}}_\theta^m\,\vec{\kappa}^m,\vec{\kappa}^m\right\rangle_{\Gamma^m}^h & \langle\vec{\kappa}^m,\vec{\omega}^m\rangle_{\Gamma^m}^h \\ \langle\vec{\kappa}^m,\vec{\omega}^m\rangle_{\Gamma^m}^h & \langle\vec{\omega}^m,\vec{\omega}^m\rangle_{\Gamma^m}^h \end{pmatrix}\begin{pmatrix}\lambda^m \\ \mu^m\end{pmatrix} = \begin{pmatrix} -\left\langle\nabla_s\,\vec{Y}^m,\nabla_s\,\vec{\kappa}^m\right\rangle_{\Gamma^m} - \left\langle\vec{f}^m,\vec{\kappa}^m\right\rangle_{\Gamma^m}^h \\ -\left\langle\nabla_s\,\vec{Y}^m,\nabla_s\,\vec{\omega}^m\right\rangle_{\Gamma^m} - \left\langle\vec{f}^m,\vec{\omega}^m\right\rangle_{\Gamma^m}^h \end{pmatrix}, \tag{4.3}$$

where for convenience we have re-written (4.2a) as

$$\left\langle\underline{\underline{Q}}_\theta^m\,\frac{\vec{X}^{m+1}-\vec{\mathrm{id}}}{\tau_m},\vec{\chi}\right\rangle_{\Gamma^m}^h - \left\langle\nabla_s\,\vec{Y}^{m+1},\nabla_s\,\vec{\chi}\right\rangle_{\Gamma^m} = \left\langle\vec{f}^m + \lambda^m\,\underline{\underline{Q}}_\theta^m\,\vec{\kappa}^m + \mu^m\,\vec{\omega}^m,\vec{\chi}\right\rangle_{\Gamma^m}^h \qquad \forall\ \vec{\chi} \in \underline{V}^h(\Gamma^m)\,.$$

Similarly to (3.23) we note that the linear system (4.3) is symmetric and nonnegative definite, with a unique solution unless $\vec{\kappa}^m$ is a scalar multiple of $\vec{\omega}^m$.

THEOREM. 4.1. *Let the assumptions* ($\mathcal{A}$) *hold, let* $\theta \in [0,1]$ *and let* $(\lambda^m, \mu^m)^T \in \mathbb{R}^2$ *be given. Then there exists a unique solution* $(\vec{X}^{m+1}, \vec{\kappa}^{m+1}, \vec{Y}^{m+1}) \in [\underline{V}^h(\Gamma^m)]^3$ *to* (4.2a–c).

Proof. As (4.2a–c) is linear, existence follows from uniqueness. To investigate the latter, we consider the system: Find $(\vec{X}, \vec{\kappa}, \vec{Y}) \in [\underline{V}^h(\Gamma^m)]^3$ such that

$$\left\langle \underline{\underline{Q}}^m_\theta\, \vec{X}, \vec{\chi} \right\rangle^h_{\Gamma^m} - \tau_m \left\langle \nabla_s\, \vec{Y}, \nabla_s\, \vec{\chi} \right\rangle_{\Gamma^m} = 0 \qquad \forall\, \vec{\chi} \in \underline{V}^h(\Gamma^m)\,, \tag{4.4a}$$

$$\left\langle \vec{\kappa} - \underline{\underline{Q}}^m_\theta\, \vec{Y}, \vec{\xi} \right\rangle^h_{\Gamma^m} = 0 \quad \forall\, \vec{\xi} \in \underline{V}^h(\Gamma^m)\,, \tag{4.4b}$$

$$\left\langle \underline{\underline{Q}}^m_\theta\, \vec{\kappa}, \vec{\eta} \right\rangle^h_{\Gamma^m} + \left\langle \nabla_s\, \vec{X}, \nabla_s\, \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall\, \vec{\eta} \in \underline{V}^h(\Gamma^m)\,. \tag{4.4c}$$

Choosing $\vec{\chi} = \vec{X}$ in (4.4a), $\vec{\xi} = \vec{\kappa}$ in (4.4b) and $\vec{\eta} = \vec{Y}$ in (4.4c) yields that

$$\left\langle \underline{\underline{Q}}^m_\theta\, \vec{X}, \vec{X} \right\rangle^h_{\Gamma^m} + \tau_m\, \langle \vec{\kappa}, \vec{\kappa} \rangle^h_{\Gamma^m} = 0\,, \tag{4.5}$$

and hence $\vec{\kappa} = \vec{0}$, as well as $\theta\, \vec{X} = \vec{0}$ and $(1-\theta)\, \pi^m\, [\vec{X} \,.\, \vec{\omega}^m] = 0$. If $\theta > 0$ this immediately implies that $\vec{X} = \vec{0}$. In the case $\theta = 0$ it follows from $\vec{\kappa} = \vec{0}$ and (4.4c) with $\vec{\eta} = \vec{X}$ that $\langle \nabla_s\, \vec{X}, \nabla_s\, \vec{X} \rangle_{\Gamma^m} = 0$, and so $\vec{X} = \vec{X}_c \in \mathbb{R}^3$ is constant. Hence it follows from $\vec{X}_c \,.\, \vec{\omega}^m = 0$ and assumption ($\mathcal{A}$) that $\vec{X} = \vec{0}$. Similarly, combining $\vec{X} = \vec{\kappa} = \vec{0}$ and (4.4a,b) with $\vec{\chi} = \vec{Y}$ and $\vec{\xi} = \vec{Y}$ yields that $\vec{Y} = \vec{0}$. Hence there exists a unique solution $(\vec{X}^{m+1}, \vec{\kappa}^{m+1}, \vec{Y}^{m+1}) \in [\underline{V}^h(\Gamma^m)]^3$ to (4.2a–c). □

