

Parametric finite element approximations of curvature driven interface evolutions

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Abstract

Parametric finite elements lead to very efficient numerical methods for surface evolution equations. We introduce several computational techniques for curvature driven evolution equations based on a weak formulation for the mean curvature. The approaches discussed, in contrast to many other methods, have good mesh properties that avoid mesh coalescence and very non-uniform meshes. Mean curvature flow, surface diffusion, anisotropic geometric flows, solidification, two-phase flow, Willmore and Helfrich flow as well as biomembranes are treated. We show stability results as well as results explaining the good mesh properties.

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1 Introduction

Interfaces separating different regions in space frequently appear in the natural and imaging sciences as well as in mathematics. In many situations these interfaces evolve in time

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and the evolution laws contain curvature quantities. Often an interface carries a surface energy and in the simplest case the surface energy is given by the total surface area of the interface. Frequently the surface energy decreases in time and as the negative mean curvature is the first variation of the surface area, the mean curvature naturally appears in the context of evolving interfaces. In the simplest such situation the evolution of the interface is the L^2 -gradient flow of the surface area. This leads to mean curvature flow, which will play a prominent role in this work. Many recent applications involve surface energies, which contain surface integrals of curvature quantities. An example is the Willmore functional, which is the integrated squared mean curvature. Evolution problems for surfaces involving the first variation of the Willmore functional are particularly challenging and will also be discussed in this work.

Often however, the evolution of the interface is given by laws which couple quantities on the interface to quantities which are solutions of partial differential equations in the bulk, i.e., in the surrounding regions. This happens for example in solidification phenomena in which the temperature, which solves a diffusion equation in the liquid and solid phases, influences the evolution of the interface. Other examples are interfaces driven by a flow field, which is for example the solution of a Stokes or Navier–Stokes system. These situations are much more involved and lead to challenging problems in analysis and computation.

This work deals with parametric finite element methods for evolving interfaces. We first present the main ideas for simple geometric evolution equations like the mean curvature flow. We will then couple equations on the interface to bulk equations using an unfitted finite element method, which uses a surface mesh that is independent from the bulk mesh. As examples, solidification phenomena and problems arising in two-phase fluid flow will be discussed. Upon introducing ideas on the approximation of the Willmore energy and the associated Willmore flow, we end this work with a discussion of the numerical approximation of evolution problems for biomembranes. For other numerical approaches for geometric partial differential equations, like level set methods, phase field methods and other front tracking methods, we refer to the contributions Bänsch and Schmidt (2019); Bartels (2019); Bonito et al. (2019); Du and Feng (2019); Sethian (2019); Turek (2019) in *Handbook of Numerical Analysis, Vol. XXI & XXII.*, and also to the review article Deckelnick et al. (2005a).

2 Geometry of surfaces

In this section we review basic facts about surfaces, which will be necessary later on, when we develop numerical algorithms for curvature driven flows of hypersurfaces. We will define surfaces, differential operators on surfaces, important curvature quantities as well as a divergence theorem on hypersurfaces. For a more detailed discussion of these themes we refer to do Carmo (1976); Deckelnick et al. (2005a); Kühnel (2015); Walker (2015). Readers familiar with these concepts may skip this section.

2.1 Surfaces in $\mathbb{R}^d$

We will first define the term surface. Here, and throughout, let $d \geq 2$.

Definition 2.1.

- (i) A subset $\Gamma \subset \mathbb{R}^d$ is called an n -dimensional C^k -surface, for $0 \leq n \leq d$ and $k \geq 1$, if for every point $\vec{p} \in \Gamma$ there exists an open neighbourhood $V \subset \mathbb{R}^d$ of $\vec{p}$ and a bijective C^k -map $\vec{\mathfrak{X}} : U \rightarrow V \cap \Gamma$, with $U \subset \mathbb{R}^n$ open and connected, such that the Jacobian $\nabla \vec{\mathfrak{X}} = (\partial_1 \vec{\mathfrak{X}}, \dots, \partial_n \vec{\mathfrak{X}}) : U \rightarrow \mathbb{R}^{d \times n}$ of $\vec{\mathfrak{X}}$ has full rank in U .
- (ii) The map $\vec{\mathfrak{X}}$ is called a local parameterization of Γ .
- (iii) If $n = d - 1$, then we call Γ a hypersurface.

We now define what we mean by a mapping defined on a hypersurface being differentiable.

Definition 2.2. Let $\Gamma \subset \mathbb{R}^d$ be an n -dimensional C^k -surface. A function $f : \Gamma \rightarrow \mathbb{R}$ is a C^k -function, denoted by $f \in C^k(\Gamma)$, if $f \circ \vec{\mathfrak{X}} : U \rightarrow \mathbb{R}$ is of class C^k for all C^k -parameterizations $\vec{\mathfrak{X}} : U \rightarrow \Gamma$.

With the help of a local parameterization we can define a basis of the tangent space.

Definition 2.3. Let Γ be an n -dimensional C^1 -surface with a local parameterization $\vec{\mathfrak{X}} : U \rightarrow \mathbb{R}^d$. For $\vec{p} \in \Gamma$ let $\vec{u} \in U$ be such that $\vec{p} = \vec{\mathfrak{X}}(\vec{u})$. The vectors

$$\vec{\partial}_1 = (\partial_1 \vec{\mathfrak{X}})(\vec{u}), \dots, \vec{\partial}_n = (\partial_n \vec{\mathfrak{X}})(\vec{u})$$

are linearly independent and span an n -dimensional space, which is called the tangent space and will be denoted by

$$T_{\vec{p}}\Gamma = \text{span}\{\vec{\partial}_1, \dots, \vec{\partial}_n\}.$$

Its orthogonal complement $N_{\vec{p}}\Gamma = (T_{\vec{p}}\Gamma)^\perp$ in $\mathbb{R}^d$ is called the normal space of Γ at $\vec{p}$.

Mainly oriented hypersurfaces will be of interest, which we define next.

Definition 2.4. A hypersurface Γ is called orientable, if a continuous normal vector field $\vec{\nu} : \Gamma \rightarrow \mathbb{S}^{d-1}$, with $\vec{\nu}(\vec{p}) \in N_{\vec{p}}\Gamma$ for all $\vec{p} \in \Gamma$, exists, where $\mathbb{S}^{d-1}$ is the $(d-1)$ -dimensional sphere in $\mathbb{R}^d$.

We will frequently use the following differential operators on a surface Γ .

Definition 2.5. Let $\Gamma \subset \mathbb{R}^d$ be an n -dimensional C^1 -surface, and let $f : \Gamma \rightarrow \mathbb{R}$, $\vec{f} : \Gamma \rightarrow \mathbb{R}^d$ be C^1 -functions.

(i) For $\vec{p} \in \Gamma$ and $\vec{\tau} \in T_{\vec{p}}\Gamma$ we define the directional derivative as

$$(\partial_{\vec{\tau}} f)(\vec{p}) = \lim_{\varepsilon \rightarrow 0} \frac{f(\vec{y}(\varepsilon)) - f(\vec{y}(0))}{\varepsilon} = (f \circ \vec{y})'(0),$$

where $\vec{y}: (-1, 1) \rightarrow \Gamma$ parameterizes a curve on Γ with $\vec{y}(0) = \vec{p}$ and $\vec{y}'(0) = \vec{\tau}$.

(ii) The surface gradient of f on Γ at the point $\vec{p} \in \Gamma$ is defined as

$$(\nabla_s f)(\vec{p}) = \sum_{i=1}^n (\partial_{\vec{\tau}_i} f)(\vec{p}) \vec{\tau}_i,$$

where $\{\vec{\tau}_1, \dots, \vec{\tau}_n\}$ is an orthonormal basis of $T_{\vec{p}}\Gamma$.

(iii) The surface divergence of $\vec{f}$ at the point $\vec{p} \in \Gamma$ is defined as

$$(\nabla_s \cdot \vec{f})(\vec{p}) = \sum_{i=1}^n \vec{\tau}_i \cdot (\partial_{\vec{\tau}_i} \vec{f})(\vec{p}),$$

where $\{\vec{\tau}_1, \dots, \vec{\tau}_n\}$ is again an orthonormal basis of $T_{\vec{p}}\Gamma$.

(iv) The surface Jacobian of $\vec{f}$ at the point $\vec{p} \in \Gamma$ is defined as

$$(\nabla_s \vec{f})(\vec{p}) = \sum_{i=1}^n (\partial_{\vec{\tau}_i} \vec{f})(\vec{p}) \otimes \vec{\tau}_i,$$

where $\{\vec{\tau}_1, \dots, \vec{\tau}_n\}$ is again an orthonormal basis of $T_{\vec{p}}\Gamma$.

(v) If Γ is a C^2 -surface, and $f \in C^2(\Gamma)$, then we define the Laplace–Beltrami operator and the surface Hessian of f on Γ as

$$\Delta_s f = \nabla_s \cdot (\nabla_s f) \quad \text{and} \quad \nabla_s^2 f = \nabla_s (\nabla_s f),$$

respectively.

(vi) The Laplace–Beltrami operator of $\vec{f} \in [C^2(\Gamma)]^d$, for a C^2 -surface Γ , is defined component-wise, i.e. $(\Delta_s \vec{f}) \cdot \vec{e}_i = \Delta_s (\vec{f} \cdot \vec{e}_i)$, $i = 1, \dots, d$. Here, and throughout, we let $\vec{e}_i$ denote the i -th standard basis vector in $\mathbb{R}^d$.

(vii) We define the generalized symmetrized surface Jacobian

$$\underline{D}_s(\vec{f}) = \frac{1}{2} \underline{P}_\Gamma (\nabla_s \vec{f} + (\nabla_s \vec{f})^\top) \underline{P}_\Gamma \quad \text{on } \Gamma,$$

where $\underline{P}_\Gamma$ is the orthogonal projection onto the tangent space of Γ . I.e.

$$\underline{P}_\Gamma(\vec{p}) = \sum_{i=1}^n \vec{\tau}_i \otimes \vec{\tau}_i \tag{2.1}$$

for an orthonormal basis $\{\vec{\tau}_1, \dots, \vec{\tau}_n\}$ of $T_{\vec{p}}\Gamma$.

- (viii) The surface divergence of a tensor $\underline{f} \in [C^1(\Gamma)]^{d \times d}$ is defined via $(\nabla_s \cdot \underline{f}) \cdot \vec{e}_i = \nabla_s \cdot (\underline{f}^\top \vec{e}_i)$ on Γ , for $i = 1, \dots, d$.

Remark 2.6.

- (i) It is easy to check that Definition 2.5(i) does not depend on the choice of the parameterization $\vec{y}$. Parameterizations $\vec{y}$ of curves, as 1-dimensional surfaces, are always assumed to be regular in the sense that $\vec{y}$ is continuously differentiable and such that $\vec{y}' \neq \vec{0}$ holds everywhere, recall Definition 2.1. A curve is an equivalence class of regular parameterizations, see e.g. Kühnel (2015, p. 8), where the equivalence relation is given by parameter transformations. For simplicity, from now on, we will often also call a parameterization $\vec{y}$ a curve.
- (ii) It is easy to check that Definitions 2.5(ii), 2.5(iii) and 2.5(iv) do not depend on the choice of the orthonormal basis of $T_{\vec{p}}\Gamma$.
- (iii) For $\vec{p} \in \Gamma$ it holds that

$$\begin{aligned} (\nabla_s \vec{f})(\vec{p}) \vec{\tau} &= (\partial_{\vec{\tau}} \vec{f})(\vec{p}) \quad \forall \vec{\tau} \in T_{\vec{p}}\Gamma \\ \text{and } (\nabla_s \vec{f})(\vec{p}) \vec{v} &= \vec{0} \quad \forall \vec{v} \in N_{\vec{p}}\Gamma. \end{aligned}$$

Moreover, it holds that the i -th row of $\nabla_s \vec{f}$ is the surface gradient of the i -th component of $\vec{f}$, i.e. $(\nabla_s \vec{f})^\top \vec{e}_i = \nabla_s (\vec{f} \cdot \vec{e}_i)$, $i = 1, \dots, d$.

- (iv) We remark that the second projection $\underline{P}_\Gamma$ in Definition 2.5(vii) ensures that

$$(\underline{D}_s(\vec{f}))(\vec{p}) \vec{v} = \vec{0} \quad \forall \vec{v} \in N_{\vec{p}}\Gamma, \vec{p} \in \Gamma,$$

similarly to (iii). The first projection then ensures that $(\underline{D}_s(\vec{f}))(\vec{p})$ is symmetric.

- (v) It follows directly from Definitions 2.5(ii), 2.5(iv) and (2.1) that

$$\nabla_s f = \underline{P}_\Gamma \nabla_s f \quad \text{and} \quad \nabla_s \vec{f} = (\nabla_s \vec{f}) \underline{P}_\Gamma \quad \text{on } \Gamma.$$

- (vi) We observe that if Γ is a hypersurface, then

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

with $\vec{\nu}(p)$ denoting a unit vector in $N_{\vec{p}}\Gamma$ for $\vec{p} \in \Gamma$.

The following product rules and identities hold.

Lemma 2.7. Let $\Gamma \subset \mathbb{R}^d$ be an n -dimensional C^1 -surface, and let $f : \Gamma \rightarrow \mathbb{R}$, $\vec{f}, \vec{g} : \Gamma \rightarrow \mathbb{R}^d$ and $\underline{f} : \Gamma \rightarrow \mathbb{R}^{d \times d}$ be C^1 -functions. Then it holds:

- (i)

$$\nabla_s \cdot (f \vec{g}) = \vec{g} \cdot \nabla_s f + f \nabla_s \cdot \vec{g} \quad \text{on } \Gamma,$$

(ii)

$$\nabla_s (\vec{f} \cdot \vec{g}) = (\nabla_s \vec{f})^\top \vec{g} + (\nabla_s \vec{g})^\top \vec{f} \quad \text{on } \Gamma,$$

(iii)

$$\nabla_s (f \vec{g}) = \vec{g} \otimes \nabla_s f + f \nabla_s \vec{g} \quad \text{on } \Gamma,$$

(iv)

$$\nabla_s \cdot (\underline{f}^\top \vec{g}) = \vec{g} \cdot (\nabla_s \cdot \underline{f}) + \underline{f} : \nabla_s \vec{g} \quad \text{on } \Gamma,$$

(v) and

$$\text{tr}(\nabla_s \vec{f}) = \nabla_s \cdot \vec{f} \quad \text{on } \Gamma.$$

Proof. (i)–(iv) are direct analogues of their flat counterparts, and follow easily from Definition 2.5.

(v) Using the fact that the trace is invariant under basis changes, we obtain from Remark 2.6(iii) and Definition 2.5(iii) that for $\vec{p} \in \Gamma$

$$\text{tr} \left((\nabla_s \vec{f})(\vec{p}) \right) = \sum_{i=1}^n \vec{\tau}_i \cdot (\nabla_s \vec{f})(\vec{p}) \vec{\tau}_i = \sum_{i=1}^n \vec{\tau}_i \cdot (\partial_{\vec{\tau}_i} \vec{f})(\vec{p}) = (\nabla_s \cdot \vec{f})(\vec{p}),$$

where $\{\vec{\tau}_1, \dots, \vec{\tau}_n\}$ is an orthonormal basis of $T_{\vec{p}}\Gamma$. □

It is often convenient to consider alternative representations of the differential operators introduced in Definition 2.5.

Remark 2.8.

(i) For a local parameterization $\vec{\mathfrak{X}} : U \rightarrow \Gamma$ one can define the first fundamental form, or metric tensor, $(g_{ij})_{i,j=1,\dots,n}$ as

$$g_{ij} = \vec{\partial}_i \cdot \vec{\partial}_j = \partial_i \vec{\mathfrak{X}} \cdot \partial_j \vec{\mathfrak{X}},$$

and a little linear algebra shows that

$$(\nabla_s f) \circ \vec{\mathfrak{X}} = \sum_{i,j=1}^n g^{ij} \partial_i (f \circ \vec{\mathfrak{X}}) \vec{\partial}_j \quad \text{in } U,$$

$$(\nabla_s \cdot \vec{f}) \circ \vec{\mathfrak{X}} = \sum_{i,j=1}^n g^{ij} \partial_i (\vec{f} \circ \vec{\mathfrak{X}}) \cdot \vec{\partial}_j \quad \text{in } U,$$

where $(g^{ij})_{i,j=1,\dots,n}$ is the inverse of $(g_{ij})_{i,j=1,\dots,n}$. Moreover, it holds that

$$(\Delta_s f) \circ \vec{\mathfrak{X}} = \frac{1}{\sqrt{g}} \sum_{i,j=1}^n \partial_i (\sqrt{g} g^{ij} \partial_j (f \circ \vec{\mathfrak{X}})) \quad \text{in } U,$$

where

$$g = \det((g_{ij})_{i,j=1,\dots,n}) \tag{2.2}$$

is the square of the local area element, see Amann and Escher (2009, §XI.6).

- (ii) Denoting by $\nabla_s = (\partial_{s_1}, \dots, \partial_{s_d})^\top$ the surface gradient on Γ , it holds that $\nabla_s \cdot \vec{f} = \sum_{i=1}^d \partial_{s_i} (\vec{f} \cdot \vec{e}_i)$, $\nabla_s \vec{f} = (\partial_{s_j} \vec{f} \cdot \vec{e}_i)_{i,j=1}^d$ and $\nabla_s^2 f = (\partial_{s_j} \partial_{s_i} f)_{i,j=1}^d$. Moreover, it follows from Lemma 2.7(v) that the Laplace–Beltrami operator satisfies $\Delta_s = \sum_{i=1}^d \partial_{s_i}^2$.
- (iii) If Γ is an orientable hypersurface with normal vector field $\vec{\nu}$, we obtain for an extension of the functions f and $\vec{f}$ to an open neighbourhood of Γ the formulas

$$\nabla_s f = \nabla f - (\nabla f \cdot \vec{\nu}) \vec{\nu} \quad \text{and} \quad \nabla_s \cdot \vec{f} = \nabla \cdot \vec{f} - ((\nabla \vec{f}) \cdot \vec{\nu}) \cdot \vec{\nu} \quad \text{on } \Gamma,$$

where ∇ and $\nabla \cdot$ are the gradient and the divergence in $\mathbb{R}^d$. These identities follow directly from Definition 2.5(ii),(iii) and the representation of ∇f and $\nabla \cdot \vec{f}$ with the help of an orthonormal basis.

Lemma 2.9. *Let Γ be a C^1 -hypersurface. Then the identity map id satisfies the following.*

(i)

$$\nabla_s \text{id} = \underline{P}_\Gamma \quad \text{on } \Gamma.$$

(ii) For $\vec{f} \in [C^1(\Gamma)]^d$ it holds that

$$\nabla_s \text{id} : \nabla_s \vec{f} = \nabla_s \cdot \vec{f} \quad \text{on } \Gamma,$$

where $\underline{A} : \underline{B} = \text{tr}(\underline{A}^\top \underline{B})$ denotes the Hilbert–Schmidt inner product for matrices $\underline{A}$ and $\underline{B}$.

(iii) If Γ is an orientable C^2 -surface with normal vector field $\vec{\nu}$, then

$$\Delta_s \text{id} = -(\nabla_s \cdot \vec{\nu}) \vec{\nu} \quad \text{on } \Gamma.$$

Proof. (i) The result follows from Definitions 2.5(iv), 2.5(i) and (2.1).

(ii) It follows from (i), Remark 2.6(iii) and Lemma 2.7(v) that $\nabla_s \text{id} : \nabla_s \vec{f} = \text{tr}(\nabla_s \vec{f}) = \nabla_s \cdot \vec{f}$.

(iii) Using Remark 2.8(iii), and on recalling Definition 2.5(vi),(v), we compute for $i = 1, \dots, d$

$$\begin{aligned} (\Delta_s \text{id}) \cdot \vec{e}_i &= \Delta_s (\text{id} \cdot \vec{e}_i) = \nabla_s \cdot [\nabla_s (\text{id} \cdot \vec{e}_i)] = \nabla_s \cdot [\vec{e}_i - (\vec{e}_i \cdot \vec{\nu}) \vec{\nu}] \\ &= -\nabla_s \cdot [(\vec{\nu} \cdot \vec{e}_i) \vec{\nu}] = -(\vec{\nu} \cdot \vec{e}_i) \nabla_s \cdot \vec{\nu} \quad \text{on } \Gamma, \end{aligned}$$

where we have noted that $\nabla_s (\vec{\nu} \cdot \vec{e}_i)$ is orthogonal to $\vec{\nu}$. □

2.2 Curvature

We now define the fundamental curvature quantities needed in the subsequent sections.

Definition 2.10. *Let Γ be an orientable C^2 -hypersurface with normal vector field $\vec{\nu}$.*

(i) The Weingarten map at $\vec{p} \in \Gamma$ is defined through

$$W_{\vec{p}} : T_{\vec{p}}\Gamma \rightarrow T_{\vec{p}}\Gamma, \quad W_{\vec{p}}(\vec{\tau}) = -(\partial_{\vec{\tau}} \vec{\nu})(\vec{p}).$$

(ii) The corresponding bilinear form is called the second fundamental form and is given by

$$\mathbb{I}_{\vec{p}}(\vec{\tau}_1, \vec{\tau}_2) = W_{\vec{p}}(\vec{\tau}_1) \cdot \vec{\tau}_2 = -(\partial_{\vec{\tau}_1} \vec{\nu})(\vec{p}) \cdot \vec{\tau}_2$$

for all $\vec{\tau}_1, \vec{\tau}_2 \in T_{\vec{p}}\Gamma$, $\vec{p} \in \Gamma$. It can be shown that $W_{\vec{p}}$ is self-adjoint, which implies that $\mathbb{I}_{\vec{p}}$ is symmetric, see e.g. Kühnel (2015, §3.9). Hence there exists an orthonormal basis $\{\vec{t}_1, \dots, \vec{t}_{d-1}\}$ of $T_{\vec{p}}\Gamma$, consisting of eigenvectors of $W_{\vec{p}}$ with corresponding eigenvalues $\kappa_1, \dots, \kappa_{d-1}$.

Definition 2.11.

(i) The eigenvalues $\kappa_1, \dots, \kappa_{d-1}$ of $W_{\vec{p}}$ are called the principal curvatures of Γ at $\vec{p}$.

(ii) The mean curvature κ of Γ at $\vec{p}$ is defined to be the trace of $W_{\vec{p}}$, i.e.

$$\kappa(\vec{p}) = \text{tr } W_{\vec{p}} = \kappa_1 + \dots + \kappa_{d-1}.$$

(iii) The mean curvature vector $\vec{\kappa}$ of Γ at $\vec{p}$ is defined as

$$\vec{\kappa}(\vec{p}) = \kappa(\vec{p}) \vec{\nu}(\vec{p}).$$

(iv) For $d = 3$ the Gaussian curvature $\mathcal{K}$ at $\vec{p}$ is the determinant of $W_{\vec{p}}$, i.e. the product of the principal curvatures. This means we set

$$\mathcal{K}(\vec{p}) = \det W_{\vec{p}} = \kappa_1 \kappa_2.$$

Lemma 2.12. Let Γ be an orientable C^2 -hypersurface with normal vector field $\vec{\nu}$. The Jacobian $(\nabla_s \vec{\nu})(\vec{p})$, for $\vec{p} \in \Gamma$, induces a self-adjoint linear map from $\mathbb{R}^d$ to $\mathbb{R}^d$ that collapses to $-W_{\vec{p}}$ on $T_{\vec{p}}\Gamma$ and that maps $N_{\vec{p}}\Gamma$ to zero. As a consequence, the following hold:

(i)

$$(\nabla_s \vec{\nu})^\top \vec{\nu} = (\nabla_s \vec{\nu}) \vec{\nu} = \vec{0} \quad \text{on } \Gamma,$$

(ii)

$$(\nabla_s \vec{\nu})^\top = \nabla_s \vec{\nu} \quad \text{on } \Gamma,$$

(iii)

$$\kappa = -\text{tr}(\nabla_s \vec{\nu}) \quad \text{on } \Gamma,$$

(iv) and

$$|\nabla_s \vec{\nu}|^2 = \nabla_s \vec{\nu} : \nabla_s \vec{\nu} = \kappa_1^2 + \dots + \kappa_{d-1}^2 \quad \text{on } \Gamma.$$

Proof. Let $\vec{p} \in \Gamma$. It follows from Remark 2.6(iii) and Definition 2.10 that $W_{\vec{p}}(\vec{\tau}) = -(\nabla_s \vec{\nu})(\vec{p}) \vec{\tau} = -((\nabla_s \vec{\nu})(\vec{p}))^\top \vec{\tau}$ for all $\vec{\tau} \in T_{\vec{p}}\Gamma$. Moreover, on denoting $\vec{\nu} = (\nu_1, \dots, \nu_d)^\top$, and on noting from Definition 2.5(iv) that the i -th column of $(\nabla_s \vec{\nu})^\top$ is $\nabla_s \nu_i$, we have that

$$(\nabla_s \vec{\nu})^\top \vec{\nu} = \sum_{i=1}^d \nu_i \nabla_s \nu_i = \frac{1}{2} \nabla_s |\vec{\nu}|^2 = 0.$$

Combining this with Remark 2.6(iii) yields that $(\nabla_s \vec{\nu})(\vec{p}) \vec{\nu} = ((\nabla_s \vec{\nu})(\vec{p}))^\top \vec{\nu} = \vec{0}$, and so the linear map induced by $(\nabla_s \vec{\nu})(\vec{p})$ is self-adjoint. This proves (i) and (ii). Furthermore, if $\{\vec{t}_1, \dots, \vec{t}_{d-1}\}$ is an orthonormal basis of $T_{\vec{p}}\Gamma$, consisting of eigenvectors of $W_{\vec{p}}$ with corresponding eigenvalues $\kappa_1, \dots, \kappa_{d-1}$, then $\{\vec{t}_1, \dots, \vec{t}_{d-1}, \vec{\nu}(\vec{p})\}$ is an orthonormal basis of $\mathbb{R}^d$, consisting of eigenvectors of $(\nabla_s \vec{\nu})(\vec{p})$ with corresponding eigenvalues $\kappa_1, \dots, \kappa_{d-1}, 0$. This implies (iii), on recalling Definition 2.11(ii), and (iv). $\square$

The next lemma shows that while the sign of the mean curvature κ depends on the choice of the unit normal $\vec{\nu}$, the mean curvature vector $\vec{\kappa}$ is an invariant under the change of the sign of the normal.

Lemma 2.13. *Let Γ be an orientable C^2 -hypersurface with normal vector field $\vec{\nu}$. The following formulas for the mean curvature and the mean curvature vector hold true.*

(i) *For the mean curvature it holds that*

$$\kappa = -\nabla_s \cdot \vec{\nu} \quad \text{on } \Gamma.$$

(ii) *For the mean curvature vector it holds that*

$$\vec{\kappa} = \kappa \vec{\nu} = \Delta_s \text{id} \quad \text{on } \Gamma.$$

Proof. (i) This follows from Lemma 2.12(iii) and Lemma 2.7(v).