REMARK. 4.1. *In practice it can be advantageous to consider implicit Lagrange multipliers* λ^{m+1} *and* μ^{m+1} *in order to obtain better discrete surface area and volume preservation properties. In particular, we replace* (4.2a) *with*

$$\left\langle \underline{\underline{Q}}^m_\theta\, \frac{\vec{X}^{m+1} - \vec{\mathrm{id}}}{\tau_m}, \vec{\chi} \right\rangle^h_{\Gamma^m} - \left\langle \nabla_s\, \vec{Y}^{m+1}, \nabla_s\, \vec{\chi} \right\rangle_{\Gamma^m} = \left\langle \vec{f}^m + \lambda^{m+1}\, \underline{\underline{Q}}^m_\theta\, \vec{\kappa}^{m+1} + \mu^{m+1}\, \vec{\omega}^m, \vec{\chi} \right\rangle^h_{\Gamma^m} \quad \forall\, \vec{\chi} \in \underline{V}^h(\Gamma^m) \tag{4.6}$$

and require the coupled solution $(\vec{X}^{m+1}, \vec{\kappa}^{m+1}, \vec{Y}^{m+1}) \in [\underline{V}^h(\Gamma^m)]^3$ *and* $(\lambda^{m+1}, \mu^{m+1})^T \in \mathbb{R}^2$ *to satisfy the nonlinear system* (4.6), (4.2b–d) *as well as an adapted variant of* (4.3), *where the superscript* m *is replaced by* $m+1$ *in all occurrences of* $\vec{\kappa}^m$, $\vec{Y}^m$, λ^m *and* μ^m. *In practice this nonlinear system can be solved with a fixed point iteration as follows. Let* $(\lambda^{m+1,0}, \mu^{m+1,0}) = (\lambda^m, \mu^m)$. *Then, for* $i \geq 0$, *find a solution* $(\vec{X}^{m+1,i}, \vec{\kappa}^{m+1,i}, \vec{Y}^{m+1,i}) \in [\underline{V}^h(\Gamma^m)]^3$ *to the linear system* (4.6), (4.2b–d), *where any superscript* $m+1$ *is replaced by* $m+1, i$. *Then compute* $(\lambda^{m+1,i+1}, \mu^{m+1,i+1})$ *as the unique solution to*

$$\begin{pmatrix} \left\langle \underline{\underline{Q}}^m_\theta\, \vec{\kappa}^{m+1,i}, \vec{\kappa}^{m+1,i} \right\rangle^h_{\Gamma^m} & \langle \vec{\kappa}^{m+1,i}, \vec{\omega}^m \rangle^h_{\Gamma^m} \\ \langle \vec{\kappa}^{m+1,i}, \vec{\omega}^m \rangle^h_{\Gamma^m} & \langle \vec{\omega}^m, \vec{\omega}^m \rangle^h_{\Gamma^m} \end{pmatrix} \begin{pmatrix} \lambda^{m+1,i+1} \\ \mu^{m+1,i+1} \end{pmatrix}$$
$$= \begin{pmatrix} -\left\langle \nabla_s\, \vec{Y}^{m+1,i}, \nabla_s\, \vec{\kappa}^{m+1,i} \right\rangle_{\Gamma^m} - \left\langle \vec{f}^m, \vec{\kappa}^{m+1,i} \right\rangle^h_{\Gamma^m} \\ -\left\langle \nabla_s\, \vec{Y}^{m+1,i}, \nabla_s\, \vec{\omega}^m \right\rangle_{\Gamma^m} - \left\langle \vec{f}^m, \vec{\omega}^m \right\rangle^h_{\Gamma^m} \end{pmatrix},$$

and continue the iteration until $|\lambda^{m+1,i+1}-\lambda^{m+1,i}|+|\mu^{m+1,i+1}-\mu^{m+1,i}|<10^{-8}$. *In practice this iteration always converged in less than ten steps, and at little extra computational cost compared to the linear scheme* (4.2a–d), *since the linear subsystem* (4.2a–c), *for given values of* $\vec{\kappa}^m$, λ^m, μ^m, *can be easily factorized with the help of sparse factorization packages such as UMFPACK, see Davis (2004).*

5 Solution of the algebraic equations

We introduce the matrices $M, A, A_\theta \in \mathbb{R}^{K\times K}$, $\vec{M}, \vec{\mathcal{M}}_\theta, \vec{A}, \vec{A}_\theta, \vec{\mathcal{B}}, \vec{\mathcal{R}} \in (\mathbb{R}^{3\times 3})^{K\times K}$ with entries

$$
\begin{aligned}
&M_{kl} := \langle \chi^m_l, \chi^m_k\rangle^h_{\Gamma^m}\,, \quad [\vec{\mathcal{M}}_\theta]_{kl} := M_{kl}\,\underline{\underline{Q}}^m_\theta(\vec{q}^m_k)\,, \quad A_{kl} := \langle \nabla_s\,\chi^m_l, \nabla_s\,\chi^m_k\rangle_{\Gamma^m}\,,\\
&\vec{\mathcal{B}}_{kl} := \left(\langle [\nabla_s]_j\,\chi^m_l, [\nabla_s]_i\,\chi^m_k\rangle_{\Gamma^m}\right)^3_{i,j=1}\,, \quad \vec{\mathcal{R}}_{kl} := \int_{\Gamma^m} \nabla_s\,\chi^m_l\,.\,\nabla_s\,\chi^m_k\,(\underline{\underline{\mathrm{Id}}} - \vec{\nu}^m\otimes\vec{\nu}^m)\;\mathrm{d}\mathcal{H}^2\,,\\
&[A_\theta]_{kl} := \tfrac12\left\langle \left[|\vec{\kappa}^m - \overline{\varkappa}\,\vec{\nu}^m|^2 - 2\,\vec{Y}^m\,.\,\underline{\underline{Q}}^m_\theta\,\vec{\kappa}^m + 2A^m\,\vec{\kappa}^m\,.\,\vec{\nu}^m\right]\nabla_s\,\chi^m_l, \nabla_s\,\chi^m_k\right\rangle^h_{\Gamma^m}\\
&\qquad\qquad - (1-\theta)\left\langle (\vec{G}^m(\vec{Y}^m,\vec{\kappa}^m)\,.\,\vec{\nu}^m)\,\nabla_s\,\chi^m_l, \nabla_s\,\chi^m_k\right\rangle^h_{\Gamma^m}\,,
\end{aligned}
$$

and $\vec{M}_{kl} := M_{kl}\,\underline{\underline{\mathrm{Id}}}$, $\vec{A}_{kl} := A_{kl}\,\underline{\underline{\mathrm{Id}}}$, $[\vec{A}_\theta]_{kl} := [A_\theta]_{kl}\,\underline{\underline{\mathrm{Id}}}$. It holds that $(\vec{\mathcal{B}}_{kl})^T = \vec{\mathcal{B}}_{lk} =: [\vec{\mathcal{B}}^\star]_{kl}$.