(ii) The result follows directly from (i), Definition 2.11(iii) and Lemma 2.9(iii). $\square$

Lemma 2.14. *Let Γ be an orientable C^2 -hypersurface with normal vector field $\vec{\nu}$. Let $\vec{f} \in [C^1(\Gamma)]^d$ and set $\vec{f}_T = \underline{P}_\Gamma \vec{f}$ on Γ . Then it holds that*

(i)

$$\nabla_s \cdot \vec{f} = -(\vec{f} \cdot \vec{\nu}) \kappa + \nabla_s \cdot \vec{f}_T \quad \text{on } \Gamma,$$

(ii)

$$\nabla_s \vec{f} = (\vec{f} \cdot \vec{\nu}) \nabla_s \vec{\nu} + \vec{\nu} \otimes \nabla_s (\vec{f} \cdot \vec{\nu}) + \nabla_s \vec{f}_T \quad \text{on } \Gamma,$$

(iii)

$$\underline{D}_s(\vec{f}) = (\vec{f} \cdot \vec{\nu}) \nabla_s \vec{\nu} + \frac{1}{2} (\underline{P}_\Gamma \nabla_s \vec{f}_T + (\nabla_s \vec{f}_T)^\top \underline{P}_\Gamma) \quad \text{on } \Gamma.$$

Proof. (i) Using Lemma 2.7(i), Definition 2.5(ii) and Lemma 2.13(i), we compute that

$$\nabla_s \cdot \vec{f} = \nabla_s \cdot \left((\vec{f} \cdot \vec{\nu}) \vec{\nu} \right) + \nabla_s \cdot \vec{f}_T = (\vec{f} \cdot \vec{\nu}) \nabla_s \cdot \vec{\nu} + \nabla_s \cdot \vec{f}_T = -(\vec{f} \cdot \vec{\nu}) \kappa + \nabla_s \cdot \vec{f}_T.$$

(ii) Similarly, it follows from Lemma 2.7(iii) that

$$\nabla_s \vec{f} = \nabla_s \left((\vec{f} \cdot \vec{\nu}) \vec{\nu} \right) + \nabla_s \vec{f}_T = (\vec{f} \cdot \vec{\nu}) \nabla_s \vec{\nu} + \vec{\nu} \otimes \nabla_s (\vec{f} \cdot \vec{\nu}) + \nabla_s \vec{f}_T.$$

(iii) The desired result follows immediately from (ii), Definitions 2.5(iv), 2.5(vii) and the fact that $\nabla_s \vec{\nu}$ is a symmetric mapping that maps tangent vectors to tangent vectors, recall Lemma 2.12. $\square$

In the derivation of some relevant formulas it is sometimes helpful to be able to extend functions defined on a hypersurface Γ to a neighbourhood of Γ . This then frequently allows us to use the calculus in $\mathbb{R}^d$ to compute for quantities on the surface, recall Remark 2.8(iii). Let $\Gamma \subset \mathbb{R}^d$ be a compact orientable C^2 -hypersurface without boundary and with normal vector field $\vec{\nu}$. For $\delta > 0$ we define a tubular neighbourhood

$$\mathcal{N}_\delta = \{ \vec{z} \in \mathbb{R}^d : \vec{z} = \vec{p} + \eta \vec{\nu}(\vec{p}), \vec{p} \in \Gamma, |\eta| < \delta \}$$

of Γ . In Gilbarg and Trudinger (1983, Appendix 14.6) it is shown that there is a bijective relation between $\vec{z} \in \mathcal{N}_\delta$ and $(\vec{p}, \eta) \in \Gamma \times (-\delta, \delta)$, provided that δ is small enough. We can hence define the functions $\vec{\Pi}_\Gamma(\vec{z}) = \vec{p}$ and $d_\Gamma(\vec{z}) = \eta$, and it turns out that $|d_\Gamma(\vec{z})|$ is the distance of $\vec{z}$ to Γ , where $d_\Gamma(\vec{z})$ is positive if $\vec{z}$ lies on the side towards which $\vec{\nu}$ is pointing, and negative otherwise. We call d_Γ the signed distance function to Γ , and $\vec{\Pi}_\Gamma(\vec{z})$ is the projection of $\vec{z}$ onto Γ , i.e.

$$\vec{\Pi}_\Gamma(\vec{z}) = \arg \min_{\vec{y} \in \Gamma} |\vec{y} - \vec{z}|.$$

For later use, we recall from Gilbarg and Trudinger (1983, Appendix 14.6) that, for δ sufficiently small,

$$d_\Gamma \in C^2(\mathcal{N}_\delta). \quad (2.3a)$$

It also holds that

$$\nabla d_\Gamma = \vec{\nu} \circ \vec{\Pi}_\Gamma \quad \Rightarrow \quad |\nabla d_\Gamma| = 1 \quad \text{in } \mathcal{N}_\delta, \quad (2.3b)$$

which can be shown as follows. It clearly holds that

$$\text{id} = \vec{\Pi}_\Gamma + d_\Gamma \vec{\nu} \circ \vec{\Pi}_\Gamma \quad \text{and} \quad d_\Gamma = \left(\text{id} - \vec{\Pi}_\Gamma \right) \cdot \left(\vec{\nu} \circ \vec{\Pi}_\Gamma \right) \quad \text{in } \mathcal{N}_\delta.$$

Differentiating the second identity, and observing the first, yields for $k = 1, \dots, d$

$$\begin{aligned} \partial_k d_\Gamma &= \left(\vec{e}_k - \partial_k \vec{\Pi}_\Gamma \right) \cdot \left(\vec{\nu} \circ \vec{\Pi}_\Gamma \right) - \left(\text{id} - \vec{\Pi}_\Gamma \right) \cdot \partial_k \left(\vec{\nu} \circ \vec{\Pi}_\Gamma \right) \\ &= \vec{e}_k \cdot \vec{\nu} \circ \vec{\Pi}_\Gamma - d_\Gamma \left(\vec{\nu} \circ \vec{\Pi}_\Gamma \right) \cdot \partial_k \left(\vec{\nu} \circ \vec{\Pi}_\Gamma \right) \\ &= \vec{e}_k \cdot \vec{\nu} \circ \vec{\Pi}_\Gamma - d_\Gamma \frac{1}{2} \partial_k \left| \vec{\nu} \circ \vec{\Pi}_\Gamma \right|^2 = \vec{e}_k \cdot \vec{\nu} \circ \vec{\Pi}_\Gamma \quad \text{in } \mathcal{N}_\delta, \end{aligned}$$

where we have noted that $\partial_k \vec{\Pi}_\Gamma$ is tangential in $\mathcal{N}_\delta$. This proves (2.3b).

We now extend a function f defined on Γ to $\mathcal{N}_\delta$, for δ sufficiently small, via

$$f = f \circ \vec{\Pi}_\Gamma \quad \text{in } \mathcal{N}_\delta. \quad (2.4)$$

This means that we extend f constantly in the normal direction, and so we obtain from Remark 2.8(iii) that

$$\nabla f \cdot \vec{\nu} = 0, \quad \text{and hence} \quad \nabla f = \nabla_s f \quad \text{on } \Gamma. \quad (2.5)$$

In the flat case the Schwarz theorem yields that the Hessian is symmetric. In the curved case, however, this is no longer the case. In fact, the following result holds.

Lemma 2.15. *Let Γ be an orientable C^2 -hypersurface with normal vector field $\vec{\nu}$, and let $f \in C^2(\Gamma)$. For the surface Hessian it holds that*

$$\nabla_s^2 f - (\nabla_s^2 f)^\top = [(\nabla_s \vec{\nu}) \nabla_s f] \otimes \vec{\nu} - \vec{\nu} \otimes [(\nabla_s \vec{\nu}) \nabla_s f] \quad \text{on } \Gamma.$$

Proof. Recalling from Remark 2.8(ii) the notation $\nabla_s = (\partial_{s_1}, \dots, \partial_{s_d})^\top$, and denoting $\vec{\nu} = (\nu_1, \dots, \nu_d)^\top$, the claim can be equivalently written as

$$\partial_{s_j} \partial_{s_i} f - \partial_{s_i} \partial_{s_j} f = [(\nabla_s \vec{\nu}) \nabla_s f]_i \nu_j - [(\nabla_s \vec{\nu}) \nabla_s f]_j \nu_i \quad \text{on } \Gamma, \quad (2.6)$$

for all $i, j \in \{1, \dots, d\}$. In order to prove this, we extend f to a neighbourhood of Γ as in (2.4). It follows from (2.5) that $\partial_{s_i}(\nabla f \cdot \vec{\nu}) = 0$ on Γ , and so we compute, using Remark 2.8(iii), for all $i, j = 1, \dots, d$ that

$$\partial_{s_i} \partial_{s_j} f = \partial_{s_i} (\partial_j f - (\nabla f \cdot \vec{\nu}) \nu_j) = \partial_{s_i} \partial_j f = \partial_i \partial_j f - (\nabla \partial_j f \cdot \vec{\nu}) \nu_i.$$

In addition we have, on using the Schwarz theorem and on extending $\vec{\nu}$ to the neighbourhood of Γ similarly to (2.4), and so (2.5) yields $\partial_j \vec{\nu} = \partial_{s_j} \vec{\nu}$, that

$$\begin{aligned} 0 &= \partial_{s_j} (\nabla f \cdot \vec{\nu}) = \partial_j (\nabla f \cdot \vec{\nu}) - (\nabla (\nabla f \cdot \vec{\nu}) \cdot \vec{\nu}) \nu_j \\ &= \nabla \partial_j f \cdot \vec{\nu} + \nabla f \cdot \partial_j \vec{\nu} - (\nabla (\nabla f \cdot \vec{\nu}) \cdot \vec{\nu}) \nu_j = \nabla \partial_j f \cdot \vec{\nu} + \nabla_s f \cdot \partial_{s_j} \vec{\nu}. \end{aligned}$$

Combining the above with the Schwarz theorem and Lemma 2.12(ii) yields that

$$\begin{aligned} \partial_{s_j} \partial_{s_i} f - \partial_{s_i} \partial_{s_j} f &= (\nabla_s f \cdot \partial_{s_i} \vec{\nu}) \nu_j - (\nabla_s f \cdot \partial_{s_j} \vec{\nu}) \nu_i \\ &= (\nabla_s f \cdot \nabla_s \nu_i) \nu_j - (\nabla_s f \cdot \nabla_s \nu_j) \nu_i \\ &= [(\nabla_s \vec{\nu}) \nabla_s f]_i \nu_j - [(\nabla_s \vec{\nu}) \nabla_s f]_j \nu_i. \end{aligned}$$

This proves (2.6). □

Lemma 2.16. *Let Γ be an orientable C^3 -hypersurface with normal vector field $\vec{\nu}$. It holds that*

$$\nabla_s \varkappa = -\Delta_s \vec{\nu} - |\nabla_s \vec{\nu}|^2 \vec{\nu} \quad \text{on } \Gamma.$$

Proof. Using the same notation as in the proof of Lemma 2.15, it follows from Lemma 2.12(ii), Lemma 2.15, Lemma 2.13(i) and Lemma 2.12(i) that, for $j = 1, \dots, d$,

$$\begin{aligned}
\Delta_s \nu_j &= \sum_{i=1}^d \partial_{s_i} \partial_{s_i} \nu_j = \sum_{i=1}^d \partial_{s_i} \partial_{s_j} \nu_i \\
&= \sum_{i=1}^d (\partial_{s_j} \partial_{s_i} \nu_i - [(\nabla_s \vec{\nu}) \nabla_s \nu_i]_i \nu_j + [(\nabla_s \vec{\nu}) \nabla_s \nu_i]_j \nu_i) \\
&= \partial_{s_j} (\nabla_s \cdot \vec{\nu}) - \nu_j \sum_{i=1}^d |\nabla_s \nu_i|^2 + (\nabla_s \nu_j) \cdot \sum_{i=1}^d (\nabla_s \nu_i) \nu_i \\
&= \partial_{s_j} (\nabla_s \cdot \vec{\nu}) - \nu_j |\nabla_s \vec{\nu}|^2 + (\nabla_s \nu_j) \cdot (\nabla_s \vec{\nu})^\top \vec{\nu} = -\partial_{s_j} \kappa - \nu_j |\nabla_s \vec{\nu}|^2.
\end{aligned}$$

This yields the claim. $\square$

2.3 The divergence theorem

Definition 2.17.

- (i) A subset $\Gamma \subset \mathbb{R}^d$ is called an n -dimensional C^k -surface with boundary, for $1 \leq n \leq d$ and $k \geq 1$, if for each point $\vec{p} \in \Gamma$ one of the following conditions is satisfied.
 - (a) There exist an open neighbourhood $V \subset \mathbb{R}^d$ of $\vec{p}$ and a bijective C^k -map $\vec{\mathfrak{X}} : U \rightarrow V \cap \Gamma$, with $U \subset \mathbb{R}^n$ open and connected, such that the Jacobian $\nabla \vec{\mathfrak{X}} : U \rightarrow \mathbb{R}^{d \times n}$ of $\vec{\mathfrak{X}}$ has full rank in U .
 - (b) There exist open and connected sets $U \subset \mathbb{R}^n$, $V \subset \mathbb{R}^d$, with $\vec{0} \in U$ and $\vec{p} \in V$, and an injective C^k -map $\vec{\mathfrak{X}} : U \rightarrow \mathbb{R}^d$, such that $\vec{\mathfrak{X}}(\vec{0}) = \vec{p}$ and

$$\vec{\mathfrak{X}}(U \cap (\mathbb{R}^{n-1} \times \mathbb{R}_{\geq 0})) = V \cap \Gamma.$$

- (ii) The maps $\vec{\mathfrak{X}} : U \rightarrow \mathbb{R}^d$ in (a) and (b) are called local parameterizations of Γ . In the latter case, we call $\vec{\mathfrak{X}}$ a local boundary parameterization of Γ .
- (iii) If $n = d - 1$, then we call Γ a hypersurface with boundary.

Remark 2.18.

- (i) A boundary point of Γ is a point on Γ for which the second condition in the definition is fulfilled. The set of all boundary points is called the boundary of Γ and is denoted by $\partial\Gamma$.
- (ii) If Γ is a C^k -hypersurface with boundary, its boundary $\partial\Gamma$ is either empty or a $(d-2)$ -dimensional surface without boundary, see Agricola and Friedrich (2002, §3.1) for details.

- (iii) If $\partial\Gamma$ is empty, we say that Γ is a surface without boundary. If, in addition, Γ is compact, then we call Γ a closed surface. Here we note that Definition 2.17 implies that any bounded hypersurface is compact.
- (iv) All the definitions and results in §2.1 and §2.2 have been stated for $\vec{p} \in \Gamma \setminus \partial\Gamma$. However, they easily generalize to $\vec{p} \in \partial\Gamma$ for a surface with boundary. The only required changes are as follows. In Definition 2.2, U is replaced by $U \cap (\mathbb{R}^{n-1} \times \mathbb{R}_{\geq 0})$, and similarly in Remark 2.8(i). In addition, in Definition 2.5(i), we choose a curve $\vec{y} : (-1, 0] \rightarrow \Gamma$.

Definition 2.19. Let Γ be an n -dimensional C^1 -surface in $\mathbb{R}^d$, $f : \Gamma \rightarrow \mathbb{R}$ a function and let $\vec{\mathfrak{X}} : U \rightarrow \Gamma$ be a local parameterization of $\Gamma \setminus \partial\Gamma$. Then, on recalling (2.2), we define

$$\int_{\vec{\mathfrak{X}}(U)} f \, d\mathcal{H}^n = \int_U f \circ \vec{\mathfrak{X}} \sqrt{g} \, d\mathcal{L}^n, \quad (2.7)$$

for all functions f such that $f \circ \vec{\mathfrak{X}}$ is integrable, where $\mathcal{L}^n$ is the n -dimensional Lebesgue measure. For a local boundary parameterization $\vec{\mathfrak{X}}$ of Γ , we replace U with $U \cap (\mathbb{R}^{n-1} \times \mathbb{R}_{\geq 0})$ in (2.7). The integral $\int_{\Gamma} f \, d\mathcal{H}^n$ is defined using a partition of unity and the definition (2.7), see Amann and Escher (2009, §XII.1) for details. The induced measure, defined by $\mathcal{H}^n(\Gamma) = \int_{\Gamma} 1 \, d\mathcal{H}^n$, is called the n -dimensional Hausdorff measure in $\mathbb{R}^d$.

Definition 2.20. For a C^1 -hypersurface Γ with boundary it holds that for $\vec{p} \in \partial\Gamma$ the tangent space $T_{\vec{p}}\partial\Gamma$ is $(d-2)$ -dimensional, $T_{\vec{p}}\Gamma$ is $(d-1)$ -dimensional and $T_{\vec{p}}\partial\Gamma \subset T_{\vec{p}}\Gamma$. We can hence choose a unique vector $\vec{\mu}(\vec{p}) \in T_{\vec{p}}\Gamma$, which we call the outer unit conormal, such that

- (i) $|\vec{\mu}(\vec{p})| = 1$,
- (ii) $\vec{\mu}(\vec{p}) \in N_{\vec{p}}\partial\Gamma$,
- (iii) there exists a curve $\vec{y} : (-1, 0] \rightarrow \Gamma$ on Γ with $\vec{y}(0) = \vec{p}$ and $\vec{y}'(0) = \vec{\mu}(\vec{p})$.

We will frequently use the following generalization of the divergence theorem on hypersurfaces.

Theorem 2.21. Let Γ be a compact orientable C^2 -hypersurface with normal vector field $\vec{\nu}$, and let $\vec{f} \in [C^1(\Gamma)]^d$. Then it holds that

$$\int_{\Gamma} \nabla_s \cdot \vec{f} + \varkappa \vec{f} \cdot \vec{\nu} \, d\mathcal{H}^{d-1} = \int_{\partial\Gamma} \vec{f} \cdot \vec{\mu} \, d\mathcal{H}^{d-2},$$

where $\vec{\mu}$ is the outer unit conormal to $\partial\Gamma$.

Proof. The result is well-known for tangential vector fields $\vec{f}$, for which $\varkappa \vec{f} \cdot \vec{\nu}$ is not present. This special case can be shown on surfaces similarly to the case of flat domains

in $\mathbb{R}^d$, see e.g. Amann and Escher (2009, §XII.3) or Agricola and Friedrich (2002, §3.8). In the case of a nontangential vector field $\vec{f}$, we define the tangential vector field

$$\vec{h} = \vec{f} - (\vec{f} \cdot \vec{\nu}) \vec{\nu}$$

and compute, on using Lemma 2.7(i), $\nabla_s(\vec{f} \cdot \vec{\nu})$ being orthogonal to $\vec{\nu}$ and Lemma 2.13(i), that

$$\nabla_s \cdot \vec{h} = \nabla_s \cdot \vec{f} - (\vec{f} \cdot \vec{\nu}) \nabla_s \cdot \vec{\nu} = \nabla_s \cdot \vec{f} + \kappa \vec{f} \cdot \vec{\nu}.$$

Using the divergence theorem for $\vec{h}$, taking into account that $\vec{h} \cdot \vec{\mu} = \vec{f} \cdot \vec{\mu}$, we obtain the assertion of the theorem. $\square$

Remark 2.22.

- (i) *The following integration by parts rule is a direct consequence of Theorem 2.21, Lemma 2.7(i) and Definition 2.5(ii). Let $f \in C^2(\Gamma)$ and $\eta \in C^1(\Gamma)$. Then it holds that*

$$\int_{\Gamma} \eta \Delta_s f + \nabla_s f \cdot \nabla_s \eta \, d\mathcal{H}^{d-1} = \int_{\partial\Gamma} \eta \nabla_s f \cdot \vec{\mu} \, d\mathcal{H}^{d-2}.$$

- (ii) *Moreover, for $f \in C^1(\Gamma)$ we obtain the Gauss–Green formula*

$$\int_{\Gamma} \nabla_s f + f \kappa \vec{\nu} \, d\mathcal{H}^{d-1} = \int_{\partial\Gamma} f \vec{\mu} \, d\mathcal{H}^{d-2},$$

by choosing $\vec{f} = f \vec{e}_i$, $i = 1, \dots, d$, in Theorem 2.21, and applying Lemma 2.7(i).

- (iii) *Let $\vec{f} \in [C^2(\Gamma)]^d$ and $\vec{\eta} \in [C^1(\Gamma)]^d$. Then it follows from (i) and Remark 2.6(iii) that*

$$\int_{\Gamma} \vec{\eta} \cdot \Delta_s \vec{f} + \nabla_s \vec{f} : \nabla_s \vec{\eta} \, d\mathcal{H}^{d-1} = \int_{\partial\Gamma} \vec{\eta} \cdot (\nabla_s \vec{f}) \vec{\mu} \, d\mathcal{H}^{d-2}.$$

On noting that for symmetric matrices $\underline{A} \in \mathbb{R}^{d \times d}$ it holds that $\underline{P}_{\Gamma} \underline{A} \underline{P}_{\Gamma} : \underline{B} = \underline{P}_{\Gamma} \underline{A} \underline{P}_{\Gamma} : \frac{1}{2} \underline{P}_{\Gamma} (\underline{B} + \underline{B}^T) \underline{P}_{\Gamma}$ on Γ for all $\underline{B} \in \mathbb{R}^{d \times d}$, we obtain furthermore that

$$\int_{\Gamma} \vec{\eta} \cdot (\nabla_s \cdot \underline{D}_s(\vec{f})) + \underline{D}_s(\vec{f}) : \underline{D}_s(\vec{\eta}) \, d\mathcal{H}^{d-1} = \int_{\partial\Gamma} \vec{\eta} \cdot \underline{D}_s(\vec{f}) \vec{\mu} \, d\mathcal{H}^{d-2},$$

where we have recalled Definition 2.5(vii) and used Theorem 2.21 with Lemma 2.7(iv) and Remark 2.6(iv).

- (iv) *Of fundamental importance in the development of numerical approximations for curvature driven evolution equations is the following identity. Let $\vec{\eta} \in [C^1(\Gamma)]^d$. Then it follows from (iii), Lemma 2.13(ii), Lemma 2.9(i) and Definition 2.20 that*

$$\int_{\Gamma} \kappa \vec{\eta} \cdot \vec{\nu} + \nabla_s \text{id} : \nabla_s \vec{\eta} \, d\mathcal{H}^{d-1} = \int_{\partial\Gamma} \vec{\eta} \cdot \vec{\mu} \, d\mathcal{H}^{d-2}.$$

- (v) *For numerical approximations of the Weingarten map, recall Definition 2.10(i), the following identity is of use. Let $\underline{\eta} \in [C^1(\Gamma)]^{d \times d}$. Then it follows from Theorem 2.21, with $\vec{f} = \underline{\eta}^T \vec{\nu}$, on recalling Lemma 2.7(iv), that*

$$\int_{\Gamma} \nabla_s \vec{\nu} : \underline{\eta} + \vec{\nu} \cdot [\kappa \underline{\eta} \vec{\nu} + \nabla_s \cdot \underline{\eta}] \, d\mathcal{H}^{d-1} = \int_{\partial\Gamma} \vec{\nu} \cdot \underline{\eta} \vec{\mu} \, d\mathcal{H}^{d-2}.$$

2.4 Evolving surfaces and transport theorems

We are mainly interested in evolving hypersurfaces. Hence we now consider hypersurfaces which evolve in a time interval $[0, T]$ and define the term evolving hypersurface.

Definition 2.23.

- (i) Let $(\Gamma(t))_{t \in [0, T]}$ be a family of C^k -hypersurfaces (with or without boundary), for $k \geq 1$. The set

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

is called a C^k -evolving hypersurface if it is a C^k -hypersurface with boundary in $\mathbb{R}^{d+1}$, such that $T_{(\vec{p}, t)} \mathcal{G}_T \neq \mathbb{R}^d \times \{0\}$ for all $(\vec{p}, t) \in \mathcal{G}_T$. We will often identify $\mathcal{G}_T$ with $(\Gamma(t))_{t \in [0, T]}$, and call the latter also a C^k -evolving hypersurface.

- (ii) Let $\mathcal{G}_T$ be a C^1 -evolving hypersurface and $(\vec{p}_0, t_0) \in \mathcal{G}_T$. We assume that $\mathcal{G}_T$ allows for a continuous vector field $\vec{\nu} : \mathcal{G}_T \rightarrow \mathbb{R}^d$, such that $\vec{\nu}(\cdot, t)$ is a unit normal to $\Gamma(t)$. Furthermore, let $\vec{\gamma} : (t_0 - \delta, t_0 + \delta) \rightarrow \mathbb{R}^d$, for some $\delta > 0$, with $\vec{\gamma}(t) \in \Gamma(t)$ and $\vec{\gamma}(t_0) = \vec{p}_0$ be a smooth curve in $\mathbb{R}^d$. Then the normal velocity of $\Gamma(t_0)$ at $\vec{p}_0$ is defined as

$$\mathcal{V}(\vec{p}_0, t_0) = \vec{\nu}(\vec{p}_0, t_0) \cdot \vec{\gamma}'(t_0).$$

- (iii) Let $\mathcal{G}_T$ be a C^k -evolving hypersurface satisfying the assumptions in (ii). Then we call $\mathcal{G}_T$ a C^k -evolving orientable hypersurface.

Remark 2.24. Let $\mathcal{G}_T$ be a C^1 -evolving orientable hypersurface.

- (i) The condition $T_{(\vec{p}, t)} \mathcal{G}_T \neq \mathbb{R}^d \times \{0\}$, for all $(\vec{p}, t) \in \mathcal{G}_T$, guarantees the existence of a curve $\vec{\gamma}$ in Definition 2.23(ii), recall Remark 2.6(i).
- (ii) It is easy to show that $\mathcal{V}$ does not depend on the curve $\vec{\gamma}$. To see this, we note that $(\vec{\gamma}'(t_0), 1) \in T_{(\vec{p}_0, t_0)} \mathcal{G}_T$. Hence, on letting $\{\vec{\tau}_1, \dots, \vec{\tau}_{d-1}\}$ denote a basis of $T_{\vec{p}_0} \Gamma(t_0)$, we have that $\{(\vec{\tau}_1, 0), \dots, (\vec{\tau}_{d-1}, 0), (\vec{\gamma}'(t_0), 1)\}$ is a basis of $T_{(\vec{p}_0, t_0)} \mathcal{G}_T$. Then it follows from Definition 2.23(ii) that $\vec{\gamma}'(t_0) = \mathcal{V}(\vec{p}_0, t_0) \vec{\nu}(\vec{p}_0, t_0) + \sum_{i=1}^{d-1} \alpha_i \vec{\tau}_i$ for some $\alpha_i \in \mathbb{R}$, $i = 1, \dots, d-1$, and so $(\mathcal{V}(\vec{p}_0, t_0) \vec{\nu}(\vec{p}_0, t_0), 1) \in T_{(\vec{p}_0, t_0)} \mathcal{G}_T$. In addition, we observe that there exists a unique vector $(\vec{\omega}, 1) \in T_{(\vec{p}_0, t_0)} \mathcal{G}_T$ with $\vec{\omega}$ parallel to $\vec{\nu}(\vec{p}_0, t_0)$. Therefore we have that $\vec{\omega} = \mathcal{V}(\vec{p}_0, t_0) \vec{\nu}(\vec{p}_0, t_0)$, and so $\mathcal{V}(\vec{p}_0, t_0)$ does not depend on $\vec{\gamma}$.
- (iii) Moreover, we observe that $(1 + \mathcal{V}^2)^{-\frac{1}{2}} (\vec{\nu}, -\mathcal{V})$ is a continuous normal vector field on $\mathcal{G}_T$, and so $\mathcal{G}_T$ is an orientable hypersurface in $\mathbb{R}^{d+1}$.
- (iv) If $\mathcal{G}_T$ is a C^2 -evolving hypersurface, then it is even easier to show that $\mathcal{V}$ does not depend on the curve $\vec{\gamma}$. In order to do so, we choose a C^1 -function f defined in a small neighbourhood of $\mathcal{G}_T$ such that $f = 0$ on $\mathcal{G}_T$, and such that $\nabla f(\vec{z}, t) \neq \vec{0}$ for

all $(\vec{z}, t) \in \mathcal{G}_T$. A possible choice for $f(\cdot, t)$ is the signed distance function $d_\Gamma(\cdot, t)$ to $\Gamma(t)$, recall (2.3). We then compute for a curve y as in Definition 2.23(ii) that

$$0 = \frac{d}{dt} f(\vec{y}(t), t) = (\nabla f)(\vec{y}(t), t) \cdot \vec{y}'(t) + (\partial_t f)(\vec{y}(t), t).$$

As $\vec{\nu} = \nabla f / |\nabla f|$, we obtain

$$\mathcal{V}(\vec{p}_0, t_0) = \vec{\nu}(\vec{p}_0, t_0) \cdot \vec{y}'(t_0) = - \left(\frac{\partial_t f}{|\nabla f|} \right) (\vec{p}_0, t_0),$$

where the right hand side does not depend on $\vec{y}$.

Typically we will consider evolving hypersurfaces that are given by a global parameterization as follows.

Definition 2.25. Let $\mathcal{G}_T$ be a C^k -evolving hypersurface, and let Υ be a C^k -hypersurface in $\mathbb{R}^d$, with $k \geq 1$.

- (i) A C^k -map $\vec{x} : \Upsilon \times [0, T] \rightarrow \mathbb{R}^d$ such that $\vec{x}(\cdot, t)$ is a diffeomorphism from Υ to $\Gamma(t)$ for all $t \in [0, T]$ is called a global parameterization of $\mathcal{G}_T$.
- (ii) The full velocity of $\Gamma(t)$ on $\mathcal{G}_T$, induced by the parameterization $\vec{x}$, is defined by

$$\vec{\mathcal{V}}(\vec{x}(\vec{q}, t), t) = (\partial_t \vec{x})(\vec{q}, t) \quad \forall (\vec{q}, t) \in \Upsilon \times [0, T].$$

- (iii) The tangential velocity of $\Gamma(t)$ on $\mathcal{G}_T$, induced by the parameterization $\vec{x}$, is defined by

$$\vec{\mathcal{V}}_T = \underline{P}_\Gamma \vec{\mathcal{V}} \quad \text{on } \Gamma(t),$$

recall (2.1).