Then we can formulate (4.2a–c) as: Find $(\vec{Y}^{m+1}, \delta\vec{X}^{m+1}, \vec{\kappa}^{m+1}) \in (\mathbb{R}^3)^{3K}$ such that

$$
\begin{pmatrix} \vec{A} & -\frac{1}{\tau_m}\vec{\mathcal{M}}_\theta & 0\\ 0 & \vec{A} & \vec{\mathcal{M}}_\theta\\ \vec{\mathcal{M}}_\theta & 0 & -\vec{M}\end{pmatrix}
\begin{pmatrix} \vec{Y}^{m+1}\\ \delta\vec{X}^{m+1}\\ \vec{\kappa}^{m+1}\end{pmatrix}
= \begin{pmatrix} [\vec{\mathcal{B}}^\star - \vec{\mathcal{B}} + \vec{\mathcal{R}}]\,\vec{Y}^m + \vec{A}_\theta\,\vec{X}^m + \vec{b}_\theta - \lambda^m\,\vec{\mathcal{M}}_\theta\,\vec{\kappa}^m - \mu^m\,\vec{M}\,\vec{\omega}^m\\ -\vec{A}\,\vec{X}^m\\ (A^m - \overline{\varkappa})\,\vec{M}\,\vec{\omega}^m\end{pmatrix},
$$

where, with the obvious abuse of notation, $\delta\vec{X}^{m+1} = (\delta\vec{X}^{m+1}_1,\ldots,\delta\vec{X}^{m+1}_K)^T$, $\vec{Y}^{m+1} = (\vec{Y}^{m+1}_1,\ldots,\vec{Y}^{m+1}_K)^T$ and $\vec{\kappa}^{m+1} = (\vec{\kappa}^{m+1}_1,\ldots,\vec{\kappa}^{m+1}_K)^T$ are the vectors of coefficients with respect to the standard basis for $\vec{X}^{m+1}-\vec{X}^m$, $\vec{Y}^{m+1}$ and $\vec{\kappa}^{m+1}$, respectively. In addition, $\vec{b}_\theta \in (\mathbb{R}^3)^K$ with

$$
[\vec{b}_\theta]_k = \left\langle \left[(\overline{\varkappa} - A^m)\,\vec{\kappa}^m + (1-\theta)\,\vec{G}^m(\vec{Y}^m,\vec{\kappa}^m)\right].\,\nabla_s\,\chi^m_k, \vec{\nu}^m\right\rangle^h_{\Gamma^m}.
$$

6 Numerical computations

We note that we implemented the approximations within the finite element toolbox ALBERTA, see Schmidt and Siebert (2005). The arising systems of linear equations were solved with the help of the sparse factorization package UMFPACK, see Davis (2004). For the computations involving volume preserving Willmore flow and Helfrich flow, we always employ the implicit Lagrange multiplier formulation discussed in Remark 4.1.

For the fully discrete scheme (4.2a–d) we need to prescribe initial data A^0, $\vec\kappa^0$ and $\vec Y^0$. Given the initial triangulation Γ^0, we define

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

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

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

Throughout this section we use uniform time steps $\tau_m = \tau$, $m = 0,\ldots,M-1$, and set $\tau = 10^{-3}$ unless stated otherwise. In addition, unless stated otherwise, we fix $\beta = \overline{\varkappa} = 0$ and $\lambda^m = \mu^m = 0$ for $m = 0,\ldots,M-1$. At times we will discuss the discrete energy of the numerical solutions, which, similarly to (3.10), is defined by

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

6.1 Numerical results for Willmore flow

We begin with a numerical simulation of Willmore flow for a torus with large radius $R = 2$ and small radius $r = 1$. Here $K = 2048$, $J = 4096$ and $\tau = 2\times10^{-4}$, as in Barrett *et al.* (2008b, Fig. 7). See Figure 1 for the results for the scheme (4.2a–d) with $\theta = 0$. We note that the discrete surface approaches the Clifford torus, which is the minimum of the Willmore energy (1.1) among all genus 1 surfaces, see Marques and Neves (2014). The Clifford torus is a standard torus with a ratio of large radius R and small radius r of $\frac{R}{r} = \sqrt2$, which leads to a Willmore energy of $E(\Gamma(t)) = 4\,\pi^2$. In our simulation the discrete energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec\kappa^{m+1})$ decreases to a value below $4\,\pi^2$, which is due to spatial discretization errors. For finer meshes this difference converges to zero. As a comparison, we repeat the same experiment now for (4.2a–d) with $\theta = 1$. Now the scheme is not able to integrate the solution until the final time $T = 2$ due to coalescence of mesh points. We show the evolution only until time $t = 1.4$, by which time several degenerate elements have appeared, which leads to an oscillatory behaviour of the discrete energy in time, see Figure 2. The behaviour shown in Figure 2 is fairly generic for the scheme (4.2a–d) with $\theta = 1$. The scheme with $\theta = 0$, on the other hand, often incorporates a good tangential motion, which means that the numerical solutions can be integrated for longer. That is why from now on we will always attempt to use $\theta = 0$ in all our simulations.