- (iv) We define the rate of deformation tensor of $\Gamma(t)$ by

$$\underline{D}_s(\vec{\mathcal{V}}) \quad \text{on } \Gamma(t),$$

recall Definition 2.5(vii).

Remark 2.26.

- (i) For the normal velocity of an evolving orientable hypersurface $\mathcal{G}_T$ defined in Definition 2.23(ii) it holds that

$$\mathcal{V} = \vec{\mathcal{V}} \cdot \vec{\nu} \quad \text{on } \mathcal{G}_T.$$

Hence we have that

$$\vec{\mathcal{V}} = \mathcal{V} \vec{\nu} + \vec{\mathcal{V}}_T \quad \text{on } \mathcal{G}_T.$$

Here we stress that $\mathcal{V}$ does not depend on the parameterization $\vec{x}$, while $\vec{\mathcal{V}}_T$ clearly does.

- (ii) The expression “rate of deformation tensor” for $\underline{D}_s(\vec{\mathcal{V}})$ is justified, because it encodes how $\Gamma(t)$ is locally deformed due to the motion induced by $\vec{x}$. This will be made rigorous in Lemma 2.30, below.

For the velocity field $\vec{\mathcal{V}}$ on $\mathcal{G}_T$ we have the following properties. Here and throughout, for notational convenience, we often identify $\Gamma(t) \times \{t\}$ with $\Gamma(t)$.

Lemma 2.27. *Let $\mathcal{G}_T$ a C^2 -evolving orientable hypersurface with a global parameterization leading to the velocity field $\vec{\mathcal{V}}$.*

- (i) It holds that

$$\nabla_s \cdot \vec{\mathcal{V}} = -\mathcal{V} \kappa + \nabla_s \cdot \vec{\mathcal{V}}_T \quad \text{on } \Gamma(t).$$

- (ii) Moreover, it holds that

$$\nabla_s \vec{\mathcal{V}} = \mathcal{V} \nabla_s \vec{\nu} + \vec{\nu} \otimes \nabla_s \mathcal{V} + \nabla_s \vec{\mathcal{V}}_T \quad \text{on } \Gamma(t).$$

- (iii) Finally, for the rate of deformation tensor it holds that

$$\underline{D}_s(\vec{\mathcal{V}}) = \mathcal{V} \nabla_s \vec{\nu} + \frac{1}{2} (\underline{P}_\Gamma \nabla_s \vec{\mathcal{V}}_T + (\nabla_s \vec{\mathcal{V}}_T)^\top \underline{P}_\Gamma) \quad \text{on } \Gamma(t).$$

Proof. The desired results follow immediately from Lemma 2.14, on noting $\vec{\mathcal{V}}(\cdot, t) \in [C^1(\Gamma(t))]^d$ and Remark 2.26(i). $\square$

It is often convenient to also consider local parameterizations of $\Gamma(t)$, as defined in Definition 2.17. To this end, let $\vec{\varphi} : U \rightarrow \mathbb{R}^d$, $U \subset \mathbb{R}^{d-1}$ open and connected, be a local parameterization of Υ . Then

$$\vec{\mathfrak{X}}(t) = \vec{x}(\cdot, t) \circ \vec{\varphi} \quad \text{in } U, \quad t \in [0, T], \quad (2.8)$$

defines a local parameterization of $\Gamma(t)$.

We now define the time derivative of a function $f : \mathcal{G}_T \rightarrow \mathbb{R}$. We cannot differentiate $f(\vec{p}, t)$ directly with respect to t due to the fact that $\vec{p}$ might not lie on $\Gamma(t)$ for different times t . When differentiating with respect to t , we need to move the point $\vec{p}$. There is hence some ambiguity in defining the time derivative.

Definition 2.28. *Let $\mathcal{G}_T$ be a C^1 -evolving hypersurface with a global parameterization $\vec{x} : \Upsilon \times [0, T] \rightarrow \mathbb{R}^d$, and let $f \in C^1(\mathcal{G}_T)$.*

- (i) The expression

$$(\partial_t^\circ f)(\vec{x}(\vec{q}, t), t) = \frac{d}{dt} f(\vec{x}(\vec{q}, t), t) \quad \forall (\vec{q}, t) \in \Upsilon \times [0, T]$$

is the time derivative following the parameterizations $\vec{x}(\cdot, t)$ of f on $\Gamma(t)$. It is also called the material time derivative induced by $\vec{x}$.

(ii) The normal time derivative of f on $\Gamma(t)$ is defined as

$$\partial_t^\square f = \partial_t^\circ f - \vec{\mathcal{V}}_T \cdot \nabla_s f.$$

Remark 2.29.

(i) The quantity $\partial_t^\circ f$ depends on the parameterization $\vec{x}$. Moreover, it holds that $\vec{\mathcal{V}} = \partial_t^\circ \text{id}$ on $\Gamma(t)$ and $\vec{\mathcal{V}} \circ \vec{\mathcal{X}} = \partial_t \vec{\mathcal{X}}$ in U .

For the following observations, we assume that f is extended to a neighbourhood of $\mathcal{G}_T$.

(ii) It holds that

$$\partial_t^\circ f = \partial_t f + \vec{\mathcal{V}} \cdot \nabla f \quad \text{on } \Gamma(t),$$

where ∇f denotes the gradient in $\mathbb{R}^d$ of the extension f .

(iii) Moreover, we have that

$$\partial_t^\square f = \partial_t f + \mathcal{V} \vec{\nu} \cdot \nabla f \quad \text{on } \Gamma(t).$$

Taking Remark 2.24(ii) into account, we observe, in particular, that $\partial_t^\square f$ does not depend on $\vec{x}$. In fact, $\partial_t^\square f$ is the derivative of f in the direction $(\mathcal{V} \vec{\nu}, 1)$, where the vector $(\mathcal{V} \vec{\nu}, 1)$ is a space time tangential vector of the evolving surface $\mathcal{G}_T$. I.e.

$$\partial_t^\square f = \partial_{(\mathcal{V} \vec{\nu}, 1)} f \quad \text{on } \mathcal{G}_T,$$

recall Definition 2.5(i).

(iv) Taking a curve $t \mapsto \vec{y}(t) \in \mathbb{R}^d$ such that $\vec{y}(t) \in \Gamma(t)$ and $\vec{y}'(t) = (\mathcal{V} \vec{\nu}) \circ \vec{y}$, we obtain from (iii) that

$$(\partial_t^\square f)(\vec{y}(t), t) = \frac{d}{dt} f(\vec{y}(t), t).$$

For the time-dependent metric tensor $(g_{ij}(t))_{i,j=1,\dots,d-1}$, which, similarly to Remark 2.8(i), is defined via

$$g_{ij}(t) = \partial_i \vec{\mathcal{X}}(t) \cdot \partial_j \vec{\mathcal{X}}(t) \quad \text{in } U, \tag{2.9}$$

for $\vec{\mathcal{X}}(t) = \vec{x}(\cdot, t) \circ \vec{\varphi}$, recall (2.8), we obtain the following lemma. Here and throughout, for notational convenience, we often omit the dependence on t .

Lemma 2.30. Let $\mathcal{G}_T$ a C^2 -evolving hypersurface with a global parameterization $\vec{x}$ leading to the velocity field $\vec{\mathcal{V}}$, and let the metric tensor be defined by (2.9). Then it holds that

$$\partial_t g_{ij} = 2((\underline{D}_s(\vec{\mathcal{V}}) \circ \vec{\mathcal{X}}) \partial_i \vec{\mathcal{X}}) \cdot \partial_j \vec{\mathcal{X}} \quad \text{in } U,$$

where $\underline{D}_s(\vec{\mathcal{V}})$ is the rate of deformation tensor, recall Definition 2.25(iv).

Proof. We introduce the shorthand notation $\vec{\partial}_i = \partial_i \vec{\mathfrak{X}}$, $i = 1, \dots, d-1$, and recall from Remark 2.29(i) that $\vec{\mathcal{V}} \circ \vec{\mathfrak{X}} = \partial_t \vec{\mathfrak{X}}$ in U . Then we compute, using Remark 2.6(iii),

$$\begin{aligned} \partial_t g_{ij} &= \partial_t (\partial_i \vec{\mathfrak{X}} \cdot \partial_j \vec{\mathfrak{X}}) = \partial_i (\vec{\mathcal{V}} \circ \vec{\mathfrak{X}}) \cdot \vec{\partial}_j + \vec{\partial}_i \cdot \partial_j (\vec{\mathcal{V}} \circ \vec{\mathfrak{X}}) \\ &= ((\nabla_s \vec{\mathcal{V}}) \circ \vec{\mathfrak{X}} \vec{\partial}_i) \cdot \vec{\partial}_j + \vec{\partial}_i \cdot (\nabla_s \vec{\mathcal{V}}) \circ \vec{\mathfrak{X}} \vec{\partial}_j \\ &= (\nabla_s \vec{\mathcal{V}} + (\nabla_s \vec{\mathcal{V}})^\top) \circ \vec{\mathfrak{X}} \vec{\partial}_i \cdot \vec{\partial}_j. \end{aligned}$$

As $\vec{\partial}_i$ and $\vec{\partial}_j$ are tangential, the claim follows. $\square$

In order to compute the first variation of area, it is crucial to know how the area element $\sqrt{g}$ evolves in time, recall Definition 2.19. This is studied in the next lemma.

Lemma 2.31. *Let $\mathcal{G}_T$ a C^2 -evolving orientable hypersurface with a global parameterization $\vec{x}$ leading to the velocity field $\vec{\mathcal{V}}$, and let the metric tensor be defined by (2.9). It holds that*

$$\partial_t \sqrt{g} = (\nabla_s \cdot \vec{\mathcal{V}}) \circ \vec{\mathfrak{X}} \sqrt{g} = (-\mathcal{V} \varkappa + \nabla_s \cdot \vec{\mathcal{V}}_T) \circ \vec{\mathfrak{X}} \sqrt{g} \quad \text{in } U,$$

where

$$g(t) = \det((g_{ij}(t))_{i,j=1,\dots,d-1}).$$

Proof. Jacobi's formula for the derivative of the determinant, see e.g. Eck et al. (2017, Lemma 5.3), for $\underline{G}(t) = (g_{ij}(t))_{i,j=1,\dots,d-1}$, gives

$$\partial_t \det \underline{G}(t) = \det \underline{G}(t) \operatorname{tr}(\underline{G}^{-1}(t) \partial_t \underline{G}(t)).$$

As $g(t) = \det \underline{G}(t)$, and since $\underline{G}(t)$ is symmetric, we obtain from the proof of Lemma 2.30 that

$$\begin{aligned} \partial_t \sqrt{g} &= \partial_t \sqrt{\det \underline{G}} = \frac{1}{2} \sqrt{g} \operatorname{tr}(\underline{G}^{-1} \partial_t \underline{G}) = \frac{1}{2} \sqrt{g} \underline{G}^{-1} : \partial_t \underline{G} \\ &= \frac{1}{2} \sqrt{g} \sum_{i,j=1}^{d-1} g^{ij} \partial_t g_{ij} = \sqrt{g} \sum_{i,j=1}^{d-1} g^{ij} \partial_i (\vec{\mathcal{V}} \circ \vec{\mathfrak{X}}) \cdot \vec{\partial}_j \vec{\mathfrak{X}} \\ &= \sqrt{g} (\nabla_s \cdot \vec{\mathcal{V}}) \circ \vec{\mathfrak{X}}, \end{aligned}$$

where in the last step we have recalled Remark 2.8(i). The second identity is then a direct consequence of Lemma 2.27(i). $\square$

We can now prove a transport theorem for evolving hypersurfaces, which will be crucial for many arguments that follow.

Theorem 2.32. *Let $\mathcal{G}_T$ be a compact C^2 -evolving orientable hypersurface with a global parameterization leading to the velocity field $\vec{\mathcal{V}}$, and let $f \in C^1(\mathcal{G}_T)$. Then it holds that*

$$\begin{aligned} \frac{d}{dt} \int_{\Gamma(t)} f \, d\mathcal{H}^{d-1} &= \int_{\Gamma(t)} (\partial_t^\circ f + f \nabla_s \cdot \vec{\mathcal{V}}) \, d\mathcal{H}^{d-1} \\ &= \int_{\Gamma(t)} (\partial_t^\circ f + f \nabla_s \cdot \vec{\mathcal{V}}_T - f \mathcal{V} \varkappa) \, d\mathcal{H}^{d-1} \\ &= \int_{\Gamma(t)} (\partial_t^\square f - f \mathcal{V} \varkappa) \, d\mathcal{H}^{d-1} + \int_{\partial\Gamma(t)} f \vec{\mathcal{V}} \cdot \vec{\mu} \, d\mathcal{H}^{d-2}, \end{aligned}$$

where $\vec{\mu}$ is the outer unit conormal to $\partial\Gamma$.

Proof. We first consider an f with support in the image of a single time-dependent local parameterization $\vec{\mathfrak{X}}(t) = \vec{x}(\cdot, t) \circ \vec{\varphi}$, recall (2.8). In this case we can compute from Definition 2.19, Definition 2.28(i) and Lemma 2.31 that

$$\begin{aligned} \frac{d}{dt} \int_{\Gamma(t)} f \, d\mathcal{H}^{d-1} &= \frac{d}{dt} \int_{\vec{x}(\vec{\varphi}(U), t)} f \, d\mathcal{H}^{d-1} \\ &= \frac{d}{dt} \int_U f(\vec{x}(\vec{\varphi}(\vec{u}), t), t) \sqrt{g} \, d\mathcal{L}^{d-1} \\ &= \int_U (\partial_t^\circ f + f \nabla_s \cdot \vec{\mathcal{V}}) \circ \vec{\mathfrak{X}} \sqrt{g} \, d\mathcal{L}^{d-1} \\ &= \int_{\Gamma(t)} (\partial_t^\circ f + f \nabla_s \cdot \vec{\mathcal{V}}) \, d\mathcal{H}^{d-1}. \end{aligned}$$

Using a partition of unity argument now proves the first identity in the claim. Lemma 2.27(i) yields the second identity, and Definition 2.28(ii) and Lemma 2.7(i) then give the last identity, on noting from Theorem 2.21 and Definition 2.20 that

$$\begin{aligned} \int_{\Gamma(t)} \nabla_s \cdot (f \vec{\mathcal{V}}_T) \, d\mathcal{H}^{d-1} &= - \int_{\Gamma(t)} \kappa f \vec{\mathcal{V}}_T \cdot \vec{\nu} \, d\mathcal{H}^{d-1} + \int_{\partial\Gamma(t)} f \vec{\mathcal{V}}_T \cdot \vec{\mu} \, d\mathcal{H}^{d-2} \\ &= \int_{\partial\Gamma(t)} f \vec{\mathcal{V}} \cdot \vec{\mu} \, d\mathcal{H}^{d-2}. \end{aligned}$$

□

We also have the following transport theorem for moving domains.

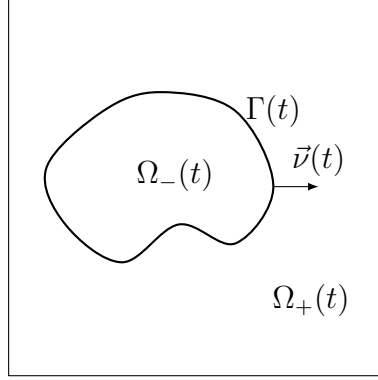
Theorem 2.33. *Let $\mathcal{G}_T$ be a compact C^2 -evolving orientable hypersurface, such that $\Gamma(t)$ is bounding a domain $\Omega(t) \subset \mathbb{R}^d$, for $t \in [0, T]$. We assume that $\vec{\nu}(t)$ is the outer unit normal to $\Omega(t)$ on $\Gamma(t)$, and that $f \in C^1(\mathfrak{D}_T)$, where*

$$\mathfrak{D}_T = \bigcup_{t \in [0, T]} (\Omega(t) \times \{t\}).$$

Then it holds that

$$\frac{d}{dt} \int_{\Omega(t)} f \, d\mathcal{L}^d = \int_{\Omega(t)} \partial_t f \, d\mathcal{L}^d + \int_{\Gamma(t)} f \mathcal{V} \, d\mathcal{H}^{d-1}. \quad (2.10)$$

Proof. A proof can be found in Prüss and Simonett (2016, Chapter 2). If the moving domain is transported with a velocity field $\vec{\mathcal{V}}_{\mathfrak{D}} : \mathfrak{D}_T \rightarrow \mathbb{R}^d$, with $\vec{\mathcal{V}}_{\mathfrak{D}} \cdot \vec{\nu} = \mathcal{V}$ on $\mathcal{G}_T$, then the theorem can be shown similarly to Theorem 2.32. An alternative proof would integrate (2.10), and use the divergence theorem in space-time, see e.g. Eck et al. (2017, §7.3). □

Figure 1: A sketch of the domain Ω in the case $d = 2$.

Remark 2.34. *If the moving domain $\mathfrak{D}_T$ is transported with a velocity field $\vec{\mathcal{V}}_{\mathfrak{D}} : \mathfrak{D}_T \rightarrow \mathbb{R}^d$, we obtain the Reynolds transport theorem*

$$\begin{aligned} \frac{d}{dt} \int_{\Omega(t)} f \, d\mathcal{L}^d &= \int_{\Omega(t)} \partial_t f \, d\mathcal{L}^d + \int_{\Gamma(t)} f \vec{\mathcal{V}}_{\mathfrak{D}} \cdot \vec{\nu} \, d\mathcal{H}^{d-1} \\ &= \int_{\Omega(t)} \partial_t f + \nabla \cdot (f \vec{\mathcal{V}}_{\mathfrak{D}}) \, d\mathcal{L}^d, \end{aligned}$$

where we have used the divergence theorem in $\mathbb{R}^d$, and where we once again assumed that $\vec{\nu}(t)$ is the outer unit normal to $\Omega(t)$ on $\Gamma(t)$.

Using Theorem 2.33, one can also show a transport theorem for two-phase moving domains. To this end, let $\Omega \subset \mathbb{R}^d$ be a fixed, bounded domain. Suppose that $\mathcal{G}_T$ is a compact C^2 -evolving orientable hypersurface with $\Gamma(t) \subset \Omega$, such that $\overline{\Gamma(t)}$ encloses a region $\Omega_-(t) \subset \Omega$, with $\Gamma(t) = \partial\Omega_-(t)$, for all $t \in [0, T]$. Let $\Omega_+(t) = \Omega \setminus \overline{\Omega_-(t)}$, and let $\vec{\nu}(t)$ denote the outer normal to $\Omega_-(t)$ on $\Gamma(t)$, see Figure 1. We have

$$\overline{\Omega} = \overline{\Omega_-(t)} \cup \overline{\Omega_+(t)}, \quad \overline{\Omega_-(t)} \cap \overline{\Omega_+(t)} = \Gamma(t), \quad \partial\Omega_+(t) = \Gamma(t) \cup \partial\Omega.$$

Now let

$$\mathfrak{D}_{\pm, T} = \bigcup_{t \in [0, T]} (\Omega_{\pm}(t) \times \{t\}),$$

and let $f_{\pm} : \mathfrak{D}_{\pm, T} \rightarrow \mathbb{R}$ be given such that each $f_{\pm}$ has a continuous extension to $\overline{\mathfrak{D}_{\pm, T}}$. Defining $f : \mathfrak{D}_{-, T} \cup \mathfrak{D}_{+, T} \rightarrow \mathbb{R}$ as

$$f(\cdot, t) = f_-(\cdot, t) \mathcal{X}_{\Omega_-(t)} + f_+(\cdot, t) \mathcal{X}_{\Omega_+(t)} \quad \forall t \in [0, T], \quad (2.11)$$

where, here and throughout, $\mathcal{X}_{\mathfrak{A}}$ defines the characteristic function for a set $\mathfrak{A}$, we let

$$[f]_{-}^+(\vec{z}, t) = \lim_{\substack{\vec{y} \rightarrow \vec{z} \\ \vec{y} \in \Omega_+(t)}} f(\vec{y}, t) - \lim_{\substack{\vec{y} \rightarrow \vec{z} \\ \vec{y} \in \Omega_-(t)}} f(\vec{y}, t) \quad \forall (\vec{z}, t) \in \mathcal{G}_T. \quad (2.12)$$

Then we obtain that following result.

Theorem 2.35. *Let $\mathcal{G}_T \subset \Omega \times [0, T]$ be a compact C^2 -evolving orientable hypersurface, such that $\Gamma(t)$ is bounding a domain $\Omega_-(t) \subset \mathbb{R}^d$, for $t \in [0, T]$. We assume that $\vec{\nu}(t)$ is the outer unit normal to $\Omega_-(t)$ on $\Gamma(t)$, and that $f_\pm \in C^1(\overline{\Omega}_{\pm, T})$. Then, for f as defined in (2.11), it holds that*

$$\frac{d}{dt} \int_{\Omega} f \, d\mathcal{L}^d = \int_{\Omega_-(t)} \partial_t f \, d\mathcal{L}^d + \int_{\Omega_+(t)} \partial_t f \, d\mathcal{L}^d - \int_{\Gamma(t)} [f]_{-}^{+} \nu \, d\mathcal{H}^{d-1}.$$

Proof. The claim follows directly from Theorem 2.33. $\square$

Remark 2.36. *We naturally extend (2.12) to vector-valued quantities. For example, if f , as defined in (2.11), has a continuous extension to $\overline{\Omega} \times [0, T]$, and such that each $\nabla f_{\pm}$ has a continuous extension to $\overline{\Omega}_{\pm, T}$, then we define*

$$\begin{aligned} [\partial_{\vec{\nu}} f]_{-}^{+}(\vec{z}, t) &= \lim_{\substack{\vec{y} \rightarrow \vec{z} \\ \vec{y} \in \Omega_{+}(t)}} (\nabla f_{+})(\vec{y}, t) \cdot \vec{\nu}(\vec{z}, t) - \lim_{\substack{\vec{y} \rightarrow \vec{z} \\ \vec{y} \in \Omega_{-}(t)}} (\nabla f_{-})(\vec{y}, t) \cdot \vec{\nu}(\vec{z}, t) \\ &\quad \forall (\vec{z}, t) \in \mathcal{G}_T. \end{aligned} \tag{2.13}$$

For such an f , integration by parts in $\mathbb{R}^d$ immediately yields that

$$\begin{aligned} &\int_{\Omega_-(t) \cup \Omega_+(t)} \eta \Delta f \, d\mathcal{L}^d \\ &= \int_{\partial\Omega} \eta \partial_{\vec{\nu}_{\Omega}} f \, d\mathcal{H}^{d-1} - \int_{\Gamma(t)} \eta [\partial_{\vec{\nu}} f]_{-}^{+} \, d\mathcal{H}^{d-1} - \int_{\Omega} \nabla f \cdot \nabla \eta \, d\mathcal{L}^d \end{aligned}$$

for all $\eta \in C^1(\overline{\Omega})$, where $\vec{\nu}_{\Omega}$ denotes the outer unit normal to Ω on $\partial\Omega$.

2.5 Time derivatives of the normal

We also frequently need time derivatives of the normal. The relevant results are stated in the following lemma.

Lemma 2.37. *Let $\mathcal{G}_T$ be a C^2 -evolving orientable hypersurface.*

- (i) *Let $\vec{\mathcal{V}}$ be the velocity field induced by a global parameterization of $\mathcal{G}_T$. Then it holds that*

$$\partial_t^{\circ} \vec{\nu} = -(\nabla_s \vec{\mathcal{V}})^{\top} \vec{\nu} \quad \text{on } \Gamma(t).$$

- (ii) *The normal time derivative of $\vec{\nu}$ satisfies*

$$\partial_t^{\square} \vec{\nu} = -\nabla_s \mathcal{V} \quad \text{on } \Gamma(t).$$

Proof. (i) For $\vec{p} \in \Gamma(t)$, with $\vec{p} = \vec{x}(\vec{\varphi}(\vec{u}, t), t) = \vec{\mathfrak{X}}(\vec{u}, t)$, recall (2.8), we define a basis $\{\vec{\tau}_1, \dots, \vec{\tau}_{d-1}\}$ of the tangent space $T_{\vec{p}}\Gamma(t)$ via $\vec{\tau}_i(\vec{p}) = \partial_i \vec{\mathfrak{X}}(\vec{u}, t)$, $i = 1, \dots, d-1$. We also recall from Remark 2.29(i) that $\vec{\mathcal{V}} \circ \vec{\mathfrak{X}} = \partial_t \vec{\mathfrak{X}}$ and hence note that

$$\begin{aligned} \partial_t^{\circ} \vec{\tau}_i &= \partial_t [(\partial_i \vec{\mathfrak{X}}) \circ \vec{\mathfrak{X}}^{-1}] = [\partial_i (\partial_t \vec{\mathfrak{X}})] \circ \vec{\mathfrak{X}}^{-1} = [\partial_i (\vec{\mathcal{V}} \circ \vec{\mathfrak{X}})] \circ \vec{\mathfrak{X}}^{-1} = \partial_{\vec{\tau}_i} \vec{\mathcal{V}} \\ &= (\nabla_s \vec{\mathcal{V}}) \vec{\tau}_i \quad \text{on } \Gamma(t), \end{aligned}$$

where for the last step we have recalled Remark 2.6(iii). As $\vec{\nu} \cdot \vec{\tau}_i = 0$, it follows for $i = 1, \dots, d-1$ that

$$(\partial_t^\circ \vec{\nu}) \cdot \vec{\tau}_i = -\vec{\nu} \cdot \partial_t^\circ \vec{\tau}_i = -\vec{\nu} \cdot ((\nabla_s \vec{\mathcal{V}}) \vec{\tau}_i) = -((\nabla_s \vec{\mathcal{V}})^\top \vec{\nu}) \cdot \vec{\tau}_i \quad \text{on } \Gamma(t).$$

Since $\{\vec{\tau}_1, \dots, \vec{\tau}_{d-1}\}$ is a basis of the tangent space $T_{\vec{p}}\Gamma(t)$, we obtain, on using $(\partial_t^\circ \vec{\nu}) \cdot \vec{\nu} = \frac{1}{2} \partial_t^\circ |\vec{\nu}|^2 = 0$ and the fact that $\vec{\nu} \cdot (\nabla_s \vec{\mathcal{V}})^\top \vec{\nu} = (\nabla_s \vec{\mathcal{V}}) \vec{\nu} \cdot \vec{\nu} = 0$, recall Remark 2.6(iii), that

$$\partial_t^\circ \vec{\nu} = -(\nabla_s \vec{\mathcal{V}})^\top \vec{\nu} \quad \text{on } \Gamma(t).$$

(ii) Let $\vec{x}$ be an arbitrary global parameterization of $\mathcal{G}_T$, with induced velocity field $\vec{\mathcal{V}}$. Using Definition 2.28(ii), Lemma 2.12, the result from (i) and Lemma 2.7(ii), we compute

$$\begin{aligned} \partial_t^\square \vec{\nu} &= \partial_t^\circ \vec{\nu} - (\nabla_s \vec{\nu}) \vec{\mathcal{V}}_T = \partial_t^\circ \vec{\nu} - (\nabla_s \vec{\nu})^\top \vec{\mathcal{V}}_T = -(\nabla_s \vec{\mathcal{V}})^\top \vec{\nu} - (\nabla_s \vec{\nu})^\top \vec{\mathcal{V}}_T \\ &= -(\nabla_s \vec{\mathcal{V}})^\top \vec{\nu} - (\nabla_s \vec{\nu})^\top \vec{\mathcal{V}} = -\nabla_s (\vec{\mathcal{V}} \cdot \vec{\nu}) = -\nabla_s \mathcal{V} \quad \text{on } \Gamma(t). \end{aligned}$$

□

2.6 Time derivatives of the mean curvature

In order to be able to compute the first variation of energies that depend on the mean curvature, for example with the help of Theorem 2.32, we need expressions for the time derivatives of curvature.

We begin with the following commutator rule for time derivatives and surface differential operators.

Lemma 2.38. *Let $\mathcal{G}_T$ be a C^2 -evolving orientable hypersurface with a global parameterization leading to the velocity field $\vec{\mathcal{V}}$, and let $f : \mathcal{G}_T \rightarrow \mathbb{R}$, $\vec{f} : \mathcal{G}_T \rightarrow \mathbb{R}^d$ be C^1 -functions. Then we have the following results:*

(i)

$$\partial_t^\circ \nabla_s f - \nabla_s \partial_t^\circ f = [\nabla_s \vec{\mathcal{V}} - 2 \underline{\underline{D}}_s(\vec{\mathcal{V}})] \nabla_s f \quad \text{on } \Gamma(t).$$

(ii)

$$\partial_t^\circ \nabla_s \vec{f} - \nabla_s \partial_t^\circ \vec{f} = (\nabla_s \vec{f}) [\nabla_s \vec{\mathcal{V}} - 2 \underline{\underline{D}}_s(\vec{\mathcal{V}})]^\top \quad \text{on } \Gamma(t).$$

(iii)

$$\partial_t^\circ (\nabla_s \cdot \vec{f}) - \nabla_s \cdot (\partial_t^\circ \vec{f}) = [\nabla_s \vec{\mathcal{V}} - 2 \underline{\underline{D}}_s(\vec{\mathcal{V}})] : \nabla_s \vec{f} \quad \text{on } \Gamma(t).$$

Proof. (i) We extend f to a neighbourhood of $\mathcal{G}_T$, such that the extension from $\Gamma(t)$ is constant in the $\vec{\nu}$ -direction, recall (2.4). On noting (2.5) and Lemma 2.37(i), it holds on $\Gamma(t)$ that

$$\begin{aligned} 0 &= \partial_t^\circ (\nabla f \cdot \vec{\nu}) = \partial_t^\circ (\nabla_s f \cdot \vec{\nu}) = (\partial_t^\circ \nabla_s f) \cdot \vec{\nu} + \nabla_s f \cdot \partial_t^\circ \vec{\nu} \\ &= (\partial_t^\circ \nabla_s f) \cdot \vec{\nu} - (\nabla_s f) \cdot (\nabla_s \vec{\mathcal{V}})^\top \vec{\nu} = (\partial_t^\circ \nabla_s f) \cdot \vec{\nu} - ((\nabla_s \vec{\mathcal{V}}) \nabla_s f) \cdot \vec{\nu}. \end{aligned}$$

As $\nabla_s \partial_t^\circ f$ is tangential, we obtain

$$(\partial_t^\circ \nabla_s f - \nabla_s \partial_t^\circ f) \cdot \vec{\nu} = ((\nabla_s \vec{\mathcal{V}}) \nabla_s f) \cdot \vec{\nu}.$$

We now identify the tangential part of $\partial_t^\circ \nabla_s f - \nabla_s \partial_t^\circ f$, recall (2.1). We compute, on noting (2.5), Remark 2.6(v), Remark 2.29(ii), Remark 2.8(iii), Lemma 2.7(ii) and Remark 2.6(iii) that

$$\begin{aligned} \underline{P}_\Gamma (\partial_t^\circ \nabla_s f - \nabla_s \partial_t^\circ f) &= \underline{P}_\Gamma \partial_t^\circ \nabla f - \nabla_s \partial_t^\circ f \\ &= \underline{P}_\Gamma (\partial_t \nabla f + (\nabla^2 f) \vec{\mathcal{V}}) - \nabla_s (\partial_t f + \vec{\mathcal{V}} \cdot \nabla f) \\ &= \underline{P}_\Gamma (\partial_t \nabla f + (\nabla^2 f) \vec{\mathcal{V}}) - \underline{P}_\Gamma \nabla \partial_t f - \nabla_s (\vec{\mathcal{V}} \cdot \nabla f) \\ &= \underline{P}_\Gamma (\nabla^2 f) \vec{\mathcal{V}} - (\nabla_s \vec{\mathcal{V}})^\top \nabla f - \underline{P}_\Gamma \sum_{i=1}^d \vec{\mathcal{V}} \cdot \vec{e}_i \nabla \partial_i f \\ &= -(\nabla_s \vec{\mathcal{V}})^\top \nabla_s f. \end{aligned}$$

Combining the above, on recalling Definition 2.5(vii) and Remark 2.6(v), yields that

$$\begin{aligned} \partial_t^\circ \nabla_s f - \nabla_s \partial_t^\circ f &= \underline{P}_\Gamma (\partial_t^\circ \nabla_s f - \nabla_s \partial_t^\circ f) + (\underline{\text{Id}} - \underline{P}_\Gamma) (\partial_t^\circ \nabla_s f - \nabla_s \partial_t^\circ f) \\ &= -(\nabla_s \vec{\mathcal{V}})^\top \nabla_s f + (\underline{\text{Id}} - \underline{P}_\Gamma) (\nabla_s \vec{\mathcal{V}}) \nabla_s f = [\nabla_s \vec{\mathcal{V}} - 2 \underline{D}_s(\vec{\mathcal{V}})] \nabla_s f, \end{aligned}$$

which shows the claim.

(ii) It follows from (i) and Remark 2.6(iii) that

$$\begin{aligned} (\partial_t^\circ \nabla_s \vec{f} - \nabla_s \partial_t^\circ \vec{f})^\top \vec{e}_i &= (\partial_t^\circ \nabla_s - \nabla_s \partial_t^\circ) (\vec{f} \cdot \vec{e}_i) \\ &= [\nabla_s \vec{\mathcal{V}} - 2 \underline{D}_s(\vec{\mathcal{V}})] (\nabla_s \vec{f})^\top \vec{e}_i, \end{aligned}$$

for $i = 1, \dots, d$, and this proves the desired result.

(iii) Using (ii) and Lemma 2.7(v), we compute

$$\begin{aligned} \partial_t^\circ (\nabla_s \cdot \vec{f}) - \nabla_s \cdot (\partial_t^\circ \vec{f}) &= \text{tr} \left(\partial_t^\circ (\nabla_s \vec{f}) - \nabla_s (\partial_t^\circ \vec{f}) \right) \\ &= \text{tr} \left((\nabla_s \vec{f}) [\nabla_s \vec{\mathcal{V}} - 2 \underline{D}_s(\vec{\mathcal{V}})]^\top \right) = [\nabla_s \vec{\mathcal{V}} - 2 \underline{D}_s(\vec{\mathcal{V}})] : \nabla_s \vec{f}, \end{aligned}$$

which yields the desired result. $\square$

We now obtain formulas for the time derivatives of the mean curvature.

Lemma 2.39. *Let $\mathcal{G}_T$ be a C^3 -evolving orientable hypersurface.*

(i) *Let $\vec{\mathcal{V}}_T$ be the tangential velocity field induced by a global parameterization of $\mathcal{G}_T$. Then it holds that*

$$\partial_t^\circ \varkappa = \Delta_s \mathcal{V} + \mathcal{V} |\nabla_s \vec{\nu}|^2 + \vec{\mathcal{V}}_T \cdot \nabla_s \varkappa \quad \text{on } \Gamma(t).$$

(ii) *The normal time derivative of the mean curvature satisfies*

$$\partial_t^\square \kappa = \Delta_s \mathcal{V} + \mathcal{V} |\nabla_s \vec{v}|^2 \quad \text{on } \Gamma(t).$$

Proof. (i) It follows from Lemma 2.13(i), Lemma 2.38(iii), Lemma 2.37(i), Lemma 2.27(ii), (iii) and Lemma 2.12 that

$$\begin{aligned} \partial_t^\circ \kappa &= -\partial_t^\circ (\nabla_s \cdot \vec{v}) = -\nabla_s \cdot (\partial_t^\circ \vec{v}) - [\nabla_s \vec{\mathcal{V}} - 2 \underline{D}_s(\vec{\mathcal{V}})] : \nabla_s \vec{v} \\ &= \nabla_s \cdot ((\nabla_s \vec{\mathcal{V}})^\top \vec{v}) + \mathcal{V} |\nabla_s \vec{v}|^2 + \nabla_s \vec{\mathcal{V}}_T : \nabla_s \vec{v} \\ &= \nabla_s \cdot (\nabla_s \mathcal{V} + (\nabla_s \vec{\mathcal{V}}_T)^\top \vec{v}) + \mathcal{V} |\nabla_s \vec{v}|^2 + \nabla_s \vec{\mathcal{V}}_T : \nabla_s \vec{v}. \end{aligned}$$

As $\vec{\mathcal{V}}_T \cdot \vec{v} = 0$, we obtain from Lemma 2.7(ii) and Lemma 2.12(ii) that $(\nabla_s \vec{\mathcal{V}}_T)^\top \vec{v} = -(\nabla_s \vec{v}) \vec{\mathcal{V}}_T$, and hence Lemma 2.7(i) implies that

$$\begin{aligned} \partial_t^\circ \kappa &= \Delta_s \mathcal{V} - \nabla_s \cdot ((\nabla_s \vec{v}) \vec{\mathcal{V}}_T) + \mathcal{V} |\nabla_s \vec{v}|^2 + \nabla_s \vec{\mathcal{V}}_T : \nabla_s \vec{v} \\ &= \Delta_s \mathcal{V} - (\Delta_s \vec{v}) \cdot \vec{\mathcal{V}}_T - \nabla_s \vec{v} : \nabla_s \vec{\mathcal{V}}_T + \mathcal{V} |\nabla_s \vec{v}|^2 + \nabla_s \vec{\mathcal{V}}_T : \nabla_s \vec{v} \\ &= \Delta_s \mathcal{V} - (\Delta_s \vec{v}) \cdot \vec{\mathcal{V}}_T + \mathcal{V} |\nabla_s \vec{v}|^2. \end{aligned}$$

Combining this with Lemma 2.16 yields the desired result.

(ii) On choosing an arbitrary global parameterization of $\mathcal{G}_T$, with induced tangential velocity field $\vec{\mathcal{V}}_T$, the claim follows from (i) and Definition 2.28(ii). $\square$

2.7 Gauss–Bonnet theorem

In the case $d = 3$, we can consider curves $\mathfrak{g}$ on a hypersurface Γ . For any curve in $\mathbb{R}^3$, we can define the curvature vector

$$\vec{\kappa}_{\mathfrak{g}} = \text{id}_{ss} \quad \text{on } \mathfrak{g}, \quad (2.14)$$

where ∂_s^2 denotes the second derivative with respect to arclength on γ . We note that (2.14) is invariant under a change of parameterization of the curve.

Later we will need the Gauss–Bonnet theorem, which uses (2.14) for the special case $\mathfrak{g} = \partial\Gamma \subset \Gamma$.

Theorem 2.40 (Gauss–Bonnet). *Let Γ be a compact orientable C^2 –hypersurface in $\mathbb{R}^3$. Then it holds that*

$$\int_{\Gamma} \mathcal{K} \, d\mathcal{H}^2 = 2\pi \, \text{m}(\Gamma) + \int_{\partial\Gamma} \vec{\kappa}_{\partial\Gamma} \cdot \vec{\mu} \, d\mathcal{H}^1,$$

where $\vec{\mu}$ is the outer unit conormal to $\partial\Gamma$, and where $\text{m}(\Gamma) \in \mathbb{Z}$ is the Euler characteristic of Γ .

For a definition of the Euler characteristic and a proof of the Gauss–Bonnet formula we refer to Kühnel (2015, §4F).

3 Parametric finite elements

In this section we discuss the main concepts that are necessary for the numerical approximation of curvature driven evolution equations with the help of parametric finite elements. Readers familiar with these concepts, and readers more interested in the actual finite element approximations discussed in this work, may skip this section and go directly to the appropriate sections below.

3.1 Polyhedral surfaces

In order to approximate a smooth surface we use polyhedral surfaces as follows. The idea of using polyhedral surfaces to approximate the curvature driven evolution of hypersurfaces goes back to Dziuk (1991).

Definition 3.1.

- (i) *A subset $\Gamma^h \subset \mathbb{R}^d$ is called an n -dimensional polyhedral surface for $1 \leq n \leq d$, with or without boundary, if it is the finite union of closed, nondegenerate n -simplices, where the intersection of any two simplices is either empty or a common k -simplex, $0 \leq k < n$.*
- (ii) *If $n = d - 1$, then we call Γ^h a polyhedral hypersurface.*
- (iii) *If $n = 1$, then we call Γ^h a polygonal curve.*

Remark 3.2.

- (i) *The boundary of a polyhedral surface Γ^h , as a C^0 -surface, is defined as in Definition 2.17, and is denoted by $\partial\Gamma^h$. Of course, $\partial\Gamma^h$ is given as the union of all $(n - 1)$ -simplices, that form part of the boundary of exactly one of the n -simplices that make up Γ^h . If $\partial\Gamma^h$ is empty, then we call Γ^h a closed polyhedral surface.*
- (ii) *For a polyhedral hypersurface Γ^h with boundary, the outer conormal to Γ^h is well-defined almost everywhere on $\partial\Gamma^h$, where locally we use the definition Definition 2.20.*
- (iii) *In order to define geometric quantities for, and finite element spaces on polyhedral surfaces, it is often convenient to define Γ^h in terms of a triangulation. To this end, from now on, we let an n -dimensional polyhedral surface be given by*

$$\Gamma^h = \bigcup_{j=1}^J \overline{\sigma_j},$$

where $\{\sigma_j\}_{j=1}^J$ is a family of disjoint, (relatively) open n -simplices, such that $\overline{\sigma_i} \cap \overline{\sigma_j}$ for $i \neq j$ is either empty or a common k -simplex of $\overline{\sigma_i}$ and $\overline{\sigma_j}$, $0 \leq k < n$. For later use, we denote the vertices of Γ^h by $\{\vec{q}_k\}_{k=1}^K$, and assume that the vertices of σ_j are given by $\{\vec{q}_{j,k}\}_{k=1}^{n+1}$, $j = 1, \dots, J$.

Definition 3.3. Let $\Gamma^h = \bigcup_{j=1}^J \bar{\sigma}_j$ be an n -dimensional polyhedral surface, as described in Remark 3.2(iii), with vertices $\{\vec{q}_k\}_{k=1}^K$.

- (i) We define the finite element spaces of continuous piecewise linear functions on Γ^h via

$$\begin{aligned} V(\Gamma^h) &= \{\chi \in C(\Gamma^h) : \chi|_{\sigma_j} \text{ is affine for } j = 1, \dots, J\}, \\ \underline{V}(\Gamma^h) &= [V(\Gamma^h)]^d, \quad \underline{\underline{V}}(\Gamma^h) = [V(\Gamma^h)]^{d \times d}. \end{aligned}$$

We let $\{\phi_k^{\Gamma^h}\}_{k=1}^K$ denote the standard basis of $V(\Gamma^h)$, i.e.

$$\phi_i^{\Gamma^h}(\vec{q}_j) = \delta_{ij}, \quad i, j = 1, \dots, K.$$

Moreover, we let $\pi_{\Gamma^h} : C(\Gamma^h) \rightarrow V(\Gamma^h)$ be the standard interpolation operator, i.e.

$$\pi_{\Gamma^h} \eta = \sum_{k=1}^K \eta(\vec{q}_k) \phi_k^{\Gamma^h} \quad \forall \eta \in C(\Gamma^h),$$

and similarly $\bar{\pi}_{\Gamma^h} : [C(\Gamma^h)]^d \rightarrow \underline{V}(\Gamma^h)$.

- (ii) We define the spaces of piecewise constant functions on Γ^h via

$$\begin{aligned} V_c(\Gamma^h) &= \{\chi \in L^\infty(\Gamma^h) : \chi|_{\sigma_j} \text{ is constant for } j = 1, \dots, J\}, \\ \underline{V}_c(\Gamma^h) &= [V_c(\Gamma^h)]^d, \quad \underline{\underline{V}}_c(\Gamma^h) = [V_c(\Gamma^h)]^{d \times d}. \end{aligned}$$

- (iii) We let $\langle \cdot, \cdot \rangle_{\Gamma^h}$ denote the L^2 -inner product on Γ^h , with $|\cdot|_{\Gamma^h}$ the associated L^2 -norm, and we extend these definitions to any n -dimensional piecewise C^1 -surface Γ . For piecewise continuous, $u, v \in L^\infty(\Gamma^h)$, with possible jumps across the edges of $\{\sigma_j\}_{j=1}^J$, we introduce the mass lumped inner product $\langle \cdot, \cdot \rangle_{\Gamma^h}^h$ as

$$\langle u, v \rangle_{\Gamma^h}^h = \frac{1}{n+1} \sum_{j=1}^J \mathcal{H}^n(\sigma_j) \sum_{k=1}^{n+1} (u v)((\vec{q}_{j,k})^-), \quad (3.1)$$

where $u((\vec{q})^-) = \lim_{\sigma_j \ni \vec{p} \rightarrow \vec{q}} u(\vec{p})$. The definition (3.1) is naturally extended to vector- and tensor-valued functions. We also let

$$|u|_{\Gamma^h}^h = \left(\langle u, u \rangle_{\Gamma^h}^h \right)^{\frac{1}{2}}, \quad (3.2)$$

which on $V(\Gamma^h)$ defines the norm induced by (3.1). We extend (3.2) to vector-valued functions to obtain a norm on $\underline{V}(\Gamma^h)$.

Remark 3.4. It follows from Definition 3.3 that

$$\langle \eta, 1 \rangle_{\Gamma^h}^h = \langle \pi_{\Gamma^h} \eta, 1 \rangle_{\Gamma^h} \quad \forall \eta \in C(\Gamma^h).$$

3.1.1 Orientation

In order to discuss the orientation of a polyhedral hypersurface, we begin with the definition of the wedge product in $\mathbb{R}^d$.

Definition 3.5. Let $\vec{v}_1, \dots, \vec{v}_{d-1} \in \mathbb{R}^d$. Then the wedge product

$$\vec{z} = \vec{v}_1 \wedge \dots \wedge \vec{v}_{d-1}$$

is the unique vector $\vec{z} \in \mathbb{R}^d$ such that $\vec{b} \cdot \vec{z} = \det(\vec{v}_1, \dots, \vec{v}_{d-1}, \vec{b})$ for all $\vec{b} \in \mathbb{R}^d$.

Remark 3.6.

- (i) The wedge product is the usual cross product of two vectors in $\mathbb{R}^3$, and the anti-clockwise rotation through $\frac{\pi}{2}$ of a vector in $\mathbb{R}^2$.
- (ii) The wedge product $\vec{v}_1 \wedge \dots \wedge \vec{v}_{d-1}$ is perpendicular to each of the $(d-1)$ vectors $\vec{v}_1, \dots, \vec{v}_{d-1}$, and has length equal to the volume of the parallelotope spanned by them.
- (iii) The measure of a $(d-1)$ -simplex σ , with vertices $\{\vec{q}_k\}_{k=1}^d$, can be computed via

$$\mathcal{H}^{d-1}(\sigma) = \frac{1}{d-1} |(\vec{q}_2 - \vec{q}_1) \wedge \dots \wedge (\vec{q}_d - \vec{q}_1)|.$$

We recall the following definition of orientable polyhedral hypersurface from Matveev (2006, p. 20).

Definition 3.7. We say that the polyhedral hypersurface $\Gamma^h = \bigcup_{j=1}^J \overline{\sigma_j}$ is orientable, if it is possible to consistently orientate the simplices $\{\sigma_j\}_{j=1}^J$, e.g. by choosing the order $\{\vec{q}_{j,k}\}_{k=1}^d$ for the vertices of σ_j , $j = 1, \dots, J$, in such a way, that on nonempty intersections $\overline{\sigma_i} \cap \overline{\sigma_j}$ that form a $(d-2)$ -simplex, the two orientations induced by σ_i and σ_j are opposite to each other.

Remark 3.8. For a polyhedral hypersurface in $\mathbb{R}^3$, each triangle is oriented by choosing a direction around the boundary of the triangle. On each triangle, this gives a direction to every edge of the triangle. If this can be done in such a way, that two neighbouring edges are always pointing in the opposite direction, then the surface is orientable. An example for a non-orientable polyhedral hypersurface in $\mathbb{R}^3$ is a triangulation of the Möbius strip. Of course, for $d = 2$ we are dealing with polygonal curves, and they are always orientable.

Definition 3.9. Let $\Gamma^h = \bigcup_{j=1}^J \overline{\sigma_j}$ be an orientable polyhedral hypersurface Γ^h , with a consistent ordering of the vertices $\{\vec{q}_{j,k}\}_{k=1}^d$ for each σ_j , $j = 1, \dots, J$. Then we define the consistent, piecewise constant unit normal $\vec{\nu}^h \in \underline{V}_c(\Gamma^h)$ via

$$\vec{\nu}^h = \frac{(\vec{q}_{j,2} - \vec{q}_{j,1}) \wedge \dots \wedge (\vec{q}_{j,d} - \vec{q}_{j,1})}{|(\vec{q}_{j,2} - \vec{q}_{j,1}) \wedge \dots \wedge (\vec{q}_{j,d} - \vec{q}_{j,1})|} \quad \text{on } \sigma_j,$$

$j = 1, \dots, J$, recall Definition 3.5.

Remark 3.10. *Of course, changing the orientation of Γ^h will change the sign of $\vec{v}^h$. For the majority of the approximations introduced in this work, the choice of normal is not important. We will clearly state the choice of the sign of $\vec{v}^h$ in situations where it is critical.*

Definition 3.11. *Let Γ^h be an orientable polyhedral hypersurface with unit normal $\vec{v}^h$. Then we define the vertex normal vector $\vec{\omega}^h \in \underline{V}(\Gamma^h)$ to be the mass-lumped L^2 -projection of $\vec{v}^h$ onto $\underline{V}(\Gamma^h)$, i.e.*

$$\langle \vec{\omega}^h, \vec{\varphi} \rangle_{\Gamma^h}^h = \langle \vec{v}^h, \vec{\varphi} \rangle_{\Gamma^h} \quad \forall \vec{\varphi} \in \underline{V}(\Gamma^h). \quad (3.3)$$

Remark 3.12. *It is easy to see that, for $k = 1, \dots, K$,*

$$\vec{\omega}^h(\vec{q}_k) = \frac{1}{\mathcal{H}^{d-1}(\Lambda_k)} \sum_{\sigma_j \in \mathcal{T}_k} \mathcal{H}^{d-1}(\sigma_j) \vec{v}_{|\sigma_j}^h, \quad (3.4)$$

where

$$\Lambda_k = \bigcup_{\sigma_j \in \mathcal{T}_k} \overline{\sigma_j} \quad \text{and} \quad \mathcal{T}_k = \{\sigma_j : \vec{q}_k \in \overline{\sigma_j}\}.$$

In particular, we note that one can interpret $\vec{\omega}^h(\vec{q}_k)$ as a weighted normal at the vertex $\vec{q}_k$ of Γ^h . It follows from (3.1) and (3.3) that

$$\langle \chi \vec{\omega}^h, \vec{\varphi} \rangle_{\Gamma^h}^h = \langle \chi \vec{v}^h, \vec{\varphi} \rangle_{\Gamma^h}^h \quad \forall \chi \in V(\Gamma^h), \vec{\varphi} \in \underline{V}(\Gamma^h). \quad (3.5)$$

Combining (3.5) and (3.3) yields that

$$\langle \vec{\omega}^h, \vec{\varphi} \rangle_{\Gamma^h}^h = \langle \vec{v}^h, \vec{\varphi} \rangle_{\Gamma^h}^h = \langle \vec{v}^h, \vec{\varphi} \rangle_{\Gamma^h} \quad \forall \vec{\varphi} \in \underline{V}(\Gamma^h). \quad (3.6)$$

3.1.2 Polygonal curves

Most of the above definitions simplify dramatically when Γ^h is a polygonal curve. Given a closed polygonal curve $\Gamma^h = \bigcup_{j=1}^J \overline{\sigma_j}$, we can parameterize Γ^h with the help of a finite element function defined on the periodic unit interval $\mathbb{I} = \mathbb{R}/\mathbb{Z}$.

Definition 3.13. *Let $\mathbb{I} = \bigcup_{j=1}^J I_j$ be decomposed into the intervals $I_j = [q_{j-1}, q_j]$, given by the nodes $q_j = jh$, $h = J^{-1}$, for $j = 0, \dots, J$. We make use of the periodicity of $\mathbb{R}/\mathbb{Z}$, i.e. $q_J = q_0$, $q_{J+1} = q_1$ and so on.*

- (i) *We define the finite element spaces of periodic, continuous piecewise linear functions in $\mathbb{I}$ via*

$$\begin{aligned} V^h(\mathbb{I}) &= \{\chi \in C(\mathbb{I}) : \chi|_{I_j} \text{ is affine for } j = 1, \dots, J\}, \\ \underline{V}^h(\mathbb{I}) &= [V^h(\mathbb{I})]^d. \end{aligned}$$

- (ii) We let $\langle \cdot, \cdot \rangle_{\mathbb{I}}$ denote the L^2 -inner product on $\mathbb{I}$. For piecewise continuous functions, $u, v \in L^\infty(\mathbb{I})$, with possible jumps at the nodes $\{q_j\}_{j=1}^J$, we introduce the mass lumped inner product on $\mathbb{I}$ as

$$\langle u, v \rangle_{\mathbb{I}}^h = \frac{1}{2} h \sum_{j=1}^J [(u v)(q_j^-) + (u v)(q_{j-1}^+)].$$

Remark 3.14. Given a closed polygonal curve $\Gamma^h = \bigcup_{j=1}^J \overline{\sigma_j}$, we can now find a function $\vec{X}^h \in \underline{V}^h(\mathbb{I})$ such that $\Gamma^h = \vec{X}^h(\mathbb{I})$. Then the following hold.

- (i) It follows Remark 2.8(i) that

$$\begin{aligned} (\nabla_s f) \circ \vec{X}^h &= \partial_s (f \circ \vec{X}^h) \vec{X}_s^h && \text{in } I_j, \\ (\nabla_s \cdot \vec{f}) \circ \vec{X}^h &= \partial_s (\vec{f} \circ \vec{X}^h) \cdot \vec{X}_s^h && \text{in } I_j, \end{aligned}$$

for $j = 1, \dots, J$, where $\vec{X}_s^h = \partial_s \vec{X}^h$ and $\partial_s = |\partial_1 \vec{X}^h|^{-1} \partial_1$ denotes differentiation with respect to the arclength of Γ^h . From now on we define the shorthand notation $\vec{X}_\rho^h = \partial_1 \vec{X}^h$, i.e. $\rho \in \mathbb{I}$ plays the role of the parameterization variable.

- (ii) We have that

$$\langle f, 1 \rangle_{\Gamma^h} = \left\langle f \circ \vec{X}^h, |\vec{X}_\rho^h| \right\rangle_{\mathbb{I}} \quad \text{and} \quad \langle f, 1 \rangle_{\Gamma^h}^h = \left\langle f \circ \vec{X}^h, |\vec{X}_\rho^h| \right\rangle_{\mathbb{I}}^h.$$

- (iii) For the normal $\vec{\nu}^h$ on Γ^h defined as in Definition 3.9 and Remark 3.6(i), it holds that

$$\vec{\nu}^h \circ \vec{X}^h = -(\vec{X}_s^h)^\perp \quad \text{in } I_j, \quad (3.7)$$

if $\overline{\sigma_j} = [\vec{q}_{j,1}^h, \vec{q}_{j,2}^h] = [\vec{X}^h(q_{j-1}), \vec{X}^h(q_j)]$, for $j = 1, \dots, J$. Here $\cdot^\perp$, acting on $\mathbb{R}^2$, denotes clockwise rotation by $\frac{\pi}{2}$.

- (iv) In order to find a simple expression for the vertex normal $\vec{\omega}^h$ on Γ^h defined as in Definition 3.11, we let $\vec{h}_j = \vec{X}^h(q_j) - \vec{X}^h(q_{j-1})$, $j = 1, \dots, J+1$, which according to Definition 3.1(i) are nonzero. Then (3.7) reduces to

$$(\vec{\nu}^h \circ \vec{X}^h)|_{I_j} = \vec{\nu}_j^h = -\frac{\vec{h}_j^\perp}{|\vec{h}_j|} \quad j = 1, \dots, J+1.$$

Hence, on recalling (3.4), we obtain the weighted vertex normals

$$\begin{aligned} \vec{\omega}^h(\vec{X}^h(q_j)) &= \frac{|\vec{h}_j| \vec{\nu}_j^h + |\vec{h}_{j+1}| \vec{\nu}_{j+1}^h}{|\vec{h}_j| + |\vec{h}_{j+1}|} = -\frac{(\vec{h}_j + \vec{h}_{j+1})^\perp}{|\vec{h}_j| + |\vec{h}_{j+1}|} \\ &= -\frac{(\vec{X}^h(q_{j+1}) - \vec{X}^h(q_{j-1}))^\perp}{|\vec{h}_j| + |\vec{h}_{j+1}|} \quad j = 1, \dots, J. \end{aligned} \quad (3.8)$$

3.2 Stability estimates

Lemma 3.15. *Let $\Gamma^h = \bigcup_{j=1}^J \overline{\sigma_j}$ be a two-dimensional polyhedral surface. Then we have for $j = 1, \dots, J$ that*

$$\frac{1}{2} \int_{\sigma_j} |\nabla_s \vec{X}|^2 d\mathcal{H}^2 \geq \mathcal{H}^2(\vec{X}(\sigma_j)) \quad \forall \vec{X} \in \underline{V}(\Gamma^h) \quad (3.9)$$

with equality for $\vec{X} = \text{id}|_{\Gamma^h} \in \underline{V}(\Gamma^h)$.