Following Barrett *et al.* (2008b, Fig. 8), we also present some numerical experiments for a sickle torus. Here the initial sickle torus has large radius $R = 2$ and the small radius r varies continuously in the interval $[1, 1.75]$. We set $K = 2048$, $J = 4096$ and $\tau = 2\times10^{-4}$, as in Barrett *et al.* (2008b, Fig. 8). For this simulation we observe some undesirable mesh effects, and a small increase in the energy, when $\theta = 0$. For $\theta = 0.1$

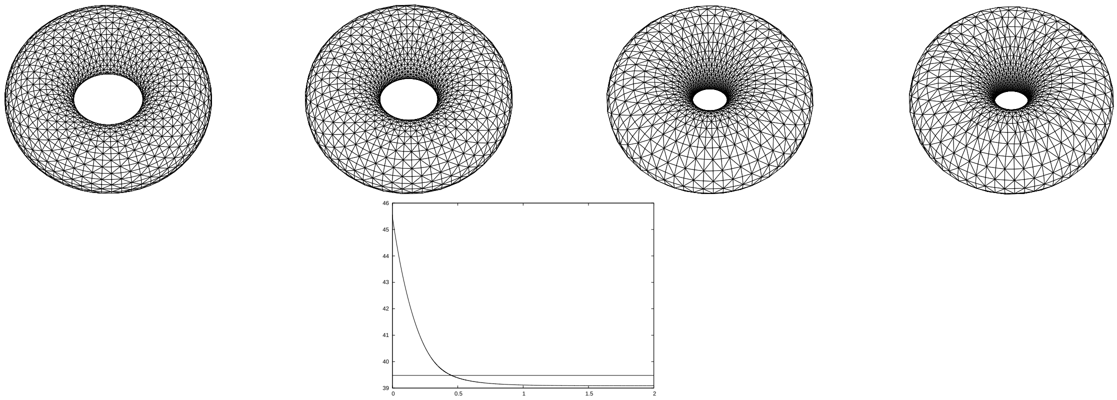

Figure 1: ($\theta = 0$) Willmore flow for a torus. A plot of Γ^m at times $t = 0,\ 0.1,\ 0.5,\ 2$. Below a plot of the discrete energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec{\kappa}^{m+1})$. The horizontal line shows $4\,\pi^2$.

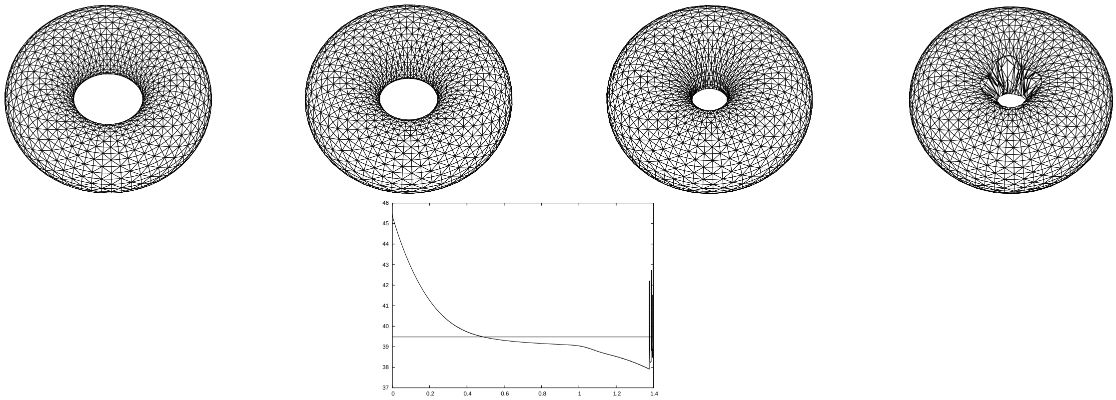

Figure 2: ($\theta = 1$) Willmore flow for a torus. A plot of Γ^m at times $t = 0,\ 0.1,\ 0.5,\ 1.4$. Below a plot of the discrete energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec{\kappa}^{m+1})$. The horizontal line shows $4\,\pi^2$.

we obtain better numerical results, with a monotonically decreasing discrete energy. For completeness we also present the run for $\theta = 1$, where a coalescence of mesh points leads to a highly oscillating energy plot in time. See Figures 3–5 for the results for the scheme (4.2a–d) with $\theta = 0$, $\theta = 0.1$ and $\theta = 1$, respectively.

6.2 Numerical results for Helfrich flow

For a numerical simulation of Helfrich flow, we start with a tubular shape of total dimension $4 \times 1 \times 1$. Here $K = 1154$, $J = 2304$ and $\tau = 10^{-3}$, as in Barrett *et al.* (2008b, Fig. 14). For this run the relative loss of area and volume is 0.15% and -0.03%, respectively. See Figure 6 for the results for the scheme (4.2a–d) with $\theta = 0$.

Following Barrett *et al.* (2008b, Fig. 15), we also consider Helfrich flow for a flat disc of total dimension $4 \times 4 \times 1$. For the discretization parameters as in Barrett *et al.* (2008b, Fig. 15) we observe undesirable mesh deformations for the scheme (4.2a–d), which means that the system matrix becomes numerically singular at time $t = 1.2$. Hence we use the

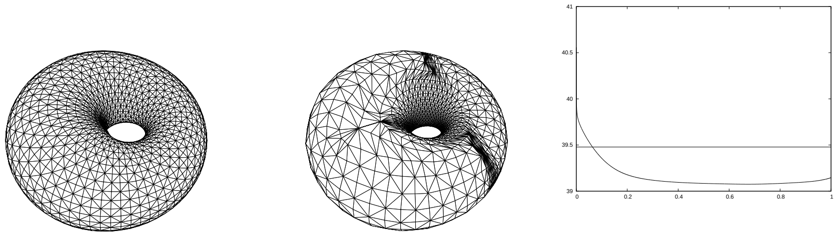

Figure 3: ($\theta = 0$) Willmore flow for a sickle torus. A plot of Γ^m at times $t = 0,\ 1$. On the right a plot of the discrete energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec\kappa^{m+1})$. The horizontal line shows $4\,\pi^2$.