Proof. We note that the integrands in (3.9) are constant. In particular, we recall from Definition 2.5(iv) that, for $\vec{X} \in \underline{V}(\Gamma^h)$,

$$\nabla_s \vec{X} = \sum_{i=1}^2 (\partial_{\vec{\tau}_i} \vec{X}) \otimes \vec{\tau}_i \quad \text{and} \quad |\nabla_s \vec{X}|^2 = \sum_{i=1}^2 |\partial_{\vec{\tau}_i} \vec{X}|^2 \quad \text{on } \sigma_j, \quad (3.10a)$$

and so

$$\nabla_s \text{id} = \sum_{i=1}^2 \vec{\tau}_i \otimes \vec{\tau}_i \quad \text{and} \quad |\nabla_s \text{id}|^2 = 2 \quad \text{on } \sigma_j, \quad (3.10b)$$

where $\{\vec{\tau}_1, \vec{\tau}_2\}$ is an orthonormal basis for the tangent plane of σ_j . Moreover, it holds that

$$\mathcal{H}^2(\vec{X}(\sigma_j)) = \int_{\sigma_j} \sqrt{g} d\mathcal{H}^2, \quad (3.11)$$

where, similarly to (2.7) and (2.2),

$$g = \det \left(\partial_{\vec{\tau}_i} \vec{X} \cdot \partial_{\vec{\tau}_j} \vec{X} \right)_{i,j=1,2} = |\partial_{\vec{\tau}_1} \vec{X}|^2 |\partial_{\vec{\tau}_2} \vec{X}|^2 - \left(\partial_{\vec{\tau}_1} \vec{X} \cdot \partial_{\vec{\tau}_2} \vec{X} \right)^2.$$

Next, we note that

$$\sqrt{g} \leq |\partial_{\vec{\tau}_1} \vec{X}| |\partial_{\vec{\tau}_2} \vec{X}| \leq \frac{1}{2} \left(|\partial_{\vec{\tau}_1} \vec{X}|^2 + |\partial_{\vec{\tau}_2} \vec{X}|^2 \right), \quad (3.12)$$

with equality if and only if $\partial_{\vec{\tau}_1} \vec{X} \cdot \partial_{\vec{\tau}_2} \vec{X} = 0$ and $|\partial_{\vec{\tau}_1} \vec{X}| = |\partial_{\vec{\tau}_2} \vec{X}|$. The desired results (3.9) then follow immediately on combining (3.10), (3.11) and (3.12). $\square$

Remark 3.16. *A result like that in Lemma 3.15 is not true for an n -dimensional polyhedral surface with $n \neq 2$. In this case*

$$\mathcal{H}^n(\vec{X}(\sigma_j)) = \int_{\sigma_j} \sqrt{g} d\mathcal{H}^n,$$

where $g = \det \left(\partial_{\vec{\tau}_i} \vec{X} \cdot \partial_{\vec{\tau}_j} \vec{X} \right)_{i,j=1,\dots,n}$, with $\{\vec{\tau}_1, \dots, \vec{\tau}_n\}$ being an orthonormal basis for the tangent space of σ_j , scales with respect to $\vec{X}$ with the power n . Whereas

$$|\nabla_s \vec{X}|^2 = \sum_{i=1}^n \left| \partial_{\vec{\tau}_i} \vec{X} \right|^2$$

scales to the power two. Hence a simple scaling argument shows that there can be no constant c_0 such that

$$c_0 \int_{\sigma_j} |\nabla_s \vec{X}|^2 d\mathcal{H}^n \geq \mathcal{H}^n(\vec{X}(\sigma_j)) \quad \forall \vec{X} \in \underline{V}(\Gamma^h).$$

This shows that the estimate in Lemma 3.15 can only be used for 2-dimensional polyhedral surfaces.

Despite the above remark, we are able to prove the following crucial stability bound, which will be extensively used in later sections, for $n = 1$ as well as for $n = 2$.

Lemma 3.17. *Let $\Gamma^h = \bigcup_{j=1}^J \overline{\sigma_j}$ be a n -dimensional polyhedral surface, and let $\vec{X} \in \underline{V}(\Gamma^h)$. Then it holds, in the case $n = 1$, that*

$$\left\langle \nabla_s \vec{X}, \nabla_s (\vec{X} - \text{id}) \right\rangle_{\Gamma^h} \geq \mathcal{H}^1(\vec{X}(\Gamma^h)) - \mathcal{H}^1(\Gamma^h) + \left| |\nabla_s \vec{X}| - 1 \right|_{\Gamma^h}^2.$$

Moreover, in the case $n = 2$, we have that

$$\left\langle \nabla_s \vec{X}, \nabla_s (\vec{X} - \text{id}) \right\rangle_{\Gamma^h} \geq \mathcal{H}^2(\vec{X}(\Gamma^h)) - \mathcal{H}^2(\Gamma^h) + \frac{1}{2} \left| \nabla_s (\vec{X} - \text{id}) \right|_{\Gamma^h}^2.$$

Proof. For $n = 2$ it follows from Lemma 3.15 that

$$\begin{aligned} & \left\langle \nabla_s \vec{X}, \nabla_s (\vec{X} - \text{id}) \right\rangle_{\Gamma^h} \\ &= \frac{1}{2} \left[\left| \nabla_s \vec{X} \right|_{\Gamma^h}^2 - \left| \nabla_s \text{id} \right|_{\Gamma^h}^2 + \left| \nabla_s (\vec{X} - \text{id}) \right|_{\Gamma^h}^2 \right] \\ &\geq \mathcal{H}^2(\vec{X}(\Gamma^h)) - \mathcal{H}^2(\Gamma^h) + \frac{1}{2} \left| \nabla_s (\vec{X} - \text{id}) \right|_{\Gamma^h}^2. \end{aligned}$$

For $n = 1$, we let $\vec{h}_j = \vec{q}_{j,2} - \vec{q}_{j,1}$, and similarly $\vec{h}_j^{\vec{X}} = \vec{X}(\vec{q}_{j,2}) - \vec{X}(\vec{q}_{j,1})$, for $j = 1, \dots, J$. Then, on using ideas from Dziuk (1999b, Theorem 2), it follows from the Cauchy–Schwarz inequality that

$$\begin{aligned} \left\langle \nabla_s \vec{X}, \nabla_s (\vec{X} - \text{id}) \right\rangle_{\Gamma^h} &= \sum_{j=1}^J \left[\frac{|\vec{h}_j^{\vec{X}}|^2 - \vec{h}_j^{\vec{X}} \cdot \vec{h}_j}{|\vec{h}_j|} \right] \\ &= \sum_{j=1}^J \left[\frac{(|\vec{h}_j^{\vec{X}}| - |\vec{h}_j|)^2 + |\vec{h}_j^{\vec{X}}| |\vec{h}_j| - \vec{h}_j^{\vec{X}} \cdot \vec{h}_j}{|\vec{h}_j|} + |\vec{h}_j^{\vec{X}}| - |\vec{h}_j| \right] \\ &\geq \sum_{j=1}^J \left[|\vec{h}_j^{\vec{X}}| - |\vec{h}_j| + \left(\frac{|\vec{h}_j^{\vec{X}}|}{|\vec{h}_j|} - \frac{|\vec{h}_j|}{|\vec{h}_j|} \right)^2 |\vec{h}_j| \right] \\ &= \mathcal{H}^1(\vec{X}(\Gamma^h)) - \mathcal{H}^1(\Gamma^h) + \left| |\nabla_s \vec{X}| - 1 \right|_{\Gamma^h}^2. \end{aligned} \tag{3.13}$$

□

The result in Lemma 3.17 is relevant for semi-implicit time discretizations. For fully implicit discretizations we need the following result.

Lemma 3.18. *Let $\Gamma^h = \bigcup_{j=1}^J \bar{\sigma}_j$ be a polygonal curve, and let $\vec{X} \in \underline{V}(\Gamma^h)$. Then it holds that*

$$\left\langle \nabla_s \vec{\text{id}}, \nabla_s (\vec{\text{id}} - \vec{X}) \right\rangle_{\Gamma^h} \geq \mathcal{H}^1(\Gamma^h) - \mathcal{H}^1(\vec{X}(\Gamma^h)).$$

Proof. Using the same notation as in the proof of Lemma 3.17, we have that

$$\begin{aligned} \left\langle \nabla_s \vec{\text{id}}, \nabla_s (\vec{\text{id}} - \vec{X}) \right\rangle_{\Gamma^h} &= \sum_{j=1}^J \left[\frac{|\vec{h}_j|^2 - \vec{h}_j \cdot \vec{h}_j^{\vec{X}}}{|\vec{h}_j|} \right] \\ &\geq \sum_{j=1}^J \left[|\vec{h}_j| - |\vec{h}_j^{\vec{X}}| \right] = \mathcal{H}^1(\Gamma^h) - \mathcal{H}^1(\vec{X}(\Gamma^h)). \end{aligned}$$

□

Remark 3.19. *A result analogous to Lemma 3.18 for n -dimensional polyhedral surfaces with $n > 1$ is not true. To see this, we construct the following counterexample. Let Γ^h be given by a single n -simplex, and let $\{\vec{\tau}_1, \dots, \vec{\tau}_n\}$ be an orthonormal basis for the tangent space of Γ^h . Now choose $\vec{X} \in \underline{V}(\Gamma^h)$ such that $\partial_{\vec{\tau}_1} \vec{X} = \alpha \vec{\tau}_1$ and $\partial_{\vec{\tau}_i} \vec{X} = \varepsilon \vec{\tau}_i$, $i = 2, \dots, n$, for $\alpha, \varepsilon \in \mathbb{R}_{>0}$. Then it holds that $\mathcal{H}^n(\vec{X}(\Gamma^h)) = \int_{\Gamma^h} \sqrt{\det \left(\partial_{\vec{\tau}_i} \vec{X} \cdot \partial_{\vec{\tau}_j} \vec{X} \right)_{i,j=1,\dots,n}} d\mathcal{H}^n = \alpha \varepsilon^{n-1} \mathcal{H}^n(\Gamma^h)$. Moreover, $|\nabla_s \vec{\text{id}}|^2 = n$ and $\nabla_s \vec{\text{id}} : \nabla_s \vec{X} = \alpha + (n-1)\varepsilon$ on Γ^h , and so*

$$\left\langle \nabla_s \vec{\text{id}}, \nabla_s (\vec{\text{id}} - \vec{X}) \right\rangle_{\Gamma^h} \geq \mathcal{H}^n(\Gamma^h) - \mathcal{H}^n(\vec{X}(\Gamma^h))$$

is equivalent to $n - (\alpha + (n-1)\varepsilon) \geq 1 - \alpha \varepsilon^{n-1}$, and hence to $(n-1)(1-\varepsilon) \geq \alpha(1-\varepsilon^{n-1})$. Choosing $\varepsilon \in (0, 1)$ and $\alpha > (n-1) \frac{1-\varepsilon}{1-\varepsilon^{n-1}}$ yields a contradiction.

3.3 Curvature approximations

Given a polyhedral hypersurface $\Gamma^h = \bigcup_{j=1}^J \bar{\sigma}_j$, it is clear from Definition 2.5 that first order differential operators are well-defined almost everywhere on Γ^h , for example for functions in $V(\Gamma^h)$ or $\underline{V}(\Gamma^h)$. However, second order operators are not.

That means that discrete curvature approximations need to be defined in a suitable way. For everything that follows we assume that Γ^h is a closed hypersurface.

One way is to define the discrete Laplace–Beltrami operator $\Delta_s^{\Gamma^h} : V(\Gamma^h) \rightarrow V(\Gamma^h)$ via

$$\left\langle \Delta_s^{\Gamma^h} \chi, \zeta \right\rangle_{\Gamma^h}^h = - \left\langle \nabla_s \chi, \nabla_s \zeta \right\rangle_{\Gamma^h} \quad \forall \zeta \in V(\Gamma^h), \quad (3.14)$$

which is a discrete analogue of Remark 2.22(i). As usual, for $\vec{\chi} \in \underline{V}(\Gamma^h)$, we define $\Delta_s^{\Gamma^h} \vec{\chi}$ component-wise. Then a possible approximation to the curvature vector, recall Lemma 2.13(ii), is $\vec{\kappa}^h = \Delta_s^{\Gamma^h} \vec{\text{id}}$, i.e. $\vec{\kappa}^h \in \underline{V}(\Gamma^h)$ is the unique solution to

$$\left\langle \vec{\kappa}^h, \vec{\eta} \right\rangle_{\Gamma^h}^h = - \left\langle \nabla_s \vec{\text{id}}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h} \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h). \quad (3.15)$$

Of course, $\vec{\kappa}^h$ gives both an approximation to the mean curvature, as well as a notion of a vertex normal direction, which in general will be different to the direction defined by Definition 3.11.

Some special polyhedral hypersurfaces allow an alternative definition of mean curvature.

Definition 3.20. *A closed orientable polyhedral hypersurface Γ^h , with unit normal $\vec{\nu}^h$, is called a conformal polyhedral hypersurface, if there exists a $\kappa^h \in V(\Gamma^h)$ such that*

$$\langle \kappa^h \vec{\nu}^h, \vec{\eta} \rangle_{\Gamma^h}^h = - \langle \nabla_s \text{id}, \nabla_s \vec{\eta} \rangle_{\Gamma^h} \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h). \quad (3.16)$$

Remark 3.21.

- (i) *For a conformal polyhedral hypersurface Γ^h , the two vertex normal directions defined by $\vec{\kappa}^h$ in (3.15) and $\vec{\omega}^h$ in Definition 3.11 agree, i.e. the two vectors are parallel at each vertex of Γ^h . In particular, on recalling (3.5), it holds that*

$$\vec{\pi}_{\Gamma^h} [\kappa^h \vec{\omega}^h] = \vec{\kappa}^h.$$

- (ii) *It is discussed in Barrett et al. (2008a, §4.1) that for $d = 3$ the geometric property from (i) means that the triangulation of Γ^h is characterized by a good mesh quality. In the case $d = 2$ it holds that any conformal polygonal curve is weakly equidistributed, see the following theorem.*

Theorem 3.22. *Let Γ^h be a closed conformal polygonal curve in $\mathbb{R}^2$, as defined in Definition 3.20. Then any two neighbouring elements on Γ^h either have equal length, or they are parallel.*

Proof. We choose a $\vec{X}^h \in \underline{V}^h(\mathbb{I})$ with $\Gamma^h = \vec{X}^h(\mathbb{I})$. Then it follows from Remark 3.14 and Definition 3.20 that there exists a $\kappa^h \in V^h(\mathbb{I})$ such that

$$\left\langle \kappa^h \vec{\omega}^h \circ \vec{X}^h, \vec{\eta} |\vec{X}_\rho^h| \right\rangle_{\mathbb{I}}^h = - \left\langle \vec{X}_s^h, \vec{\eta}_s |\vec{X}_\rho^h| \right\rangle_{\mathbb{I}} \quad \forall \vec{\eta} \in \underline{V}^h(\mathbb{I}). \quad (3.17)$$

On using the notation from Remark 3.14(iv), we fix a $j \in \{1, \dots, J\}$, and then need to show that

$$|\vec{h}_j| = |\vec{h}_{j+1}| \quad \text{if} \quad \vec{h}_j \nparallel \vec{h}_{j+1}. \quad (3.18)$$

We recall from Definition 3.1(i) that $\vec{h}_j$ and $\vec{h}_{j+1}$ are nonzero. If $\vec{h}_j + \vec{h}_{j+1} = \vec{0}$, then (3.18) directly follows. Otherwise, we observe from (3.8) that

$$\vec{\omega}^h(\vec{X}^h(q_j)) = - \frac{\left(\vec{X}^h(q_{j+1}) - \vec{X}^h(q_{j-1}) \right)^\perp}{|\vec{h}_j| + |\vec{h}_{j+1}|}.$$

Hence choosing an $\vec{\eta} \in \underline{V}^h(\mathbb{I})$ in (3.17) with

$$\vec{\eta}(q_i) = \delta_{ij} \left(\vec{X}^h(q_{j+1}) - \vec{X}^h(q_{j-1}) \right) = \delta_{ij} \left(\vec{h}_j + \vec{h}_{j+1} \right),$$

for $i = 1, \dots, J$, we obtain

$$0 = \left(\frac{\vec{h}_{j+1}}{|\vec{h}_{j+1}|} - \frac{\vec{h}_j}{|\vec{h}_j|} \right) \cdot (\vec{h}_j + \vec{h}_{j+1}) = \frac{|\vec{h}_{j+1}| - |\vec{h}_j|}{|\vec{h}_j| |\vec{h}_{j+1}|} \left(|\vec{h}_j| |\vec{h}_{j+1}| - \vec{h}_j \cdot \vec{h}_{j+1} \right).$$

The Cauchy–Schwarz inequality now implies that $|\vec{h}_j| = |\vec{h}_{j+1}|$ if $\vec{h}_j$ and $\vec{h}_{j+1}$ are not parallel. $\square$

For polyhedral hypersurfaces that do not satisfy the special property in Definition 3.20, we can introduce a discrete mean curvature as follows. Find $(\vec{X}, \kappa^h) \in \underline{V}(\Gamma^h) \times V(\Gamma^h)$ such that

$$\left\langle \vec{X} - \text{id}, \chi \vec{\nu}^h \right\rangle_{\Gamma^h}^h = 0 \quad \forall \chi \in V(\Gamma^h), \quad (3.19a)$$

$$\left\langle \kappa^h \vec{\nu}^h, \vec{\eta} \right\rangle_{\Gamma^h}^h + \left\langle \nabla_s \vec{X}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h). \quad (3.19b)$$

Remark 3.23.

- (i) The system (3.19) can be viewed as a linearization of (3.16), where in some sense we allow Γ^h to deform slightly, by moving vertices tangentially.
- (ii) If $(\text{id}|_{\Gamma^h}, \kappa^h) \in \underline{V}(\Gamma^h) \times V(\Gamma^h)$ solves (3.19), then κ^h solves (3.16), and so Γ^h is a conformal polyhedral hypersurface.

Under a mild assumption, there exists a unique solution to the system (3.19).

Assumption 3.24. Let Γ^h be an orientable polyhedral hypersurface with unit normal $\vec{\nu}^h$ and vertex normal vector $\vec{\omega}^h \in \underline{V}(\Gamma^h)$.

- (i) Let $\dim \text{span}\{\vec{\omega}^h(\vec{q}_k)\}_{k=1}^K = d$.
- (ii) Let $\vec{\omega}^h(\vec{q}_k) \neq \vec{0}$, $k = 1, \dots, K$.

Remark 3.25. Assumption 3.24(i) means that the discrete vertex normals of Γ^h span the whole space $\mathbb{R}^d$. On recalling (3.3) we observe that Assumption 3.24(i) is equivalent to $\dim \left\{ \int_{\Gamma^h} \chi \vec{\nu}^h d\mathcal{H}^{d-1} : \chi \in V(\Gamma^h) \right\} = d$. Clearly, Assumption 3.24 is only violated in very rare occasions. For example, it always holds for surfaces Γ^h without self-intersections.

Lemma 3.26. Let Γ^h satisfy Assumption 3.24. Then there exists a unique solution $(\vec{X}, \kappa^h) \in \underline{V}(\Gamma^h) \times V(\Gamma^h)$ to (3.19).

Proof. As (3.19) is a linear system, where the number of unknowns equals the number of equations, it is enough to show uniqueness. We hence consider the homogeneous system and assume that $(\vec{X}_0, \kappa_0) \in \underline{V}(\Gamma^h) \times V(\Gamma^h)$ is such that

$$\left\langle \vec{X}_0, \chi \vec{\nu}^h \right\rangle_{\Gamma^h}^h = 0 \quad \forall \chi \in V(\Gamma^h), \quad (3.20a)$$

$$\left\langle \kappa_0 \vec{\nu}^h, \vec{\eta} \right\rangle_{\Gamma^h}^h + \left\langle \nabla_s \vec{X}_0, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h). \quad (3.20b)$$

Choosing $\chi = \kappa_0 \in V(\Gamma^h)$ in (3.20a) and $\vec{\eta} = \vec{X}_0 \in \underline{V}(\Gamma^h)$ in (3.20b) yields that $|\nabla_s \vec{X}_0|_{\Gamma^h}^2 = 0$, and so $\vec{X}_0$ is constant, i.e. $\vec{X}_0 = \vec{X}^c$ on Γ^h for $\vec{X}^c \in \mathbb{R}^d$. In particular, choosing $\vec{\eta} = \vec{\pi}_{\Gamma^h}[\kappa_0 \vec{\omega}^h]$ in (3.20b) yields, on recalling (3.5) and (3.2), that

$$0 = \langle \kappa_0 \vec{\omega}^h, \kappa_0 \vec{\omega}^h \rangle_{\Gamma^h}^h = \left(|\kappa_0 \vec{\omega}^h|_{\Gamma^h}^h \right)^2,$$

and so $\vec{\pi}_{\Gamma^h}[\kappa_0 \vec{\omega}^h] = \vec{0}$. Now Assumption 3.24(ii) yields that $\kappa_0 = 0$. Moreover, it follows from (3.20a), on recalling (3.6), that

$$0 = \langle \vec{X}^c, \chi \vec{\nu}^h \rangle_{\Gamma^h}^h = \langle \vec{X}^c, \chi \vec{\nu}^h \rangle_{\Gamma^h} = \vec{X}^c \cdot \int_{\Gamma^h} \chi \vec{\nu}^h d\mathcal{H}^{d-1} \quad \forall \chi \in V(\Gamma^h),$$

and so Assumption 3.24(i), recall Remark 3.25, implies that $\vec{X}^c = \vec{0}$. Hence we have shown that there exists a unique solution $(\vec{X}, \kappa^h) \in \underline{V}(\Gamma^h) \times V(\Gamma^h)$ to (3.19). $\square$

Further discrete curvature approximations can be obtained with the help of approximations to the Weingarten map, recall Definition 2.10 and Lemma 2.12. In particular, using Remark 2.22(v) leads to the following discretization of $\nabla_s \vec{\nu}$, which goes back to Heine (2004, (3.2)). Given a closed polyhedral hypersurface Γ^h and a curvature vector approximation $\vec{\kappa}^h \in \underline{V}(\Gamma^h)$, find $\underline{W}^h \in \underline{V}(\Gamma^h)$ such that

$$\langle \underline{W}^h, \underline{\chi} \rangle_{\Gamma^h} = -\langle \vec{\kappa}^h, \underline{\chi} \vec{\nu}^h \rangle_{\Gamma^h} - \langle \vec{\nu}^h, \nabla_s \cdot \underline{\chi} \rangle_{\Gamma^h} \quad \forall \underline{\chi} \in \underline{V}(\Gamma^h). \quad (3.21a)$$

For example, $\vec{\kappa}^h$ can be defined via (3.15), or via (3.15) without mass lumping, which corresponds to the choice in Heine (2004, (3.1)). We note that $\underline{W}^h$ is not necessarily symmetric, whereas $\nabla_s \vec{\nu}$ is, recall Lemma 2.12(ii). An alternative approximation of $\nabla_s \vec{\nu}$ replaces (3.21a) with

$$\langle \underline{W}^h, \underline{\chi} \rangle_{\Gamma^h}^h = -\frac{1}{2} \langle \vec{\nu}^h, (\underline{\chi} + \underline{\chi}^\top) \vec{\kappa}^h + \nabla_s \cdot (\underline{\chi} + \underline{\chi}^\top) \rangle_{\Gamma^h}^h \quad \forall \underline{\chi} \in \underline{V}(\Gamma^h), \quad (3.21b)$$

which yields $(\underline{W}^h)^\top = \underline{W}^h$, and which was considered, for example, in Barrett et al. (2017d, (4.12b)).

A slightly modified version of (3.21a) has been utilized in Barrett et al. (2008d), and is given as follows. Given Γ^h and a mean curvature approximation $\kappa^h \in V(\Gamma^h)$, find $\underline{W}^h \in \underline{V}(\Gamma^h)$ such that

$$\langle \underline{W}^h, \underline{\chi} \rangle_{\Gamma^h}^h = -\langle \kappa^h \vec{\nu}^h, \underline{\chi} \vec{\nu}^h \rangle_{\Gamma^h}^h - \langle \vec{\nu}^h, \nabla_s \cdot \underline{\chi} \rangle_{\Gamma^h} \quad \forall \underline{\chi} \in \underline{V}(\Gamma^h). \quad (3.21c)$$

Finally, piecewise constant approximations to $\nabla_s \vec{\nu}$ can be defined by

$$\nabla_s \vec{\omega}^h \in \underline{V}_c(\Gamma^h) \quad \text{and} \quad \nabla_s \left(\vec{\pi}_{\Gamma^h} \frac{\vec{\omega}^h}{|\vec{\omega}^h|} \right) \in \underline{V}_c(\Gamma^h), \quad (3.21d)$$

the latter of which clearly needs Assumption 3.24(ii) to hold, and has been employed in e.g. Barrett et al. (2008d). We note that the two approximations in (3.21d) are in general not symmetric.

Remark 3.27. For the case of curves, $d = 2$, and adopting the notation of §3.1.2, we set $\Gamma^h = \vec{X}^h(\mathbb{I})$, where $\vec{X}^h \in \underline{V}^h(\mathbb{I})$ interpolates $\vec{x}$ with $\Gamma = \vec{x}(\mathbb{I})$. Then it is shown in Deckelnick and Dziuk (2009, Lemma 2.2) that the approximation $\vec{\kappa}^h$ from (3.15) approximates the true curvature vector, $\vec{\kappa}$, of Γ with order $O(h)$ in $[L^2(\mathbb{I})]^2$ for smooth Γ . Unfortunately, for the case $d = 3$ it is shown in Heine (2004) that (3.15) and (3.21a) are not convergent on general meshes, see also Hildebrandt et al. (2006). Similar conclusions can be drawn from the numerical experiments in Barrett et al. (2008d, §4.2.1), and also apply to (3.21b–c). However, we note that the approximations (3.21d) and (3.19) behave better in practice, see Tables 2 and 5 and Tables 3 and 6 in Barrett et al. (2008d), respectively, for closely related approximations. Moreover, one can prove convergence for higher order piecewise continuous approximations of Γ and $\vec{\kappa}$, see Heine (2004). Even though (3.15) may not be convergent for continuous piecewise linears, it turns out that the use of such an approximation does lead to convergence in approximating geometric flows; see e.g. §4.7.1 below.

3.4 Evolving polyhedral surfaces and transport theorems

We now define discrete analogues to evolving hypersurfaces, their velocity fields and material time derivatives. For more details we refer to Dziuk and Elliott (2013, §5.4).

Definition 3.28.

- (i) Let $(\Gamma^h(t))_{t \in [0, T]}$ be a family of polyhedral hypersurfaces, such that each $\Gamma^h(t)$ admits a triangulation of the form Remark 3.2(iii) for fixed J and K , and such that the position of each vertex $\vec{q}_k$, $k = 1, \dots, K$, is a C^1 -function in time. Then the set

$$\mathcal{G}_T^h = \bigcup_{t \in [0, T]} (\Gamma^h(t) \times \{t\})$$

is called an evolving polyhedral hypersurface. We will often identify $\mathcal{G}_T^h$ with $(\Gamma^h(t))_{t \in [0, T]}$, and call the latter also an evolving polyhedral hypersurface.

- (ii) The velocity of $\Gamma^h(t)$ on $\mathcal{G}_T^h$ is defined by

$$\vec{\mathcal{V}}^h(\vec{z}, t) = \sum_{k=1}^K \left[\frac{d}{dt} \vec{q}_k(t) \right] \phi_k^{\Gamma^h(t)}(\vec{z}) \quad \forall (\vec{z}, t) \in \mathcal{G}_T^h,$$

where we have recalled the notation from Definition 3.3(i).

- (iii) We define the finite element spaces

$$V(\mathcal{G}_T^h) = \{\chi \in C(\mathcal{G}_T^h) : \chi(\cdot, t) \in V(\Gamma^h(t)) \quad \forall t \in [0, T]\}$$

and $\underline{V}(\mathcal{G}_T^h) = [V(\mathcal{G}_T^h)]^d$.

(iv) Let $f \in L^\infty(\mathcal{G}_T^h)$, with $f \in C^1(\mathcal{S}_{j,T}^h)$ for $j = 1, \dots, J$, where

$$\mathcal{S}_{j,T}^h = \bigcup_{t \in [0, T]} (\overline{\sigma_j(t)} \times \{t\})$$

is a C^1 -evolving hypersurface. For $j \in \{1, \dots, J\}$, let $\vec{x} : \Upsilon \times [0, T] \rightarrow \mathbb{R}^d$ be a global parameterization of $\mathcal{S}_{j,T}^h$ such that $\vec{x}(\cdot, t) : \Upsilon \rightarrow \overline{\sigma_j(t)}$ is an affine function. Then we define the discrete time derivative of f by

$$\partial_t^{\circ, h} f = \partial_t^\circ f \quad \text{on } \mathcal{S}_{j,T}^h,$$

recall Definition 2.28(i).

(v) We define the finite element spaces

$$V_T(\mathcal{G}_T^h) = \{\chi \in V(\mathcal{G}_T^h) : \partial_t^{\circ, h} \chi \in C(\mathcal{G}_T^h)\}$$

and $\underline{V}_T(\mathcal{G}_T^h) = [V_T(\mathcal{G}_T^h)]^d$ of finite element functions on $\mathcal{G}_T^h$ with a continuous material derivative.

Remark 3.29.

(i) On introducing the short hand notation $\phi_k^h(\cdot, t) = \phi_k^{\Gamma^h(t)}$, it holds that

$$\partial_t^{\circ, h} \phi_k^h = 0 \quad \text{on } \mathcal{G}_T^h, \quad k = 1, \dots, K.$$

(ii) In general the discrete material derivative $\partial_t^{\circ, h} f$ is only defined piecewise on $\mathcal{G}_T^h$. But a direct consequence of (i) is that for $\chi \in V(\mathcal{G}_T^h)$, with $\chi(\vec{q}_k(\cdot), \cdot) \in C^1([0, T])$, $k = 1, \dots, K$, it holds that

$$(\partial_t^{\circ, h} \chi)(\vec{z}, t) = \sum_{k=1}^K \left[\frac{d}{dt} \chi(\vec{q}_k(t), t) \right] \phi_k^{\Gamma^h(t)}(\vec{z}) \quad \forall (\vec{z}, t) \in \mathcal{G}_T^h,$$

i.e. we can choose a continuous representation of $\partial_t^{\circ, h} \chi$, and hence $\chi \in V_T(\mathcal{G}_T^h)$.

(iii) We have that $\vec{\mathcal{V}}^h \in \underline{V}(\mathcal{G}_T^h)$ with $\vec{\mathcal{V}}^h = \partial_t^{\circ, h} \text{id}$ on $\mathcal{G}_T^h$.

(iv) On extending f to a neighbourhood of $\mathcal{S}_{j,T}^h$, $j = 1, \dots, J$, it holds that

$$\partial_t^{\circ, h} f = \partial_t f + \vec{\mathcal{V}}^h \cdot \nabla f \quad \text{on } \mathcal{S}_{j,T}^h,$$

recall Remark 2.29(ii).

Theorem 3.30. Let $\mathcal{G}_T^h$ be an evolving polyhedral hypersurface, and let $\eta, \zeta \in V_T(\mathcal{G}_T^h)$.

(i) It holds that

$$\frac{d}{dt} \langle \eta, \zeta \rangle_{\Gamma^h(t)} = \left\langle \partial_t^{\circ, h} \eta, \zeta \right\rangle_{\Gamma^h(t)} + \left\langle \eta, \partial_t^{\circ, h} \zeta \right\rangle_{\Gamma^h(t)} + \left\langle \eta \zeta, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}.$$

(ii) It holds that

$$\frac{d}{dt} \langle \eta, \zeta \rangle_{\Gamma^h(t)}^h = \left\langle \partial_t^{\circ, h} \eta, \zeta \right\rangle_{\Gamma^h(t)}^h + \left\langle \eta, \partial_t^{\circ, h} \zeta \right\rangle_{\Gamma^h(t)}^h + \left\langle \eta \zeta, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h.$$

Proof. (i) Using the transport theorem, Theorem 2.32, on each evolving simplex $\sigma_j(t)$ of $\Gamma^h(t)$, and using the assumptions $\eta, \zeta \in V_T(\mathcal{G}_T^h)$, leads to

$$\begin{aligned} \frac{d}{dt} \langle \eta, \zeta \rangle_{\Gamma^h(t)} &= \frac{d}{dt} \sum_{j=1}^J \int_{\sigma_j(t)} \eta \zeta \, d\mathcal{H}^{d-1} \\ &= \sum_{j=1}^J \int_{\sigma_j(t)} \partial_t^{\circ, h} (\eta \zeta) + \eta \zeta \nabla_s \cdot \vec{\mathcal{V}}^h \, d\mathcal{H}^{d-1} \\ &= \left\langle \partial_t^{\circ, h} \eta, \zeta \right\rangle_{\Gamma^h(t)} + \left\langle \eta, \partial_t^{\circ, h} \zeta \right\rangle_{\Gamma^h(t)} + \left\langle \eta \zeta, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}. \end{aligned}$$

(ii) This proof is analogous to (i) and can be found in Barrett et al. (2015b, Lemma 3.1). $\square$

Theorem 3.31. Let $\mathcal{G}_T^h$ be an evolving polyhedral hypersurface, such that $\Gamma^h(t)$ is bounding a domain $\Omega^h(t) \subset \mathbb{R}^d$, for $t \in [0, T]$. We assume that $\vec{\nu}^h(t)$ is the outer unit normal to $\Omega^h(t)$ on $\Gamma^h(t)$, and that $f \in C^1(\mathfrak{D}_T^h)$, where

$$\mathfrak{D}_T^h = \bigcup_{t \in [0, T]} (\Omega^h(t) \times \{t\}).$$

Then it holds that

$$\frac{d}{dt} \int_{\Omega^h(t)} f \, d\mathcal{L}^d = \int_{\Omega^h(t)} \partial_t f \, d\mathcal{L}^d + \left\langle f, \vec{\mathcal{V}}^h \cdot \vec{\nu}^h \right\rangle_{\Gamma^h(t)}.$$

Proof. This follows as in Eck et al. (2017, §7.3) using a variant of the divergence theorem for Lipschitz domains. $\square$

3.5 Further results for evolving polyhedral surfaces

We state discrete analogues of Lemma 2.37 and Lemma 2.38.

Lemma 3.32. Let $\mathcal{G}_T^h$ be an evolving polyhedral hypersurface. Then it holds that

$$\partial_t^{\circ, h} \vec{\nu}^h = -(\nabla_s \vec{\mathcal{V}}^h)^\top \vec{\nu}^h \quad \text{a.e. on } \Gamma^h(t).$$

Proof. Similarly to the proof of Theorem 3.30(i), we appeal to Lemma 2.37(i) on each evolving simplex $\sigma_j(t)$ of $\Gamma^h(t)$. $\square$

Lemma 3.33. Let $\mathcal{G}_T^h$ be an evolving polyhedral hypersurface, and let $\eta \in V_T(\mathcal{G}_T^h)$, $\vec{\eta} \in \underline{V}_T(\mathcal{G}_T^h)$. Then we have the following results, where we recall from Definition 2.5(vii) that $\underline{D}_s(\vec{\mathcal{V}}^h) = \frac{1}{2} \underline{P}_{\Gamma^h} (\nabla_s \vec{\mathcal{V}}^h + (\nabla_s \vec{\mathcal{V}}^h)^\top) \underline{P}_{\Gamma^h}$ almost everywhere on $\Gamma^h(t)$.

(i)

$$\partial_t^{\circ,h} \nabla_s \eta - \nabla_s \partial_t^{\circ,h} \eta = [\nabla_s \vec{\mathcal{V}}^h - 2 \underline{\underline{D}}_s(\vec{\mathcal{V}}^h)] \nabla_s \eta \quad a.e. \text{ on } \Gamma^h(t).$$

(ii)

$$\partial_t^{\circ,h} \nabla_s \vec{\eta} - \nabla_s \partial_t^{\circ,h} \vec{\eta} = (\nabla_s \vec{\eta}) [\nabla_s \vec{\mathcal{V}}^h - 2 \underline{\underline{D}}_s(\vec{\mathcal{V}}^h)]^\top \quad a.e. \text{ on } \Gamma^h(t).$$

(iii)

$$\partial_t^{\circ,h} (\nabla_s \cdot \vec{\eta}) - \nabla_s \cdot (\partial_t^{\circ,h} \vec{\eta}) = [\nabla_s \vec{\mathcal{V}}^h - 2 \underline{\underline{D}}_s(\vec{\mathcal{V}}^h)] : \nabla_s \vec{\eta} \quad a.e. \text{ on } \Gamma^h(t).$$

Proof. Similarly to the proof of Theorem 3.30(i), we appeal to Lemma 2.38 on each evolving simplex $\sigma_j(t)$ of $\Gamma^h(t)$. $\square$

4 Mean curvature flow

The main ideas needed to numerically solve curvature driven evolution equations are most easily introduced with the help of the mean curvature flow. For a family of closed evolving hypersurfaces $(\Gamma(t))_{t \in [0, T]}$ in $\mathbb{R}^d$, $d \geq 2$, we consider at each time the total surface area $|\Gamma(t)| = \mathcal{H}^{d-1}(\Gamma(t))$. In this section we will only consider closed surfaces $\Gamma(t)$, i.e. surfaces which are compact and without boundary. The transport theorem, Theorem 2.32, gives

$$\frac{d}{dt} |\Gamma(t)| = - \langle \varkappa, \mathcal{V} \rangle_{\Gamma(t)}, \quad (4.1)$$

where $\varkappa$ is the mean curvature of $\Gamma(t)$, $\mathcal{V}$ is its normal velocity, and where we recall that $\langle \cdot, \cdot \rangle_{\Gamma(t)}$ denotes the L^2 -inner product on $\Gamma(t)$. Here we used that $\Gamma(t)$ has no boundary. We hence obtain that the geometric evolution law for an evolving hypersurface

$$\mathcal{V} = \varkappa \quad \text{on } \Gamma(t) \quad (4.2)$$

most efficiently decreases the surface area, and hence it is also called the L^2 -gradient flow of $|\Gamma(t)|$, see e.g. Mantegazza (2011); Garcke (2013) for details. This law is the most fundamental curvature driven evolution law and has been studied in detail both analytically and numerically, we refer to Huisken (1984); Gage and Hamilton (1986); Giga (2006); Mantegazza (2011); Garcke (2013) and Deckelnick et al. (2005a), and the references therein, for details.

4.1 Weak formulation

In this section we want to introduce, for mean curvature flow, ideas introduced by the present authors to approximate curvature driven evolution laws for hypersurfaces. These ideas lead to stable approximations, which, in addition, are such that the quality of the mesh approximating the evolving surface in general remains good. In fact, the latter property is crucial, as many parametric approaches suffer from mesh degeneracies during the evolution. These degeneracies may even lead to situations, where the resulting algorithms break down during the evolution. The ideas presented in this section will then

be the basis for more complex evolution laws studied later on. We will also compare our approach to other methods in the literature dealing with mean curvature flow.

The basis of our approach is a weak formulation, which we introduce next. The goal is to write the evolution law $\mathcal{V} = \kappa$ in a weak form. To this end, we firstly note that the evolution law, for a global parameterization $\vec{x} : \Upsilon \times [0, T] \rightarrow \mathbb{R}^d$, and corresponding orientable hypersurfaces $\Gamma(t) = \vec{x}(\Upsilon, t)$, recall Definition 2.25, can be written as

$$\vec{\mathcal{V}} \cdot \vec{\nu} = \kappa, \quad \kappa \vec{\nu} = \Delta_s \text{id} \quad \text{on } \Gamma(t), \quad (4.3)$$

where we have noted Remark 2.26(i) and Lemma 2.13(ii). On recalling from Remark 2.22(iv) the weak formulation of the second identity, we propose the following weak formulation for mean curvature flow. Given a closed hypersurface $\Gamma(0)$, find an evolving hypersurface $(\Gamma(t))_{t \in [0, T]}$ with a global parameterization and induced velocity field $\vec{\mathcal{V}}$, and $\kappa \in L^2(\mathcal{G}_T)$ as follows. For almost all $t \in (0, T)$, find $(\vec{\mathcal{V}}(\cdot, t), \kappa(\cdot, t)) \in [L^2(\Gamma(t))]^d \times L^2(\Gamma(t))$ such that

$$\left\langle \vec{\mathcal{V}}, \chi \vec{\nu} \right\rangle_{\Gamma(t)} - \langle \kappa, \chi \rangle_{\Gamma(t)} = 0 \quad \forall \chi \in L^2(\Gamma(t)), \quad (4.4a)$$

$$\langle \kappa \vec{\nu}, \vec{\eta} \rangle_{\Gamma(t)} + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d. \quad (4.4b)$$

We note here that we consider closed surfaces and hence no boundary term appears in (4.4b). Using the weak formulation (4.4b) of $\kappa \vec{\nu} = \Delta_s \text{id}$ was the fundamental idea of Dziuk (1991), which made it possible to approximate smooth surfaces and their mean curvature by piecewise smooth surfaces. Finally we remark that $H^1(\Gamma(t))$ denotes the usual Sobolev space of square integrable functions on $\Gamma(t)$ with square integrable surface gradient, and we refer to Wloka (1987, I §4) for an introduction to Sobolev spaces on compact C^1 -surfaces.

4.2 Finite element approximation

Given an initial polyhedral hypersurface Γ^0 the plan is to construct polyhedral hypersurfaces Γ^m , $m = 1, \dots, M$, which approximate the true continuous solution $\Gamma(t_m)$ to the mean curvature flow at times $0 = t_0 < t_1 < \dots < t_M = T$, which form a partition of a time interval $[0, T]$ with time steps

$$\Delta t_m = t_{m+1} - t_m, \quad m = 0, \dots, M-1. \quad (4.5)$$

An idea going back to Dziuk (1991) is to parameterize Γ^{m+1} over Γ^m with the help of parameterizations $\vec{X}^{m+1} : \Gamma^m \rightarrow \mathbb{R}^d$. We recall the definitions of the finite element spaces and inner products from Definition 3.3, and then recall the following finite element approximation of (4.4) for mean curvature flow from Barrett et al. (2007b, 2008a).

Let the closed polyhedral hypersurface Γ^0 be an approximation of $\Gamma(0)$. Then, for

$m = 0, \dots, M - 1$, find $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that

$$\left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \chi \vec{\nu}^m \right\rangle_{\Gamma^m}^h - \langle \kappa^{m+1}, \chi \rangle_{\Gamma^m}^h = 0 \quad \forall \chi \in V(\Gamma^m), \quad (4.6a)$$

$$\langle \kappa^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (4.6b)$$

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

Here we recall from Definition 2.25(ii) that $\frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}$ on Γ^m is a natural approximation of $\vec{\mathcal{V}}$ on $\Gamma(t_m)$. We also remark that although the original problem was highly nonlinear, the system (4.6) is linear and easy to solve. The main reason for this is that the geometry, which enters the weak formulations via the area element, the normal vector and the surface gradients, is taken explicitly.

Remark 4.1 (Surfaces with boundary). *We recall that (4.2) was derived as the L^2 -gradient flow for $|\Gamma(t)|$ from (4.1) for an evolving hypersurface without boundary. If we allow $\partial\Gamma(t)$ to be nonempty, on the other hand, then (4.1) needs to be adapted to*

$$\frac{d}{dt} |\Gamma(t)| = - \left\langle \kappa \vec{\nu}, \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} + \left\langle \vec{\mathcal{V}}, \vec{\mu} \right\rangle_{\partial\Gamma(t)}, \quad (4.7)$$

where $\vec{\mathcal{V}}$ is the velocity field induced by a global parameterization of the evolving hypersurface, and $\vec{\mu}(t)$ denotes the outer unit conormal on $\partial\Gamma(t)$, recall Theorem 2.32. Now choosing a boundary condition that makes the last term in (4.7) vanish will ensure that (4.2) is still the L^2 -gradient flow for $|\Gamma(t)|$. The simplest such boundary condition fixes

$$\partial\Gamma(t) = \partial\Gamma(0) \quad \forall t \in (0, T]. \quad (4.8)$$

The approximation (4.6) can be easily generalized to this situation, by replacing the space $\underline{V}(\Gamma^m)$ in (4.6b) with

$$\underline{V}_D(\Gamma^m) = \left\{ \vec{\eta} \in \underline{V}(\Gamma^m) : \vec{\eta} = \vec{0} \text{ on } \partial\Gamma^m \right\}, \quad (4.9)$$

and by seeking $\vec{X}^{m+1}$ such that $\vec{X}^{m+1} - \text{id}|_{\Gamma^m} \in \underline{V}_D(\Gamma^m)$. More complicated boundary conditions can be handled in a similar way, for example the case of prescribed contact angles when the boundary $\partial\Gamma(t)$ is allowed to move along the boundary of a fixed given domain. A further related example is the evolution of a cluster of hypersurfaces, where the boundaries of a number of surfaces are required to remain attached to each other. Typically triple junction points in the plane, and triple junction lines in $\mathbb{R}^3$ are of interest, and these situations can be naturally approximated with the methods presented in this work both for mean curvature flow, as well as for more general geometric evolution equations. We refer the interested reader to the series of papers Barrett et al. (2007a,b, 2008b, 2010a,d).

Remark 4.2 (Implementation). *We note that implementing the system (4.6) is not difficult. For $d = 2$ an equivalent finite difference formulation can be derived, see §4.3.1 below.*

For $d = 3$ the scheme (4.6) can either be implemented directly in a high level computing environment like MATLAB, or within a finite element toolbox that allows the approximation of PDEs on two-dimensional hypersurfaces in $\mathbb{R}^3$. Examples for such toolboxes are ALBERTA, Schmidt and Siebert (2005); Dune, Dedner et al. (2010); and FELICITY, Walker (2018). An advantage of these toolboxes is that they allow a nearly dimension-independent implementation of the scheme, and so the cases $d = 2$ and $d = 3$ can be treated together. For the piecewise linear approximation (4.6), the only difference to standard problems on flat, stationary domains in $\mathbb{R}^{d-1}$ is then, that the vertices of the initial mesh, on which the PDE is to be approximated, have d coordinates, rather than $d - 1$, and that the vertices of the mesh are moved after each time step.

The initial mesh can either be created with the help of a simple, coarse macro-triangulation, that is then refined and transformed with the help of the capabilities of the chosen finite element toolbox. Or it can be created by using sophisticated 3D volume mesh generators, that allow to extract the surface mesh of the generated 3D volume mesh. Examples for such volume mesh generators are Gmsh, Geuzaine and Remacle (2009); CGAL, Rineau and Yvinec (2018); TIGER, Walker (2013); Cleaver, CIBC (2016); and NETGEN, Schöberl (1997).

4.3 Discrete linear systems

We now describe the linear systems arising from (4.6). We introduce the matrices $\vec{N}_{\Gamma^m} \in (\mathbb{R}^d)^{K \times K}$, $M_{\Gamma^m}, A_{\Gamma^m} \in \mathbb{R}^{K \times K}$ and $\underline{A}_{\Gamma^m} \in (\mathbb{R}^{d \times d})^{K \times K}$ with entries

$$\begin{aligned} [M_{\Gamma^m}]_{kl} &= \langle \phi_k^{\Gamma^m}, \phi_l^{\Gamma^m} \rangle_{\Gamma^m}^h, \quad [\vec{N}_{\Gamma^m}]_{kl} = \int_{\Gamma^m} \pi_{\Gamma^m} [\phi_k^{\Gamma^m} \phi_l^{\Gamma^m}] \vec{\nu}^m d\mathcal{H}^{d-1}, \\ [A_{\Gamma^m}]_{kl} &= \langle \nabla_s \phi_k^{\Gamma^m}, \nabla_s \phi_l^{\Gamma^m} \rangle_{\Gamma^m} \end{aligned} \quad (4.10)$$

and $[\underline{A}_{\Gamma^m}]_{kl} = [A_{\Gamma^m}]_{kl} \underline{\text{Id}}$, where we have recalled Definition 3.3(i). Assembling these matrices is similar to the situation of finite element methods for domains in $\mathbb{R}^{d-1}$. In addition to computing the volume of a simplex, one has to compute its normal and the surface gradients of the basis functions. The latter can be computed using the formula

$$\nabla_s \phi_k^{\Gamma^m} = \sum_{i=1}^{d-1} (\partial_{\vec{\tau}_i} \phi_k^{\Gamma^m}) \vec{\tau}_i,$$

where $\{\vec{\tau}_1, \dots, \vec{\tau}_{d-1}\}$ is an orthonormal basis of the tangent space to the simplex, recall Definition 2.5(ii). We can then formulate (4.6) as: Find $(\delta \vec{X}^{m+1}, \kappa^{m+1}) \in (\mathbb{R}^d)^K \times \mathbb{R}^K$ such that

$$\begin{pmatrix} \Delta t_m M_{\Gamma^m} & -\vec{N}_{\Gamma^m}^\top \\ \vec{N}_{\Gamma^m} & \underline{A}_{\Gamma^m} \end{pmatrix} \begin{pmatrix} \kappa^{m+1} \\ \delta \vec{X}^{m+1} \end{pmatrix} = \begin{pmatrix} 0 \\ -\underline{A}_{\Gamma^m} \vec{X}^m \end{pmatrix}, \quad (4.11)$$

where, with the obvious abuse of notation, $\delta \vec{X}^{m+1} = (\delta \vec{X}_1^{m+1}, \dots, \delta \vec{X}_K^{m+1})^\top$, $\kappa^{m+1} = (\kappa_1^{m+1}, \dots, \kappa_K^{m+1})^\top$, and $\vec{X}^m = (\vec{X}_1^m, \dots, \vec{X}_K^m)^\top$ are the vectors of coefficients with respect to the standard basis for $\vec{X}^{m+1} - \text{id}_{|\Gamma^m}$, κ^{m+1} and $\text{id}_{|\Gamma^m}$, respectively. In the following

section we will show that the above system, under very mild assumptions, is invertible. Hence it can be solved, for example, with a sparse direct solution method like UMFPACK, see Davis (2004), in an efficient way. It is also possible to solve the system iteratively, by first using a Schur complement approach to (4.11), in order to eliminate κ^{m+1} , and then use a (preconditioned) conjugate gradient solver, see e.g. Barrett et al. (2008a) for details. In fact, the Schur complement approach essentially boils down to the system (4.12), below, which we derive next.

It is also possible to rewrite the system (4.6) as an equation for $\vec{X}^{m+1}$ as the only unknown. To this end, let $\vec{\omega}^m \in \underline{V}(\Gamma^m)$ be the vertex normal to Γ^m , recall Definition 3.11. Then it follows from (3.5) that we can compute κ^{m+1} from (4.6a) via

$$\kappa^{m+1} = \frac{1}{\Delta t_m} \pi_{\Gamma^m} \left[\left(\vec{X}^{m+1} - \text{id}_{|\Gamma^m} \right) \cdot \vec{\omega}^m \right],$$

recall Definition 3.3(i). Hence we can rewrite (4.6) as: Find $\vec{X}^{m+1} \in \underline{V}(\Gamma^m)$ such that

$$\left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m} \cdot \vec{\omega}^m, \vec{\eta} \cdot \vec{\omega}^m \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m). \quad (4.12)$$

4.3.1 Curves in the plane

The system (4.6) is particularly simple in the case of closed curves. On recalling Definition 3.13, we can reformulate it as follows.

Let $\vec{X}^0 \in \underline{V}^h(\mathbb{I})$ be such that $\Gamma^0 = \vec{X}^0(\mathbb{I})$ is a polygonal approximation of $\Gamma(0)$. Then, for $m = 0, \dots, M-1$, find $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}^h(\mathbb{I}) \times V^h(\mathbb{I})$ such that

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\Delta t_m}, \chi \vec{\nu}^m \circ \vec{X}^m |\vec{X}_\rho^m| \right\rangle_{\mathbb{I}}^h - \left\langle \kappa^{m+1}, \chi |\vec{X}_\rho^m| \right\rangle_{\mathbb{I}}^h = 0 \quad \forall \chi \in V^h(\mathbb{I}), \quad (4.13a)$$

$$\left\langle \kappa^{m+1} \vec{\nu}^m \circ \vec{X}^m, \vec{\eta} |\vec{X}_\rho^m| \right\rangle_{\mathbb{I}}^h + \left\langle \vec{X}_\rho^{m+1}, \vec{\eta}_\rho |\vec{X}_\rho^m|^{-1} \right\rangle_{\mathbb{I}} = 0 \quad \forall \vec{\eta} \in \underline{V}^h(\mathbb{I}) \quad (4.13b)$$

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

It is now straightforward to rewrite (4.13) as a finite difference scheme. Let κ_j^{m+1} , $\vec{X}_j^{m+1}$, $\vec{X}_j^m$ and $\vec{\omega}_j^m$ be the values of κ^{m+1} , $\vec{X}^{m+1}$, $\vec{X}^m$ and $\vec{\omega}^m \circ \vec{X}^m$ at the node q_j , for $j = 0, \dots, J+1$. Let $\vec{h}_j^m = \vec{X}_j^m - \vec{X}_{j-1}^m$, $j = 1, \dots, J+1$. Then, on recalling (3.8), we obtain the weighted vertex normals

$$\vec{\omega}_j^m = - \frac{\left(\vec{X}_{j+1}^m - \vec{X}_{j-1}^m \right)^\perp}{|\vec{h}_j^m| + |\vec{h}_{j+1}^m|} \quad j = 1, \dots, J. \quad (4.14)$$

Equation (4.13a) can hence be rewritten in the following finite difference form

$$\frac{1}{\Delta t_m} \left(\vec{X}_j^{m+1} - \vec{X}_j^m \right) \cdot \vec{\omega}_j^m = \kappa_j^{m+1}, \quad j = 1, \dots, J. \quad (4.15a)$$

Testing (4.13b) with the standard basis functions gives the finite difference type equations

$$\kappa_j^{m+1} \vec{\omega}_j^m = \frac{2}{|\vec{h}_j^m| + |\vec{h}_{j+1}^m|} \left(\frac{\vec{X}_{j+1}^{m+1} - \vec{X}_j^{m+1}}{|\vec{h}_{j+1}^m|} - \frac{\vec{X}_j^{m+1} - \vec{X}_{j-1}^{m+1}}{|\vec{h}_j^m|} \right) \quad j = 1, \dots, J. \quad (4.15b)$$

Of course, it is now also possible to use (4.15a) in order to reduce (4.15b) to an equation for the nodal values of $\vec{X}^{m+1}$, in order to obtain a finite difference analogue of (4.12).

4.4 Existence and uniqueness

In order to show existence and uniqueness of solutions to (4.6), we recall Assumption 3.24.

Theorem 4.3. *Let Γ^m satisfy Assumption 3.24(i). Then there exists a unique solution $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to the system (4.6).*

Proof. Similarly to the proof of Lemma 3.26, existence follows from uniqueness, and so we consider the homogeneous system

$$\left\langle \vec{X}, \chi \vec{\nu}^m \right\rangle_{\Gamma^m}^h - \Delta t_m \langle \kappa, \chi \rangle_{\Gamma^m}^h = 0 \quad \forall \chi \in V(\Gamma^m), \quad (4.16a)$$

$$\langle \kappa \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m), \quad (4.16b)$$

for unknowns $(\vec{X}, \kappa) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$. Choosing $\chi = \kappa \in V(\Gamma^m)$ in (4.16a) and $\vec{\eta} = \vec{X} \in \underline{V}(\Gamma^m)$ in (4.16b) yields that

$$\left| \nabla_s \vec{X} \right|_{\Gamma^m}^2 + \Delta t_m \left(|\kappa|_{\Gamma^m}^h \right)^2 = 0, \quad (4.17)$$

where we have recalled (3.2). It follows from (4.17) that $\kappa = 0$ and $\vec{X} = \vec{X}^c$ on Γ^m , for $\vec{X}^c \in \mathbb{R}^d$. Together with (4.16a) this implies, on recalling (3.6), that

$$\left\langle \vec{X}^c, \chi \vec{\nu}^m \right\rangle_{\Gamma^m} = 0 \quad \forall \chi \in V(\Gamma^m). \quad (4.18)$$

As in the proof of Lemma 3.26 it follows from (4.18) and Assumption 3.24(i) that $\vec{X}^c = \vec{0}$. Hence we have shown that there exists a unique solution $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to (4.6). $\square$

4.5 Stability

For $d = 2$ and $d = 3$ it can be shown that the scheme (4.6) is unconditionally stable.