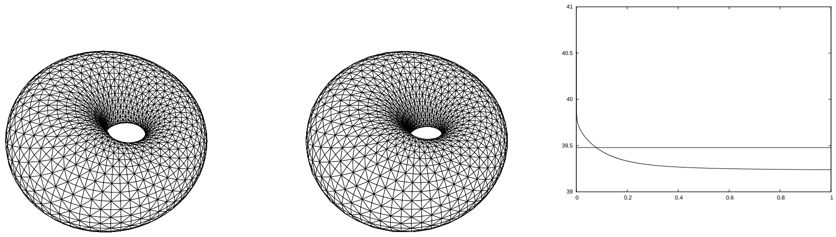

Figure 4: ($\theta = 0.1$) Willmore flow for a sickle torus. A plot of Γ^m at times $t = 0,\ 1$. On the right a plot of the discrete energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec\kappa^{m+1})$. The horizontal line shows $4\,\pi^2$.

finer discretization parameters $K = 6146$, $J = 12288$ and $\tau = 2 \times 10^{-4}$ in this paper. Then the observed relative loss of area and volume was 0.23% and 0.03%, respectively. See Figure 7 for the results for the scheme (4.2a–d).

6.3 Numerical results with spontaneous curvature effects

In this subsection, we consider flows for the free energy (1.2) with $\overline{\varkappa} < 0$. For our sign convention this means that a sphere of radius $\frac{2}{|\overline{\varkappa}|}$ will be the global energy minimizer with $E_{\overline{\varkappa}}(\Gamma(t)) = 0$.

We begin with a convergence experiment for the scheme (4.2a–d) for a radially symmetric solution to (1.4). In fact, it is easily shown that a sphere of radius $R(t)$, where $R(t)$ satisfies

$$R_t = -\tfrac{\overline{\varkappa}}{R}\left(\tfrac{2}{R} + \overline{\varkappa}\right), \quad R(0) = R_0 \in \mathbb{R}_{>0}\,, \tag{6.2}$$

is a solution to (1.4) in the case $A = \beta = 0$. The nonlinear ODE (6.2) is solved by $R(t) = z(t) - \frac{2}{\overline{\varkappa}}$, where $z(t)$ is such that $\frac{1}{2}\,(z^2(t) - z_0^2) - \frac{4}{\overline{\varkappa}}\,(z(t) - z_0) + \frac{4}{\overline{\varkappa}^2}\,\ln\frac{z(t)}{z_0} + \overline{\varkappa}^2\,t = 0$,

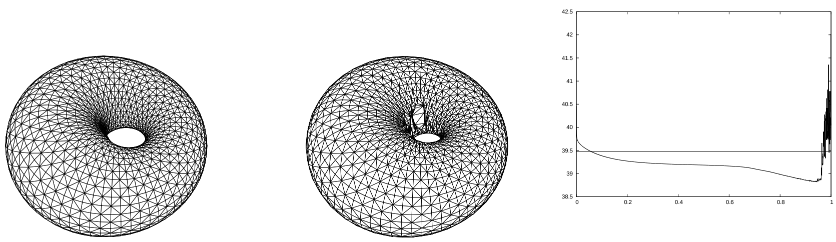

Figure 5: ($\theta = 1$) Willmore flow for a sickle torus. A plot of Γ^m at times $t = 0,\ 1$. On the right a plot of the discrete energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec\kappa^{m+1})$. The horizontal line shows $4\,\pi^2$.

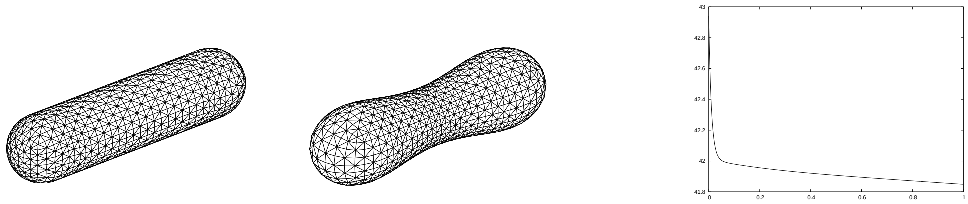

Figure 6: ($\theta = 0$) Helfrich flow for a tube. A plot of Γ^m at times $t = 0,\ 1$. On the right a plot of the discrete free energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec{\kappa}^{m+1})$.

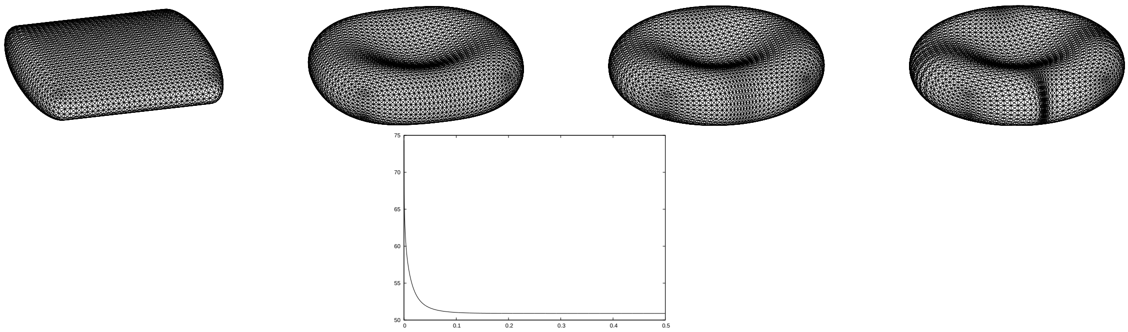

Figure 7: ($\theta = 0$) Helfrich flow for a flat plate. A plot of Γ^m at times $t = 0,\ 0.1,\ 0.25,\ 0.5$. Below a plot of the discrete free energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec{\kappa}^{m+1})$.

with $z_0 = R_0 + \frac{2}{\overline{\varkappa}}$. For the convergence experiment we set $\overline{\varkappa} = -1$ and use a sequence of four non-uniform triangulations of the unit sphere ($R_0 = 1$) to compute the error $\|\Gamma - \Gamma^h\|_{L^\infty} = \max_{m=1,\ldots,M} \max_{k=1,\ldots,K} ||\vec{q}^{\,m}_k| - R(t_m)|$ over the time interval $[0,1]$ between the true solution and the discrete solutions for the scheme (4.2a–d) in the cases $\theta = 0$ and $\theta = 1$. Here we used the time step size $\tau = 0.01\, h^2_{\Gamma^0}$, where h_{Γ^0} is the maximal edge length of Γ^0. Some of the triangulations are shown in Figure 8, where we note that $R(1) \approx 1.47$. The computed errors are reported in Table 1. It can be seen that the beneficial tangential motion in the case $\theta = 0$ leads to significantly smaller errors compared to $\theta = 1$.

In the next experiment for Willmore flow with $\overline{\varkappa} = -2$, we start with a tube of total dimension $6 \times 2 \times 2$. Here $K = 898$, $J = 1792$ and $\tau = 10^{-3}$, as in Barrett *et al.* (2008b, Fig. 19). See Figure 9 for the results for the scheme (4.2a–d). We can see that the tube evolves towards a dumbbell consisting of two "spheres" with radius close to unity.

For volume preserving Willmore flow with $\overline{\varkappa} = -3$, we start with a cigar-like shape that has a smaller radius on the right hand side. Here $K = 898$, $J = 1792$ and $\tau = 10^{-3}$,

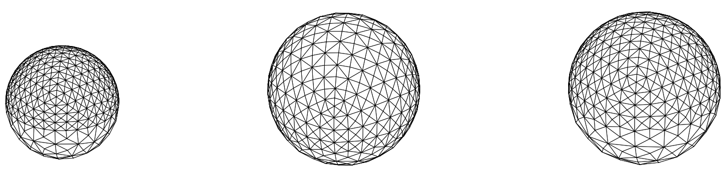

Figure 8: Triangulations of the unit sphere with $K = 490$ at time $t = 0$ (left) and at time $T = 1$ for $\theta = 0$ (middle) and $\theta = 1$ (right).

		$\theta = 0$		$\theta = 1$	
K	h_{Γ^0}	$\|\Gamma - \Gamma^h\|_{L^\infty}$	EOC	$\|\Gamma - \Gamma^h\|_{L^\infty}$	EOC
126	7.6537e-01	4.0847e-02	–	1.1230e-01	–
490	4.0994e-01	1.1435e-02	2.039173	3.6676e-02	1.792350
1938	2.0854e-01	3.0834e-03	1.939170	1.0548e-02	1.843798
7714	1.0472e-01	9.5399e-04	1.703057	2.9791e-03	1.835424

Table 1: Errors for the convergence test for the scheme (4.2a–d) with $\overline{\varkappa} = -1$ and $\beta = 0$.

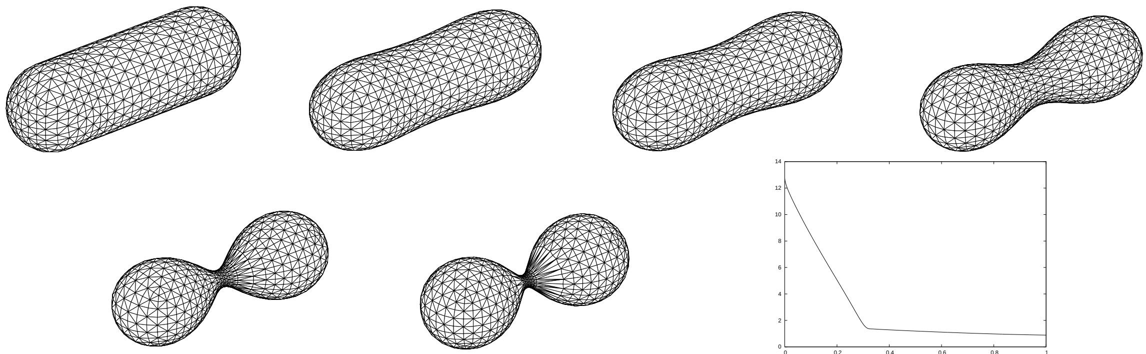

Figure 9: ($\theta = 0$) Willmore flow with $\overline{\varkappa} = -2$ for a tube. A plot of Γ^m at times $t = 0,\ 0.05,\ 0.1,\ 0.25,\ 0.5,\ 1$. On the right a plot of the discrete free energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec{\kappa}^{m+1})$.

as in Barrett *et al.* (2008b, Fig. 20). The observed relative volume loss was -0.16%. See Figure 10 for the results for the scheme (4.2a–d), where we note that part of the surface is about to pinch off.

The same experiment without volume preservation is shown in Figure 11. Here we observe that the final shape is noticeably different from the reported final shape in Barrett *et al.* (2008b, Fig. 21). However, on using finer discretization parameters for the scheme (4.2a–d), we do obtain an evolution towards three touching spheres, as in Barrett *et al.* (2008b, Fig. 21). See Figure 12, where we show the numerical results for a simulation with $K = 3586$, $J = 7168$ and $\tau = 10^{-4}$.

For Helfrich flow with $\overline{\varkappa} = -2$, we start with a disc shape of total dimension $5 \times 5 \times 1$. Here $K = 4482$, $J = 8960$ and $\tau = 10^{-4}$, which is finer than the parameters in Barrett *et al.* (2008b, Fig. 22). Here the observed relative area and volume loss was 0.23% and

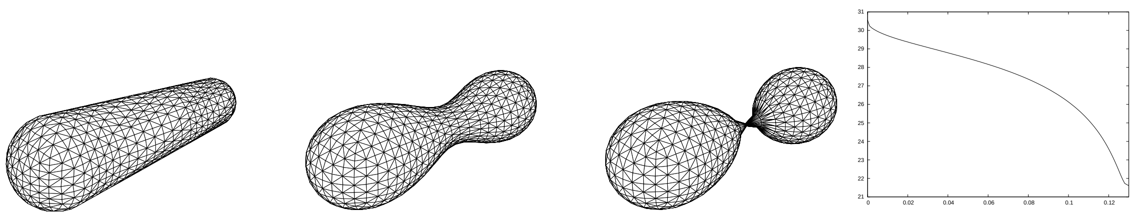

Figure 10: ($\theta = 0$) Volume preserving Willmore flow with $\overline{\varkappa} = -3$ for a stretched tube. A plot of Γ^m at times $t = 0,\ 0.1,\ 0.13$. On the right a plot of the discrete free energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec{\kappa}^{m+1})$.