Theorem 4.4. *Let $d = 2$ or $d = 3$. Let $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ be a solution to (4.6). Then we have that*

$$|\Gamma^{m+1}| + \Delta t_m \left(|\kappa^{m+1}|_{\Gamma^m}^h \right)^2 \leq |\Gamma^m|. \quad (4.19)$$

Proof. Choosing $\chi = \kappa^{m+1} \in V(\Gamma^m)$ in (4.6a) and $\vec{\eta} = \frac{1}{\Delta t_m} (\vec{X}^{m+1} - \text{id}_{|\Gamma^m}) \in \underline{V}(\Gamma^m)$ in (4.6b) yields that

$$\left\langle \nabla_s \vec{X}^{m+1}, \nabla_s (\vec{X}^{m+1} - \text{id}) \right\rangle_{\Gamma^m} + \Delta t_m \left(|\kappa^{m+1}|_{\Gamma^m}^h \right)^2 = 0. \quad (4.19)$$

In addition, we have from Lemma 3.17 that

$$\left\langle \nabla_s \vec{X}^{m+1}, \nabla_s (\vec{X}^{m+1} - \text{id}) \right\rangle_{\Gamma^m} \geq |\Gamma^{m+1}| - |\Gamma^m|. \quad (4.20)$$

Combining (4.19) and (4.20) then yields the claim. $\square$

Remark 4.5. Clearly, if $\{(\vec{X}^{m+1}, \kappa^{m+1})\}_{m=0}^{M-1}$ denote solutions to (4.6) for $m = 0, \dots, M-1$, then the above theorem immediately yields the energy bound

$$|\Gamma^k| + \sum_{m=0}^{k-1} \Delta t_m \left(|\kappa^{m+1}|_{\Gamma^m}^h \right)^2 \leq |\Gamma^0|.$$

for $k = 1, \dots, M$.

4.6 Equipartition property

Many numerical methods that use polyhedral surfaces to approximate an evolving hypersurface suffer from the fact that the meshes will have very inhomogeneous properties during the evolution. For example, mesh points can come very close to each other during the evolution, or some angles in the mesh can become rather small or rather large. This leads to very unstable and inaccurate situations. In addition, the condition number of the linear systems to be solved at each time level will become very large. In some situations, the computations cannot even be continued after some time. It is an important property of the approach discussed in this section so far, that the mesh typically behaves very well. We will discuss this below for mean curvature flow, which is the simplest possible situation. However, similar results hold true for the extension of this scheme to more complicated flows discussed in subsequent sections.

The behavior of the mesh is best explained with the help of a semidiscrete version of the scheme (4.6), where we recall Definition 3.28. Given the closed polyhedral hypersurface $\Gamma^h(0)$, find an evolving polyhedral hypersurface $\mathcal{G}_T^h$, with induced velocity $\vec{\mathcal{V}}^h \in \underline{V}(\mathcal{G}_T^h)$, and $\kappa^h \in V(\mathcal{G}_T^h)$, i.e. $\vec{\mathcal{V}}^h(\cdot, t) \in \underline{V}(\Gamma^h(t))$ and $\kappa^h(\cdot, t) \in V(\Gamma^h(t))$ for all $t \in [0, T]$, such that, for all $t \in (0, T]$,

$$\left\langle \vec{\mathcal{V}}^h, \chi \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h - \left\langle \kappa^h, \chi \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \chi \in V(\Gamma^h(t)), \quad (4.21a)$$

$$\left\langle \kappa^h \vec{\nu}^h, \vec{\eta} \right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h(t)). \quad (4.21b)$$

We can prove that the scheme (4.21) is stable, i.e. a semidiscrete analogue of Theorem 4.4 holds, and that its tangential motion ensures that any solution satisfies the property in Definition 3.20.

Theorem 4.6. *Let $(\mathcal{G}_T^h, \kappa^h)$ be a solution of (4.21).*

(i) *It holds that*

$$\frac{d}{dt} |\Gamma^h(t)| + \left(|\kappa^h|_{\Gamma^h(t)}^h \right)^2 = 0.$$

(ii) *For any $t \in (0, T]$, it holds that $\Gamma^h(t)$ is a conformal polyhedral surface. In particular, for $d = 2$, any two neighbouring elements of the curve $\Gamma^h(t)$ either have equal length, or they are parallel.*

Proof. (i) Choosing $\chi = \kappa^h(\cdot, t) \in V(\Gamma^h(t))$ in (4.21a) and $\vec{\eta} = \vec{\mathcal{V}}^h(\cdot, t) \in \underline{V}(\Gamma^h(t))$ in (4.21b) gives, on recalling Theorem 3.30 and Lemma 2.9(ii), that

$$\frac{d}{dt} |\Gamma^h(t)| = \left\langle 1, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)} = \left\langle \nabla_s \text{id}, \nabla_s \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)} = - \left\langle \kappa^h, \kappa^h \right\rangle_{\Gamma^h(t)}^h,$$

which is the claim.

(ii) This follows directly from Definition 3.20 and Theorem 3.22. $\square$

Remark 4.7. *In general it is not clear whether solutions to (4.21) exist. For example, for $d \geq 3$ the topology of the triangulation fixed by $\Gamma^h(0)$ may be such that no solutions satisfying both (4.21a) and (4.21b) exist. In those situations, the fully discrete scheme (4.6), even for very small time step sizes Δt_m , may exhibit mesh defects that would not be expected for surfaces satisfying Definition 3.20, recall Remark 3.21. An example for such defects was recently presented in Elliott and Fritz (2017, Fig. 27).*

In the case of curves, i.e. $d = 2$, the scheme (4.21) can be easily interpreted as a differential-algebraic system of equations. To this end, we adopt the notation from §4.3.1 for $\vec{X}^h(t) \in \underline{V}^h(\mathbb{I})$, and let $\vec{h}_j(t) = \vec{X}_j^h(t) - \vec{X}_{j-1}^h(t)$, $j = 1, \dots, J+1$. Then we obtain the obvious analogue of (4.14) for the vertex normals $\vec{\omega}_j^h(t)$ and, similarly to (4.15), the system (4.21) can then be written as the following differential-algebraic system of equations (DAEs). Given $\vec{X}^h(0) \in \underline{V}^h(\mathbb{I})$, for $t \in (0, T]$ find $\vec{X}^h(t) \in \underline{V}^h(\mathbb{I})$ and $\kappa^h(t) \in V^h(\mathbb{I})$ such that

$$- \left(\frac{d}{dt} \vec{X}_j^h \right) \cdot \left(\frac{(\vec{X}_{j+1}^h - \vec{X}_{j-1}^h)^\perp}{|\vec{h}_j| + |\vec{h}_{j+1}|} \right) = \kappa_j^h, \quad (4.22a)$$

$$- \kappa_j^h \frac{(\vec{X}_{j+1}^h - \vec{X}_{j-1}^h)^\perp}{|\vec{h}_j| + |\vec{h}_{j+1}|} = \frac{2}{|\vec{h}_j| + |\vec{h}_{j+1}|} \left(\frac{\vec{X}_{j+1}^h - \vec{X}_j^h}{|\vec{h}_{j+1}|} - \frac{\vec{X}_j^h - \vec{X}_{j-1}^h}{|\vec{h}_j|} \right), \quad (4.22b)$$

for $j = 1, \dots, J$.

Remark 4.8. *Equation (4.22a) only specifies one direction of $\frac{d}{dt} \vec{X}_j^h$, while the evolution of the remaining direction is enforced via the algebraic conditions in (4.22b). Hence the overall system is a highly nonlinear and degenerate differential-algebraic system of equations. The defining equations become singular where vertices coalesce. However, as is shown in Theorem 4.6(ii), in regions where the curve is not straight, this does not happen.*

So far we have discussed the linear fully discrete scheme (4.6), which is obtained as a possible time discretization of (4.21). The fully discrete scheme (4.6) will not inherit the conformality property of Theorem 4.6(ii), but solutions to (4.6) still exhibit a tangential motion that leads to a good distribution of vertices. We now discuss a fully implicit time discretization of (4.21), where the solutions are conformal polyhedral surfaces at every time step. These ideas were first presented in Barrett et al. (2011), in the case of curves.

Let the closed polyhedral hypersurface Γ^0 be an approximation of $\Gamma(0)$. Then, for $m = 0, \dots, M-1$, find a polyhedral hypersurface Γ^{m+1} , and $(\vec{X}^m, \kappa^{m+1}) \in \underline{V}(\Gamma^{m+1}) \times V(\Gamma^{m+1})$ with $\Gamma^m = \vec{X}^m(\Gamma^{m+1})$, such that

$$\left\langle \frac{\text{id} - \vec{X}^m}{\Delta t_m}, \chi \vec{\nu}^{m+1} \right\rangle_{\Gamma^{m+1}}^h - \langle \kappa^{m+1}, \chi \rangle_{\Gamma^{m+1}}^h = 0 \quad \forall \chi \in V(\Gamma^{m+1}), \quad (4.23a)$$

$$\langle \kappa^{m+1} \vec{\nu}^{m+1}, \vec{\eta} \rangle_{\Gamma^{m+1}}^h + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^{m+1}}^h = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^{m+1}). \quad (4.23b)$$

Theorem 4.9. *Let Γ^{m+1} and $(\vec{X}^m, \kappa^{m+1}) \in \underline{V}(\Gamma^{m+1}) \times V(\Gamma^{m+1})$ be a solution to (4.23).*

(i) *Then it holds that Γ^{m+1} is a conformal polyhedral surface. In particular, for $d = 2$, any two neighbouring elements of the curve Γ^{m+1} either have equal length, or they are parallel.*

(ii) *In the case $d = 2$ it holds that*

$$|\Gamma^{m+1}| + \Delta t_m \left(|\kappa^{m+1}|_{\Gamma^{m+1}}^h \right)^2 \leq |\Gamma^m|. \quad (4.24)$$

Proof. (i) This follows directly from Definition 3.20 and Theorem 3.22.

(ii) Choosing $\chi = \kappa^{m+1} \in V(\Gamma^{m+1})$ in (4.23a) and $\vec{\eta} = \frac{1}{\Delta t_m} (\text{id}|_{\Gamma^{m+1}} - \vec{X}^m) \in \underline{V}(\Gamma^{m+1})$ in (4.23b) yields that

$$\left\langle \nabla_s \text{id}, \nabla_s (\text{id} - \vec{X}^m) \right\rangle_{\Gamma^{m+1}} + \Delta t_m \left(|\kappa^{m+1}|_{\Gamma^{m+1}}^h \right)^2 = 0. \quad (4.25)$$

In addition, we have from Lemma 3.18 that

$$\left\langle \nabla_s \text{id}, \nabla_s (\text{id} - \vec{X}^m) \right\rangle_{\Gamma^{m+1}} \geq |\Gamma^{m+1}| - |\Gamma^m|. \quad (4.26)$$

Combining (4.25) and (4.26) then yields the claim. $\square$

Remark 4.10. *Similarly to Remark 4.7, in general it is not clear whether solutions to (4.23) exist. However, for $d = 2$ solutions in general appear to exist, and a small adaptation of (4.23) discussed below yields an unconditionally stable scheme that equidistributes.*

For the case of curves, $d = 2$, and building on (4.23), in Barrett et al. (2011) the present authors introduced fully discrete parametric finite element discretizations for $\mathcal{V} = \mathcal{V}$ that are unconditionally stable and that intrinsically equidistribute the vertices at each time

level. Using the notation from §4.3.1, see also Remark 3.14, we can reformulate (4.23) in the case of curves as follows.

Let $\vec{X}^0 \in \underline{V}^h(\mathbb{I})$ be such that $\Gamma^0 = \vec{X}^0(\mathbb{I})$ is a polygonal approximation of $\Gamma(0)$. Then, for $m = 0, \dots, M-1$, find $\Gamma^{m+1} = \vec{X}^{m+1}(\mathbb{I})$, with $\vec{X}^{m+1} \in \underline{V}^h(\mathbb{I})$, and $\kappa^{m+1} \in V^h(\mathbb{I})$ such that for all $\chi \in V^h(\mathbb{I})$, $\vec{\eta} \in \underline{V}^h(\mathbb{I})$

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\Delta t_m}, \chi \left(\vec{X}_\rho^{m+1} \right)^\perp \right\rangle_{\mathbb{I}}^h + \left\langle \kappa^{m+1}, \chi \left| \vec{X}_\rho^{m+1} \right| \right\rangle_{\mathbb{I}}^h = 0, \quad (4.27a)$$

$$\left\langle \kappa^{m+1} \left(\vec{X}_\rho^{m+1} \right)^\perp, \vec{\eta} \right\rangle_{\mathbb{I}}^h - \left\langle \vec{X}_\rho^{m+1}, \vec{\eta}_\rho \left| \vec{X}_\rho^{m+1} \right|^{-1} \right\rangle_{\mathbb{I}} = 0. \quad (4.27b)$$

We recall from Theorem 4.9 that solutions to (4.27) are equidistributed, at least where elements of the curve Γ^{m+1} are not locally parallel. This result can be sharpened to full equidistribution by considering the following adapted version of (4.27). For $m = 0, \dots, M-1$, find $\Gamma^{m+1} = \vec{X}^{m+1}(\mathbb{I})$, with $\vec{X}^{m+1} \in \underline{V}^h(\mathbb{I})$, and $\kappa^{m+1} \in V^h(\mathbb{I})$ such that for all $\chi \in V^h(\mathbb{I})$, $\vec{\eta} \in \underline{V}^h(\mathbb{I})$

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\Delta t_m}, \chi \left(\vec{X}_\rho^{m+1} \right)^\perp \right\rangle_{\mathbb{I}}^h + |\Gamma^{m+1}| \left\langle \kappa^{m+1}, \chi \right\rangle_{\mathbb{I}}^h = 0, \quad (4.28a)$$

$$\left\langle \kappa^{m+1} \left(\vec{X}_\rho^{m+1} \right)^\perp, \vec{\eta} \right\rangle_{\mathbb{I}}^h - |\Gamma^{m+1}|^{-1} \left\langle \vec{X}_\rho^{m+1}, \vec{\eta}_\rho \right\rangle_{\mathbb{I}} = 0. \quad (4.28b)$$

Theorem 4.11. *Let $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}^h(\mathbb{I}) \times V^h(\mathbb{I})$ be a solution of (4.28). Then it holds that*

$$\left| \vec{X}_\rho^{m+1} \right| = |\Gamma^{m+1}| \quad \text{in } I_j, \quad j = 1, \dots, J. \quad (4.29)$$

Moreover, $(\vec{X}^{m+1}, \kappa^{m+1})$ solves (4.27), and satisfies the stability estimate

$$|\Gamma^{m+1}| + \Delta t_m |\Gamma^{m+1}| \left\langle \kappa^{m+1}, \kappa^{m+1} \right\rangle_{\mathbb{I}}^h \leq |\Gamma^m|. \quad (4.30)$$

Proof. If $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}^h(\mathbb{I}) \times V^h(\mathbb{I})$ is a solution of (4.28), then on using the notation from Remark 3.14(iv), and similarly to the proof of Theorem 3.22, we fix $j \in \{1, \dots, J\}$ and choose $\vec{\eta} \in \underline{V}^h(\mathbb{I})$ in (4.28b) with

$$\vec{\eta}(q_i) = \delta_{ij} \left(\vec{X}^{m+1}(q_{j+1}) - \vec{X}^{m+1}(q_{j-1}) \right) = \delta_{ij} \left(\vec{h}_j^{m+1} + \vec{h}_{j+1}^{m+1} \right),$$

for $i = 1, \dots, J$, in order to obtain

$$0 = \left(\vec{h}_{j+1}^{m+1} - \vec{h}_j^{m+1} \right) \cdot \left(\vec{h}_{j+1}^{m+1} + \vec{h}_j^{m+1} \right) = \left| \vec{h}_{j+1}^{m+1} \right|^2 - \left| \vec{h}_j^{m+1} \right|^2. \quad (4.31)$$

Since (4.31) holds for $j = 1, \dots, J$, we obtain (4.29). It follows from (4.29) that $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}^h(\mathbb{I}) \times V^h(\mathbb{I})$ also solves (4.27), and $(\vec{X}^m \circ (\vec{X}^{m+1})^{-1}, \kappa^{m+1} \circ (\vec{X}^{m+1})^{-1}) \in \underline{V}(\Gamma^{m+1}) \times V(\Gamma^{m+1})$ is a solution to (4.23), satisfying the stability bound (4.24). Hence we obtain (4.30). $\square$

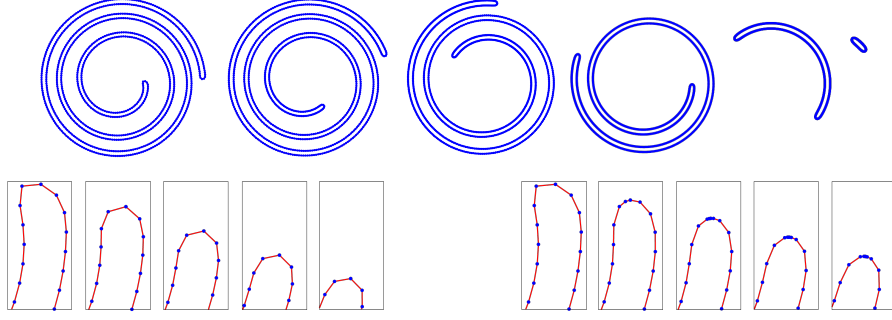


Figure 2: Mean curvature flow for a spiral. Numerical solution for the scheme (4.6) with $J = 1024$ and $\Delta t_m = \Delta t = 10^{-7}$, $m = 0, \dots, M - 1$. The discrete solution is shown at times $t = 0, 0.001, 0.005, 0.01, 0.02, 0.024$. Below we show details of the vertex distributions for the scheme (4.6) close to the inner tip (left), and compare that with the classical Dziuk scheme (4.33) (right). Coalescence for the latter scheme means that the simulation breaks down and cannot be continued.

Remark 4.12.

- (i) Clearly, (4.29) means that any solution to (4.28) is truly equidistributed.
- (ii) The system (4.28) is nonlinear, and so it can be solved either by a Newton method or with the following iteration. Given $\Gamma^{m+1,0} = \vec{X}^{m+1,0}(\mathbb{I})$, with $\vec{X}^{m+1,0} \in \underline{V}^h(\mathbb{I})$, we seek for $i \geq 0$ solutions $(\vec{X}^{m+1,i+1}, \kappa^{m+1,i+1}) \in \underline{V}^h(\mathbb{I}) \times V^h(\mathbb{I})$ such that for all $\chi \in V^h(\mathbb{I})$, $\vec{\eta} \in \underline{V}^h(\mathbb{I})$

$$\begin{aligned} \left\langle \frac{\vec{X}^{m+1,i+1} - \vec{X}^m}{\Delta t_m}, \chi \left(\vec{X}_\rho^{m+1,i} \right)^\perp \right\rangle_{\mathbb{I}}^h + |\Gamma^{m+1,i}| \langle \kappa^{m+1,i+1}, \chi \rangle_{\mathbb{I}}^h &= 0, \\ \left\langle \kappa^{m+1,i+1} \left(\vec{X}_\rho^{m+1,i} \right)^\perp, \vec{\eta} \right\rangle_{\mathbb{I}}^h - |\Gamma^{m+1,i}|^{-1} \langle \vec{X}_\rho^{m+1,i+1}, \vec{\eta}_\rho \rangle &= 0, \end{aligned}$$

and set $\Gamma^{m+1,i+1} = \vec{X}^{m+1,i+1}(\mathbb{I})$. This system has a unique solution and can be solved similarly to the discussion in §4.3. We refer to Barrett et al. (2011) for details.

As an example, we show an evolution of curve shortening flow, i.e. mean curvature flow in the case $d = 2$, computed with the scheme (4.6) in Figure 2.

4.7 Alternative parametric methods

The discussion so far was focussed on contributions of the present authors. We will now discuss other numerical methods for the numerical approximation of mean curvature flow, focussing on parametric finite element methods.

4.7.1 The classical Dziuk approach

The approach introduced by Dziuk (1991) is based on a weak formulation of

$$\vec{\mathcal{V}} = \vec{\kappa}, \quad \vec{\kappa} = \Delta_s \vec{\text{id}} \quad \text{on } \Gamma(t) \quad \Rightarrow \quad \vec{\mathcal{V}} = \Delta_s \vec{\text{id}} \quad \text{on } \Gamma(t), \quad (4.32)$$

rather than (4.3). Since $\Delta_s \vec{\text{id}} = \vec{\kappa} = \kappa \vec{\nu}$ is collinear to the normal, recall Lemma 2.13(ii), the evolving surface always moves in a direction collinear to the normal. The system to be solved, using the notation of §4.2, is then, given the closed polyhedral hypersurface Γ^m , to find $\vec{X}^{m+1} \in \underline{V}(\Gamma^m)$ such that

$$\left\langle \frac{\vec{X}^{m+1} - \vec{\text{id}}}{\Delta t_m}, \vec{\eta} \right\rangle_{\Gamma^m} + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m). \quad (4.33)$$

Existence, uniqueness and stability of this fully discrete linear system can be shown similarly to the results in §4.4 and §4.5. For the case $d = 2$ an error estimate for a semidiscrete continuous-in-time variant of (4.33) with mass lumping is shown in Dziuk (1994), on assuming that the approximated solution is sufficiently smooth. Even though for the case $d = 3$ no convergence results have been shown for either (4.33) or (4.6), in practice both approximations appear to be convergent, see e.g. Barrett et al. (2008a, Table 1).

4.7.2 The convergent finite element algorithm of Kovács, Li, Lubich

Very recently, a first proof of convergence for a numerical method for mean curvature flow for $d = 3$ was given by Kovács et al. (2018). They prove error estimates for semi- as well as full-discretizations of mean curvature flow, again assuming that the approximated solution is sufficiently smooth. They use the system

$$\vec{\mathcal{V}} = \kappa \vec{\nu}, \quad \partial_t^\circ \vec{\nu} = \Delta_s \vec{\nu} + |\nabla_s \vec{\nu}|^2 \vec{\nu}, \quad \partial_t^\circ \kappa = \Delta_s \kappa + |\nabla_s \vec{\nu}|^2 \kappa \quad \text{on } \Gamma(t).$$

The last two equations can be derived using basic geometric analysis and the law $\vec{\mathcal{V}} = \kappa \vec{\nu}$; see Lemma 2.37(i), Lemma 2.16, Lemma 2.7(iii), Lemma 2.12(i) and Lemma 2.39(i). Compared to (4.6) the approach has the disadvantages that meshes can still deteriorate, as the approximated flow is normal, similarly to the classical Dziuk approach, and that an additional system has to be solved. Of course, a clear advantage is that it is presently the only method, for which convergence can be shown for $d = 3$.

4.7.3 Alternative numerical methods that equidistribute

For the mean curvature flow of curves in the plane, the scheme (4.28) equidistributes the vertices of the polygonal approximation of the curve at every time step. In this section we discuss some alternative numerical methods that achieve the same goal.

As discussed before, it is desirable to control the tangential distribution of mesh points, and so to prevent numerical singularities such as coalescence or swallow tails, i.e. numerically induced self-intersections. In practice, many authors use mesh smoothing methods,

see e.g. Sethian (1985); Dziuk et al. (2002); Bänsch et al. (2005). However, mesh smoothing has some undesirable features, i.e. they might smoothen the solution excessively and stability results that hold for the original approximation are in general lost. For geometric evolution laws that have some conservation properties, for example flows where the enclosed area is conserved, great care must be taken to maintain the conservation properties after mesh smoothing.

In the case of an evolving curve $(\Gamma(t))_{t \in [0, T]}$, we consider parameterizations $\vec{x} : \mathbb{I} \times [0, T] \rightarrow \mathbb{R}^2$, where $\mathbb{I} = \mathbb{R}/\mathbb{Z}$ is the periodic interval $[0, 1]$, such that $\Gamma(t) = \vec{x}(\mathbb{I}, t)$, $t \in [0, T]$ are solutions of the curvature flow equation $\mathcal{V} = \kappa$. With s we denote the arclength of $\Gamma(t)$, so that the unit tangent is given by $\vec{x}_s(\rho, t) = \frac{\vec{x}_\rho(\rho, t)}{|\vec{x}_\rho(\rho, t)|}$, $\rho \in \mathbb{I}$, and a possible normal on $\Gamma(t)$ is $\vec{\nu} \circ \vec{x} = -\vec{x}_s^\perp$. The basic idea is to only consider parameterizations that satisfy

$$|\vec{x}_\rho(\rho, t)| = |\Gamma(t)| \quad \forall \rho \in \mathbb{I}, \quad t \in [0, T], \quad (4.34)$$

which means that ρ , up to a constant, is arclength. First such approaches are due to Kessler et al. (1984), and were analyzed and modified in Strain (1989); Hou et al. (1994); Mikula and Ševčovič (2001). It is also possible to discretize an evolution law for the position vector $\vec{x}$ in the form

$$\partial_t \vec{x} = (\mathcal{V} \vec{\nu}) \circ \vec{x} + \alpha \vec{x}_s \quad \text{in } \mathbb{I}, \quad (4.35)$$

where the tangential velocity is chosen such that the vertices of the polygonal approximation of $\Gamma(t)$ remain close to being equidistributed. This idea has been used in Kimura (1994), and Mikula and Ševčovič (2001) show that choosing α such that

$$\alpha_s = (\mathcal{V} \kappa) \circ \vec{x} - \frac{1}{|\Gamma(t)|} \langle \mathcal{V}, \kappa \rangle_{\Gamma(t)},$$

leads to the property (4.34), if (4.34) is fulfilled at the initial time. Also Deckelnick and Dziuk (1995) use (4.35) with

$$\alpha = \frac{\vec{x}_{\rho\rho} \cdot \vec{x}_\rho}{|\vec{x}_\rho|^3} \quad \text{in } \mathbb{I}, \quad (4.36)$$

and observe well distributed polygonal meshes in practice. In addition, an error analysis can be performed for a semidiscrete continuous-in-time finite element approximation. The resulting fully discrete scheme is particularly simple, and can be formulated as follows. Given $\vec{X}^m \in \underline{V}^h(\mathbb{I})$, find $\vec{X}^{m+1} \in \underline{V}^h(\mathbb{I})$ such that

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\Delta t_m}, \vec{\eta} \left| \vec{X}_\rho^m \right|^2 \right\rangle_{\mathbb{I}} + \left\langle \vec{X}_\rho^{m+1}, \vec{\eta}_\rho \right\rangle_{\mathbb{I}} = 0 \quad \forall \vec{\eta} \in \underline{V}^h(\mathbb{I}), \quad (4.37)$$

where we observe that the numerical computations presented in Deckelnick and Dziuk (1995) use mass lumping for the first term in (4.37). The authors in Pan and Wetton (2008); Pan (2008), on the other hand, solve $\mathcal{V} = \kappa$ with the side constraint

$$\vec{x}_\rho(\rho, t) \cdot \vec{x}_{\rho\rho}(\rho, t) = 0 \quad \forall \rho \in \mathbb{I}, \quad t \in [0, T],$$

which leads to $(\frac{1}{2}|\vec{x}_\rho|^2)_\rho = \vec{x}_\rho \cdot \vec{x}_{\rho\rho} = 0$ and hence to equidistributed parameterizations. However this approach leads to very nonlinear fully discrete problems.

4.7.4 Using the DeTurck trick to obtain good mesh properties

Mean curvature flow $\mathcal{V} = \kappa$, as a parabolic equation, has certain degeneracies, which basically stem from the fact that a reparameterization of a solution leads to another solution. It was an idea by DeTurck (1983) to use solutions of the harmonic map heat flow, in order to reparameterize the evolution of curvature flows in such a way that the reparameterized equations are strongly parabolic. Elliott and Fritz (2017) used the DeTurck trick to solve the mean curvature flow numerically. The resulting algorithm has the remarkable property, that provided the initial surface is approximated by a triangulation with a good mesh quality, the meshes will remain good during the evolution. This, roughly speaking, is due to the fact that, under appropriate assumptions, harmonic maps are conformal maps, which hence preserve angles.

The algorithm of Elliott and Fritz (2017), for the case $d = 3$, may at times lead to better meshes than the method discussed in §4.2. However, the systems to be solved are more complicated, and the approach also seems to be less flexible, e.g. when it comes to anisotropy, triple junctions and the coupling of the interface evolution to other fields. We refer to Elliott and Fritz (2017) for more details about this approach and for an error analysis in the case $d = 2$ for a semidiscrete continuous-in-time variant. This error analysis is an extension of that in Deckelnick and Dziuk (1995) for the variant with the specific tangential velocity (4.36). The error analysis in Elliott and Fritz (2017) was extended to the fully discrete case in Barrett et al. (2017a).