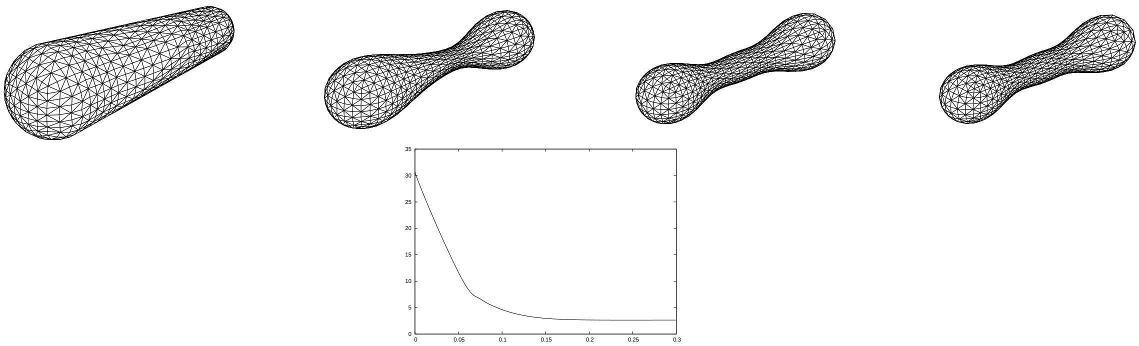

Figure 11: ($\theta = 0$) Willmore flow with $\overline{\varkappa} = -3$ for a stretched tube. A plot of Γ^m at times $t = 0,\ 0.1,\ 0.2,\ 0.3$. Below a plot of the discrete free energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec{\kappa}^{m+1})$.

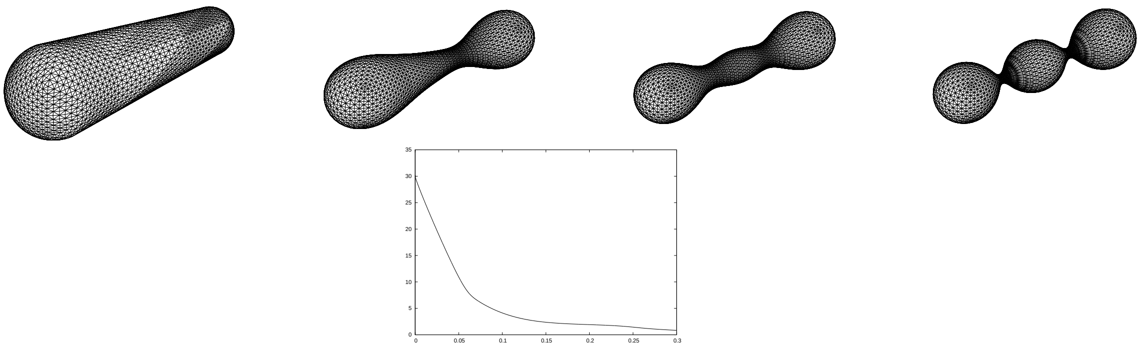

Figure 12: ($\theta = 0$) Willmore flow with $\overline{\varkappa} = -3$ for a stretched tube. A plot of Γ^m at times $t = 0,\ 0.1,\ 0.2,\ 0.3$. Below a plot of the discrete free energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec{\kappa}^{m+1})$.

-0.002%, respectively. See Figure 13 for the results for the scheme (4.2a–d).

For Helfrich flow with $\overline{\varkappa} = -2$, we start with a surface that is based on a $5 \times 5 \times \frac{3}{4}$ ellipsoid, where the "radius" varies continuously between 1 ± 0.05. Here $K = 2314$, $J = 4624$ and $\tau = 10^{-3}$, as in Barrett *et al.* (2008b, Fig. 23). The relative loss of area and volume in this experiment was 0.65% and 0.03%. See Figure 14 for the results for the scheme (4.2a–d).

6.4 Numerical results with ADE effects

We start with the same initial surface as in Figure 14 for Willmore flow with $\beta = 0.1$ and $M_0 = -150$. Here $K = 2314$, $J = 4624$ and $\tau = 10^{-3}$. See Figure 15 for the results for the scheme (4.2a–d).

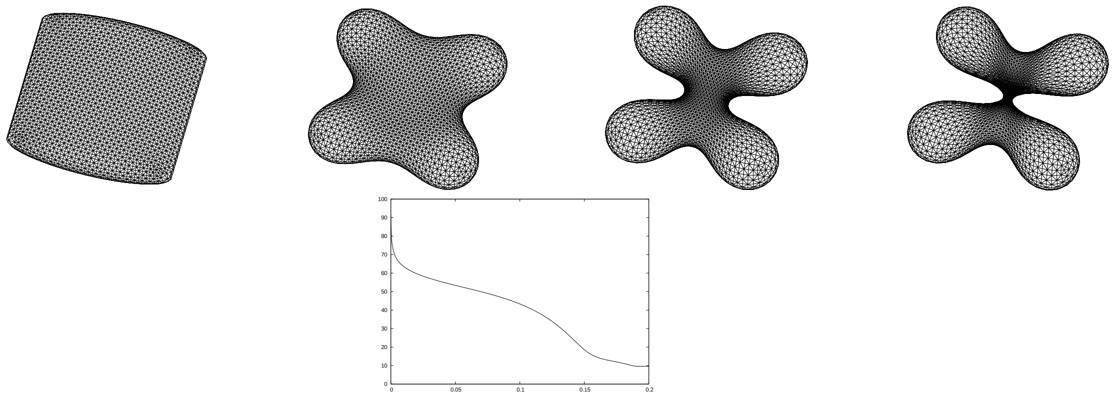

Figure 13: ($\theta = 0$) Helfrich flow with $\overline{\varkappa} = -2$ for a stretched tube. A plot of Γ^m at times $t = 0,\ 0.1,\ 0.15,\ 0.2$. Below a plot of the discrete free energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec{\kappa}^{m+1})$.

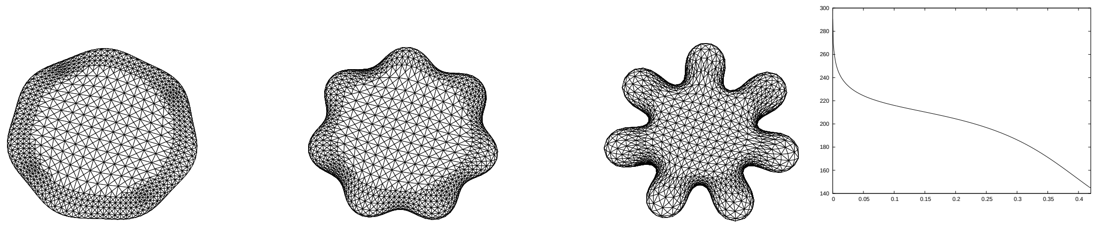

Figure 14: ($\theta = 0$) Helfrich flow with $\overline{\varkappa} = -2$. A plot of Γ^m at times $t = 0,\ 0.2,\ 0.42$. On the right a plot of the discrete free energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec{\kappa}^{m+1})$.

6.5 Numerical results for higher genus surfaces

For higher genus experiments it turns out that some form of mesh smoothing is required in practice in order to complete the simulations. This is similarly to the higher genus numerical experiments in Barrett *et al.* (2008b).

We start with a figure eight surface made up of unit cubes. Here $K = 2494$, $J = 4992$ and $\tau = 2\times 10^{-4}$, as in Barrett *et al.* (2008b, Fig. 9). Note also that we use the same mesh redistribution strategy after every time step as in Barrett *et al.* (2008b, Fig. 9). That is, after each time step we simultaneously move all the mesh points tangentially towards the average of their neighbouring vertices. In particular, we seek $\vec{X}^{m+1} \in \underline{V}^h(\Gamma^m)$ such that

$$\left\langle \vec{X}^{m+1} - \vec{\mathrm{id}}, \chi\, \vec{\nu}^m \right\rangle^h_{\Gamma^m} = 0, \qquad \forall\ \chi \in W^h(\Gamma^m), \tag{6.3a}$$

$$\left\langle \vec{X}^{m+1} - \vec{\mathrm{id}}, \chi\, \vec{\tau}^m_i \right\rangle^h_{\Gamma^m} = \left\langle \vec{z}^m - \vec{\mathrm{id}}, \chi\, \vec{\tau}^m_i \right\rangle^h_m \qquad \forall\ \chi \in V(\Gamma^m)\ ,\ i = 1 \to 2\,, \tag{6.3b}$$

where $\vec{z}^m(\vec{q}^m_k)$ is the average of the neighbouring nodes of $\vec{q}^m_k$, and where, on each element, $\{\vec{\nu}^m, \vec{\tau}^m_1, \vec{\tau}^m_2\}$ form an ONB of $\mathbb{R}^3$. See Figure 16 for the results for the scheme (4.2a–d).

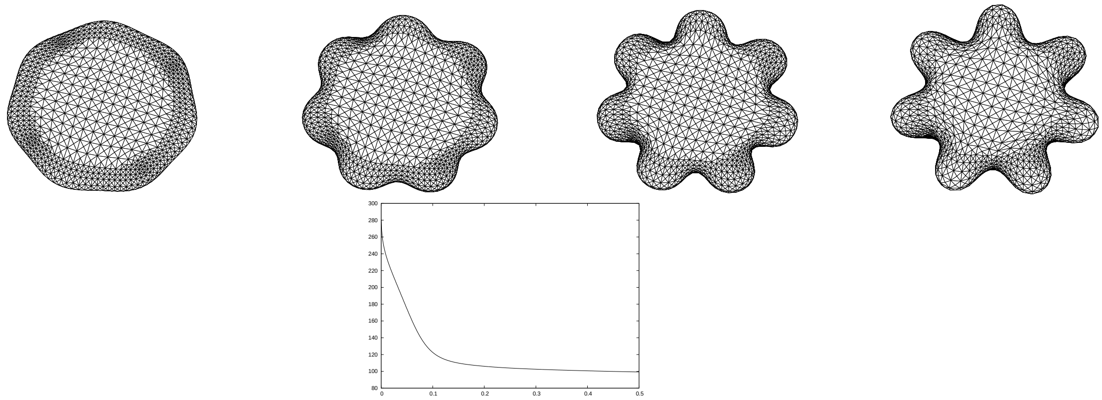

Figure 15: ($\theta = 0$) Willmore flow with $\beta = 0.1$ and $M_0 = -150$. A plot of Γ^m at times $t = 0,\ 0.05,\ 0.1,\ 0.5$. Below a plot of the discrete free energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec{\kappa}^{m+1})$.

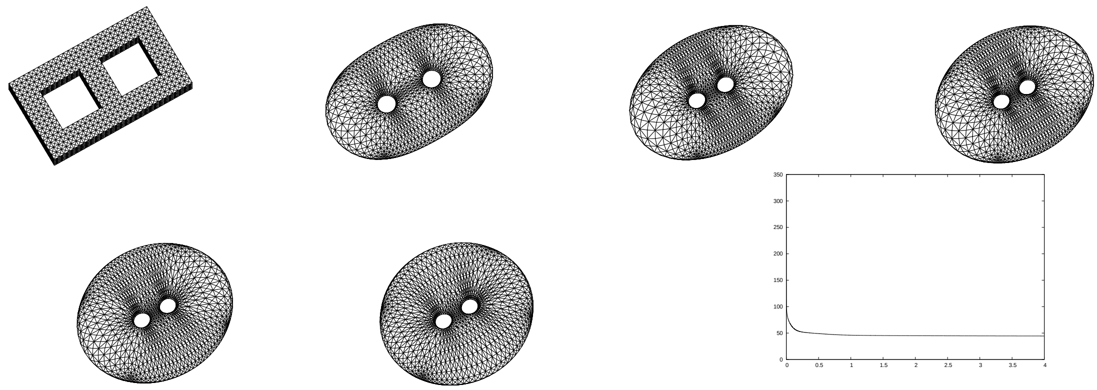

Figure 16: ($\theta = 0$) Willmore flow for a genus 2 surface. A plot of Γ^m at times $t = 0,\ 0.5,\ 1,\ 2,\ 3,\ 4$. On the right a plot of the discrete energy $E^{m+1}_{\overline{\varkappa},\beta}(\Gamma^m, \vec{\kappa}^{m+1})$.

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