4.7.5 Other numerical approaches

In some situations the surface to be computed can be written as a graph. Finite element approximations in this case have been analyzed in Dziuk (1999b) and Deckelnick and Dziuk (1999). For the case of axisymmetric surfaces moving by mean curvature flow, numerical schemes have been presented in Mayer and Simonett (2002); Barrett et al. (2019a). We also mention Mikula et al. (2014), who proposed methods for a tangential redistribution of points on evolving surfaces. They use volume-oriented and length-oriented tangential redistribution methods, which can be applied to manifolds in any dimension. Completely different approaches are the level set method and the phase field method, which are discussed, for example, in *Handbook of Numerical Analysis, Vol. XXI & XXII*.

5 Surface diffusion and other flows

In this section we extend the ideas from Section 4 to more general evolution laws for evolving hypersurfaces in $\mathbb{R}^d$, $d \geq 2$.

5.1 Properties of the surface diffusion flow

Fourth order geometric evolution equations for hypersurfaces have played an important role in the last twenty years. A basic example, which can be formulated in a very simple

way, is motion by surface diffusion

$$\mathcal{V} = -\Delta_s \kappa \quad \text{on } \Gamma(t).$$

This flow was introduced by Mullins (1957) to describe diffusion at interfaces in alloys. The flow has the remarkable property that for closed surfaces it is surface area decreasing and the enclosed volume is preserved. These two properties follow from the transport theorems as follows. If we define $\Omega(t)$ to be the domain enclosed by the closed hypersurface $\Gamma(t)$, with $\vec{\nu}(t)$ denoting the outer unit normal to $\Omega(t)$ on $\Gamma(t)$, then we obtain with the help of Theorem 2.33 that

$$\frac{d}{dt} \mathcal{L}^d(\Omega(t)) = \frac{d}{dt} \int_{\Omega(t)} 1 \, d\mathcal{L}^d = \langle 1, \mathcal{V} \rangle_{\Gamma(t)} = -\langle 1, \Delta_s \kappa \rangle_{\Gamma(t)} = 0, \quad (5.1)$$

where the last identity follows from the divergence theorem on manifolds, recall Remark 2.22(i). Furthermore, for the total surface area, $|\Gamma(t)|$, we obtain from Theorem 2.32 that

$$\frac{d}{dt} |\Gamma(t)| = -\langle \kappa, \mathcal{V} \rangle_{\Gamma(t)} = \langle \kappa, \Delta_s \kappa \rangle_{\Gamma(t)} = -|\nabla_s \kappa|_{\Gamma(t)}^2 \leq 0, \quad (5.2)$$

where for the last identity we recall once more Remark 2.22(i). In fact, the properties (5.1) and (5.2) are closely related to the fact that mathematically surface diffusion can be interpreted as the H^{-1} -gradient flow of $|\Gamma(t)|$, see e.g. Taylor and Cahn (1994).

Using the formulation

$$\vec{\mathcal{V}} \cdot \vec{\nu} = -\Delta_s \kappa, \quad \kappa \vec{\nu} = \Delta_s \text{id} \quad \text{on } \Gamma(t), \quad (5.3)$$

it is now possible to formulate a finite element approximation.

5.2 Finite element approximation for surface diffusion

Using the same notation as in §4.2, we recall the following finite element approximation of (5.3) for surface diffusion from Barrett et al. (2007a, 2008a). Let the closed polyhedral hypersurface Γ^0 be an approximation of $\Gamma(0)$. Then, for $m = 0, \dots, M-1$, find $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that

$$\left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \chi \vec{\nu}^m \right\rangle_{\Gamma^m}^h - \langle \nabla_s \kappa^{m+1}, \nabla_s \chi \rangle_{\Gamma^m} = 0 \quad \forall \chi \in V(\Gamma^m), \quad (5.4a)$$

$$\langle \kappa^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h + \langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (5.4b)$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$. Existence and uniqueness of discrete solutions for this scheme can be shown as in §4.2.

Theorem 5.1. *Let Γ^m satisfy Assumption 3.24(i). Then there exists a unique solution $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to the system (5.4).*

Proof. The proof is very similar to the proof of Theorem 4.3. For a solution $(\vec{X}, \kappa) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ of the homogeneous system

$$\left\langle \vec{X}, \chi \vec{\nu}^m \right\rangle_{\Gamma^m}^h - \Delta t_m \langle \nabla_s \kappa, \nabla_s \chi \rangle_{\Gamma^m} = 0 \quad \forall \chi \in V(\Gamma^m), \quad (5.5a)$$

$$\langle \kappa \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (5.5b)$$

we first prove $\kappa = 0$, and then proceed as in the proof of Lemma 3.26. Choosing $\chi = \kappa \in V(\Gamma^m)$ in (5.5a) and $\vec{\eta} = \vec{X} \in \underline{V}(\Gamma^m)$ in (5.5b) yields that

$$\left| \nabla_s \vec{X} \right|_{\Gamma^m}^2 + \Delta t_m \left| \nabla_s \kappa \right|_{\Gamma^m}^2 = 0.$$

We hence obtain that $\kappa = \kappa^c$ and $\vec{X} = \vec{X}^c$ on Γ^m , for $\kappa^c \in \mathbb{R}$ and $\vec{X}^c \in \mathbb{R}^d$, and so it follows from (5.5b) and (3.5) that

$$0 = \langle \kappa^c \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h = \kappa^c \langle \vec{\omega}^m, \vec{\eta} \rangle_{\Gamma^m}^h \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m). \quad (5.6)$$

If we assume that $\kappa^c \neq 0$, then choosing $\vec{\eta} = \vec{\omega}^m \in \underline{V}(\Gamma^m)$ in (5.6) yields, on recalling (3.2), that $|\vec{\omega}^m|_{\Gamma^m}^h = 0$, and so $\vec{\omega}^m = \vec{0}$. However, that clearly contradicts Assumption 3.24(i) and hence we have that $\kappa^c = 0$. Moreover, as in the proof of Lemma 3.26, we obtain from (5.5a) and Assumption 3.24(i) that $\vec{X}^c = 0$. Hence we have shown that there exists a unique solution $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to (5.4). $\square$

Similarly to §4.5, it can be shown that the scheme (5.4) is unconditionally stable for $d = 2$ and $d = 3$.

Theorem 5.2. *Let $d = 2$ or $d = 3$. Let $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ be a solution to (5.4). Then we have that*

$$|\Gamma^{m+1}| + \Delta t_m \left| \nabla_s \kappa^{m+1} \right|_{\Gamma^m}^2 \leq |\Gamma^m|.$$

Proof. Choosing $\chi = \kappa^{m+1} \in V(\Gamma^m)$ in (5.4a) and $\vec{\eta} = \frac{1}{\Delta t_m} (\vec{X}^{m+1} - \text{id}_{|\Gamma^m}) \in \underline{V}(\Gamma^m)$ in (5.4b) yields that

$$\left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \left(\vec{X}^{m+1} - \text{id} \right) \right\rangle_{\Gamma^m} + \Delta t_m \left| \nabla_s \kappa^{m+1} \right|_{\Gamma^m}^2 = 0. \quad (5.7)$$

Combining (5.7) and Lemma 3.17 yields the claim. $\square$

5.3 Volume conservation for the semidiscrete scheme

An important aspect of discretizations for geometric evolution equations is to mimic decay and conservation properties of the evolution laws on the discrete level. In this section we discuss the volume conservation properties of the scheme (5.4) for surface diffusion, recall (5.1).

On recalling Definition 3.28, we consider the following semidiscrete variant of (5.4). Given the closed polyhedral hypersurface $\Gamma^h(0)$, find an evolving polyhedral hypersurface $\mathcal{G}_T^h$ with induced velocity $\vec{\mathcal{V}}^h \in \underline{V}(\mathcal{G}_T^h)$, and $\kappa^h \in V(\mathcal{G}_T^h)$, i.e. $\vec{\mathcal{V}}^h(\cdot, t) \in \underline{V}(\Gamma^h(t))$ and $\kappa^h(\cdot, t) \in V(\Gamma^h(t))$ for all $t \in [0, T]$, such that, for all $t \in (0, T]$,

$$\left\langle \vec{\mathcal{V}}^h, \chi \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h - \left\langle \nabla_s \kappa^h, \nabla_s \chi \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \chi \in V(\Gamma^h(t)), \quad (5.8a)$$

$$\left\langle \kappa^h \vec{\nu}^h, \vec{\eta} \right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h(t)). \quad (5.8b)$$

Theorem 5.3. *Let $(\mathcal{G}_T^h, \kappa^h)$ be a solution of (5.8), and let $\Omega^h(t)$ be the domain enclosed by $\Gamma^h(t)$, for $t \in [0, T]$.*

(i) *It holds that*

$$\frac{d}{dt} |\Gamma^h(t)| + |\nabla_s \kappa^h|_{\Gamma^h(t)}^2 = 0.$$

(ii) *It holds that*

$$\frac{d}{dt} \mathcal{L}^d(\Omega^h(t)) = 0.$$

(iii) *For any $t \in (0, T]$, it holds that $\Gamma^h(t)$ is a conformal polyhedral surface. In particular, for $d = 2$, any two neighbouring elements of the curve $\Gamma^h(t)$ either have equal length, or they are parallel.*

Proof. (i) Similarly to the proof of Theorem 4.6(i), choosing $\chi = \kappa^h(\cdot, t) \in V(\Gamma^h(t))$ in (5.8a) and $\vec{\eta} = \vec{\mathcal{V}}^h(\cdot, t) \in \underline{V}(\Gamma^h(t))$ in (5.8b) gives

$$\frac{d}{dt} |\Gamma^h(t)| = \left\langle \nabla_s \text{id}, \nabla_s \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)} = - |\nabla_s \kappa^h|_{\Gamma^h(t)}^2,$$

which is the claim.

(ii) Choosing $\chi = 1$ in (5.8a) yields, on recalling Theorem 3.31, $\vec{\mathcal{V}}^h(\cdot, t) \in \underline{V}(\Gamma^h(t))$ and (3.6), that

$$\frac{d}{dt} \mathcal{L}^d(\Omega^h(t)) = \pm \left\langle \vec{\mathcal{V}}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)} = \pm \left\langle \vec{\mathcal{V}}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h = 0,$$

where the sign $\pm$ depends on whether $\vec{\nu}^h$ here is the outer/inner normal of $\Omega^h(t)$ on $\Gamma^h(t)$.

(iii) This follows directly from Definition 3.20 and Theorem 3.22. $\square$

Remark 5.4.

(i) *The result in Theorem 5.3(i) is the semidiscrete analogue of the stability result Theorem 5.2 for the fully discrete scheme (5.4), and it mimics the energy law (5.2) on the discrete level.*

- (ii) *The result in Theorem 5.3(ii) mimics the volume conservation property (5.1) on the discrete level. Moreover, while the fully discrete scheme (5.4) does not conserve the enclosed volume exactly, it does satisfy*

$$\left\langle \vec{X}^{m+1} - \vec{\text{id}}, \vec{\nu}^m \right\rangle_{\Gamma^m} = \left\langle \vec{X}^{m+1} - \vec{\text{id}}, \vec{\nu}^m \right\rangle_{\Gamma^m}^h = 0,$$

recall (3.6). On noting Theorem 3.31 this can be interpreted as a fully discrete analogue of Theorem 5.3(ii). In fact, in practice the scheme (5.4) exhibits excellent volume conservation properties, with the relative enclosed volume loss tending to zero as the time step size goes to zero.

5.4 Generalizations to other flows

The finite element approximation (5.4) for surface diffusion can easily be adapted to more general situations. The resultant discretizations will, under certain circumstances, again satisfy a stability result.

Here we consider flows of the form

$$\mathcal{V} = \mathfrak{F}(\varkappa) \quad \text{on} \quad \Gamma(t), \quad (5.9)$$

where $\mathfrak{F}$ maps functions on the closed hypersurface $\Gamma(t)$ to functions on $\Gamma(t)$. For mean curvature flow we have $\mathfrak{F}(\chi) = \chi$, while surface diffusion is obtained with $\mathfrak{F}(\chi) = -\Delta_s \chi$. If the map $\mathfrak{F}$ is such that

$$\langle \mathfrak{F}(\varkappa), \varkappa \rangle_{\Gamma(t)} \geq 0, \quad (5.10)$$

then we have, on recalling Theorem 2.32, that

$$\frac{d}{dt} |\Gamma(t)| = -\langle \mathcal{V}, \varkappa \rangle_{\Gamma(t)} = -\langle \mathfrak{F}(\varkappa), \varkappa \rangle_{\Gamma(t)} \leq 0. \quad (5.11)$$

The inequality (5.10) clearly is true for mean curvature flow, where we obtain

$$\langle \mathfrak{F}(\varkappa), \varkappa \rangle_{\Gamma(t)} = |\varkappa|_{\Gamma(t)}^2 \geq 0,$$

and also for surface diffusion, where

$$\langle \mathfrak{F}(\varkappa), \varkappa \rangle_{\Gamma(t)} = |\nabla_s \varkappa|_{\Gamma(t)}^2 \geq 0,$$

recall (5.2). Our goal now is to obtain a stability result like that in Theorem 5.2 for discretizations of flows of the form (5.9) that satisfy the energy bound (5.11). As a consistency condition for a discrete formulation, we require that there is a map $\mathfrak{F}^m : V(\Gamma^m) \rightarrow V(\Gamma^m)$ which approximates $\mathfrak{F}$ and is such that

$$\langle \mathfrak{F}^m(\chi), \chi \rangle_{\Gamma^m}^h \geq 0 \quad \forall \chi \in V(\Gamma^m). \quad (5.12)$$

We consider now the following finite element approximation of (5.9). Let the closed polyhedral hypersurface Γ^0 be an approximation of $\Gamma(0)$. Then, for $m = 0, \dots, M-1$, find $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that

$$\left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \chi \vec{\nu}^m \right\rangle_{\Gamma^m}^h - \langle \mathfrak{F}^m(\kappa^{m+1}), \chi \rangle_{\Gamma^m}^h = 0 \quad \forall \chi \in V(\Gamma^m), \quad (5.13a)$$

$$\langle \kappa^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h + \langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (5.13b)$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$. We obtain the following stability theorem, together with an existence and uniqueness result in the linear case.

Theorem 5.5.

- (i) Let Γ^m satisfy Assumption 3.24, and let $\mathfrak{F}^m : V(\Gamma^m) \rightarrow V(\Gamma^m)$ be a linear map such that (5.12) holds. Then there exists a unique solution $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to the system (5.13).
- (ii) Let $d = 2$ or $d = 3$. Let $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ be a solution to (5.13). Then we have that

$$|\Gamma^{m+1}| + \Delta t_m \langle \mathfrak{F}^m(\kappa^{m+1}), \kappa^{m+1} \rangle_{\Gamma^m}^h \leq |\Gamma^m|,$$

where both terms on the left hand side are nonnegative if $\mathfrak{F}^m$ satisfies (5.12).

Proof. (i) The proof is analogous to the proof of Lemma 3.26.

(ii) The proof is analogous to the proof of Theorem 5.2. □

Remark 5.6 (Examples).

- (i) Choosing $\mathfrak{F}(\kappa) = -\Delta_s \kappa$ and $\mathfrak{F}^m(\chi) = -\Delta_s^{\Gamma^m} \chi$, recall (3.14), we recover the results in Theorem 5.1 and Theorem 5.2 for surface diffusion. Similarly, for $\mathfrak{F}(\kappa) = \kappa$ and $\mathfrak{F}^m(\chi) = \chi$ we obtain Theorem 4.3 and Theorem 4.4 for mean curvature flow.
- (ii) Of interest are also nonlinear flows $\mathcal{V} = f(\kappa)$, i.e. $\mathfrak{F}(\kappa) = f(\kappa)$, where $f : (a, b) \rightarrow \mathbb{R}$ with $-\infty \leq a < b \leq \infty$ is a strictly monotonically increasing continuous function such that $f(0) = 0$. An example is $f(r) = |r|^{\beta-1} r$, with $\beta \in \mathbb{R}_{>0}$, which has applications in image analysis, see Alvarez et al. (1993); Sapiro and Tannenbaum (1994); Mikula and Ševčovič (2001). Here we define $\mathfrak{F}^m(\chi) = \pi_{\Gamma^m} [f(\chi)]$, recall Definition 3.3(i). For the resulting nonlinear scheme (5.13) we obtain the stability result Theorem 5.5(ii). Existence and uniqueness results for (5.13) are shown in Barrett et al. (2008a, Theorem 2.1).
- (iii) Also the volume conserving flow

$$\mathcal{V} = \mathfrak{F}(\kappa) = \kappa - f_{\Gamma(t)} \kappa \quad \text{on } \Gamma(t), \quad (5.14)$$

where we define the average

$$f_{\Gamma(t)} \varkappa = \frac{1}{|\Gamma(t)|} \int_{\Gamma(t)} \varkappa \, d\mathcal{H}^{d-1}, \quad (5.15)$$

falls into the class of functions for which stability can be shown. Here, for all $\chi \in V(\Gamma^m)$, we choose $\mathfrak{F}^m(\chi) = \chi - f_{\Gamma^m} \chi \in V(\Gamma^m)$ and obtain

$$\langle \mathfrak{F}^m(\chi), \chi \rangle_{\Gamma^m}^h = \left(|\chi - f_{\Gamma^m} \chi|_{\Gamma^m}^h \right)^2 \geq 0,$$

and so both results in Theorem 5.5 hold.

- (iv) In materials science (5.14) is called surface attachment limited kinetics (SALK). A flow interpolating between SALK and surface diffusion is

$$\mathcal{V} = -\Delta_s \left(\frac{1}{\alpha} - \frac{1}{\xi} \Delta_s \right)^{-1} \varkappa \quad \text{on } \Gamma(t),$$

where $\alpha, \xi \in \mathbb{R}_{>0}$. This flow was proposed by Taylor and Cahn (1994) and analyzed by Elliott and Garcke (1997); Escher et al. (2001) as an evolution law for interfaces in materials science. Introducing the new variable y , this flow can be restated as

$$\vec{\mathcal{V}} \cdot \vec{\nu} = -\Delta_s y, \quad \left(\frac{1}{\alpha} - \frac{1}{\xi} \Delta_s \right) y = \varkappa, \quad \varkappa \vec{\nu} = \Delta_s \vec{\text{id}} \quad \text{on } \Gamma(t).$$

Hence, for any $\chi \in V(\Gamma^m)$, the function $\mathfrak{F}^m(\chi) \in V(\Gamma^m)$ is defined via

$$\langle \mathfrak{F}^m(\chi), \eta \rangle_{\Gamma^m}^h = \langle \nabla_s Y(\chi), \nabla_s \eta \rangle_{\Gamma^m} \quad \forall \eta \in V(\Gamma^m), \quad (5.16)$$

where $Y \in V(\Gamma^m)$ solves

$$\frac{1}{\xi} \langle \nabla_s Y, \nabla_s \varphi \rangle_{\Gamma^m} + \frac{1}{\alpha} \langle Y, \varphi \rangle_{\Gamma^m}^h = \langle \chi, \varphi \rangle_{\Gamma^m}^h \quad \forall \varphi \in V(\Gamma^m). \quad (5.17)$$

Choosing $\eta = \chi$ in (5.16) and $\varphi = \chi - \frac{1}{\alpha} Y$ in (5.17) then yields that

$$\langle \mathfrak{F}^m(\chi), \chi \rangle_{\Gamma^m}^h = \langle \nabla_s Y, \nabla_s \chi \rangle_{\Gamma^m} = \frac{1}{\alpha} |\nabla_s Y|_{\Gamma^m}^2 + \xi \left(\left| \chi - \frac{1}{\alpha} Y \right|_{\Gamma^m}^h \right)^2 \geq 0,$$

and hence we obtain a stable discretization, satisfying the two results in Theorem 5.5, also in this case.

Remark 5.7 (Semidiscrete schemes and tangential motion).

- (i) Similarly to §5.3, semidiscrete variants of the schemes discussed in Remark 5.6 can also be considered. In each case they will satisfy Theorem 5.3(iii), the appropriate analogue of Theorem 5.3(i), as well as Theorem 5.3(ii) when the approximated flow is volume preserving, provided that the semidiscrete analogue of $\mathfrak{F}^m$ satisfies $\langle \mathfrak{F}^h(\chi), 1 \rangle_{\Gamma^h(t)}^h = 0$ for all $\chi \in V(\Gamma^h(t))$.

- (ii) In the case of curves, $d = 2$, for all the situations in Remark 5.6, fully discrete fully implicit schemes along the lines of (4.28) can be considered. In each case these schemes will inherit the stability properties from Remark 5.6 and, in addition, they will satisfy the strong equidistribution property (4.29). For further details we refer to Barrett et al. (2011).

5.5 Approximations with reduced or induced tangential motion

In this section we consider an alternative to (5.13b), that allows to either reduce the tangential motion or encourage tangential motion in selected directions. To this end, we assume that Γ^m satisfies Assumption 3.24(ii) and let $\vec{\tau}_i^m \in \underline{V}(\Gamma^m)$, for $i = 1, \dots, d-1$, be such that $\left\{ \frac{\vec{\omega}^m(\vec{q}_k^m)}{|\vec{\omega}^m(\vec{q}_k^m)|}, \vec{\tau}_1^m(\vec{q}_k^m), \dots, \vec{\tau}_{d-1}^m(\vec{q}_k^m) \right\}$ is an orthonormal basis of $\mathbb{R}^d$ for $k = 1, \dots, K$. Moreover, we choose coefficients $0 \leq \alpha_i^m, \delta_i^m \in V(\Gamma^m)$, $i = 1, \dots, d-1$, and forcing terms $c_i^m \in V(\Gamma^m)$, $i = 1, \dots, d-1$. Then, in place of (5.13) we consider the following approximation.

Let the closed polyhedral hypersurface Γ^0 be an approximation of $\Gamma(0)$. Then, for $m = 0, \dots, M-1$, find $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ and $\beta_i^{m+1} \in V(\Gamma^m)$, $i = 1, \dots, d-1$, such that

$$\left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \chi \vec{\nu}^m \right\rangle_{\Gamma^m}^h - \langle \mathfrak{F}^m(\kappa^{m+1}), \chi \rangle_{\Gamma^m}^h = 0 \quad \forall \chi \in V(\Gamma^m), \quad (5.18a)$$

$$\left\langle \alpha_i^m \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \xi \vec{\tau}_i^m \right\rangle_{\Gamma^m}^h - \langle \alpha_i^m [\delta_i^m \beta_i^{m+1} + c_i^m], \xi \rangle_{\Gamma^m}^h = 0 \quad \forall \xi \in V(\Gamma^m),$$

$$i = 1, \dots, d-1, \quad (5.18b)$$

$$\left\langle \kappa^{m+1} \vec{\nu}^m + \sum_{i=1}^{d-1} \alpha_i^m \beta_i^{m+1} \vec{\tau}_i^m, \vec{\eta} \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (5.18c)$$

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

Theorem 5.8.

- (i) Let Γ^m satisfy Assumption 3.24 and let $\mathfrak{F}^m : V(\Gamma^m) \rightarrow V(\Gamma^m)$ be a linear map such that (5.12) holds. Then there exists a solution $(\vec{X}^{m+1}, \kappa^{m+1}, \beta_1^{m+1}, \dots, \beta_{d-1}^{m+1}) \in \underline{V}(\Gamma^m) \times [V(\Gamma^m)]^d$ to the system (5.18), with $(\vec{X}^{m+1}, \kappa^{m+1}, \pi_{\Gamma^m} [\alpha_1^m \beta_1^{m+1}], \dots, \pi_{\Gamma^m} [\alpha_{d-1}^m \beta_{d-1}^{m+1}])$ being unique.
- (ii) Let $d = 2$ or $d = 3$. Let $(\vec{X}^{m+1}, \kappa^{m+1}, \beta_1^{m+1}, \dots, \beta_{d-1}^{m+1}) \in \underline{V}(\Gamma^m) \times [V(\Gamma^m)]^d$ be a solution to (5.18). Then we have that

$$|\Gamma^{m+1}| + \Delta t_m \langle \mathfrak{F}^m(\kappa^{m+1}), \kappa^{m+1} \rangle_{\Gamma^m}^h + \Delta t_m \langle \alpha_i^m [\delta_i^m \beta_i^{m+1} + c_i^m], \beta_i^{m+1} \rangle_{\Gamma^m}^h \leq |\Gamma^m|. \quad (5.19)$$

Proof. (i) Let

$$B_i^m(\Gamma^m) = \{\xi \in V(\Gamma^m) : \xi(\vec{q}_k^m) = 0 \text{ if } \alpha_i^m(\vec{q}_k^m) = 0, k = 1, \dots, K\},$$

for $i = 1, \dots, d-1$. We now prove the desired results by showing existence of a unique solution to the system (5.18) with $\beta_i^{m+1} \in V(\Gamma^m)$ replaced by $\beta_i^{m+1} \in B_i^m(\Gamma^m)$, and with $V(\Gamma^m)$ in (5.18b) replaced by $B_i^m(\Gamma^m)$. As usual, existence to this adapted linear system follows from uniqueness, and so we let $(\vec{X}, \kappa, b_1, \dots, b_{d-1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m) \times B_1^m(\Gamma^m) \times \dots \times B_{d-1}^m(\Gamma^m)$ be such that

$$\left\langle \vec{X}, \chi \vec{\omega}^m \right\rangle_{\Gamma^m}^h - \Delta t_m \langle \mathfrak{F}^m(\kappa), \chi \rangle_{\Gamma^m}^h = 0 \quad \forall \chi \in V(\Gamma^m), \quad (5.20a)$$

$$\left\langle \alpha_i^m \vec{X}, \xi \vec{\tau}_i^m \right\rangle_{\Gamma^m}^h - \Delta t_m \langle \alpha_i^m \delta_i^m b_i, \xi \rangle_{\Gamma^m}^h = 0 \quad \forall \xi \in B_i^m(\Gamma^m),$$

$$i = 1, \dots, d-1, \quad (5.20b)$$

$$\left\langle \kappa \vec{\omega}^m + \sum_{i=1}^{d-1} \alpha_i^m b_i \vec{\tau}_i^m, \vec{\eta} \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m), \quad (5.20c)$$

where we have observed (3.5). Choosing $\chi = \kappa \in V(\Gamma^m)$ in (5.20a), $\xi = b_i \in B_i^m(\Gamma^m)$ in (5.20b) for $i = 1, \dots, d-1$, and $\vec{\eta} = \vec{X} \in \underline{V}(\Gamma^m)$ in (5.20c) yields that

$$\Delta t_m \langle \mathfrak{F}^m(\kappa), \kappa \rangle_{\Gamma^m}^h + \Delta t_m \langle \alpha_i^m \delta_i^m b_i, b_i \rangle_{\Gamma^m}^h + \left| \nabla_s \vec{X} \right|_{\Gamma^m}^2 = 0. \quad (5.21)$$

It immediately follows from (5.21), (5.12) and our assumptions on α_i^m and δ_i^m that $\vec{X}$ is constant on Γ^m . Hence choosing $\vec{\eta} = \vec{\tau}_i^m$ in (5.20c) yields that $|\pi_{\Gamma^m}[\alpha_i^m b_i]|_{\Gamma^m}^h = 0$, and so $\pi_{\Gamma^m}[\alpha_i^m b_i] = 0$, which implies that $b_i = 0 \in B_i^m(\Gamma^m)$, for $i = 1, \dots, d-1$. The remainder of the proof proceeds as the proof of Lemma 3.26 to show that $\kappa = 0$ and $\vec{X} = \vec{0}$. This proves the uniqueness of a solution to (5.20), and hence the existence of a solution $(\vec{X}^{m+1}, \kappa^{m+1}, \beta_1^{m+1}, \dots, \beta_{d-1}^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m) \times B_1^m(\Gamma^m) \times \dots \times B_{d-1}^m(\Gamma^m)$ to the modified system discussed at the beginning of the proof. Clearly, this solution also solves the original system (5.18a), with only the values of β_i^{m+1} arbitrary where α_i^m vanishes.

(ii) Choosing $\chi = \kappa^{m+1} \in V(\Gamma^m)$ in (5.18a), $\xi = \beta_i^{m+1} \in V(\Gamma^m)$ in (5.18b) for $i = 1, \dots, d-1$ and $\vec{\eta} = \frac{1}{\Delta t_m} (\vec{X}^{m+1} - \text{id}_{|\Gamma^m}) \in \underline{V}(\Gamma^m)$ in (5.18c) yields the desired result on recalling Lemma 3.17. $\square$

Remark 5.9.

- (i) Clearly, (5.18) with $\alpha_i^m = 0$, for $i = 1, \dots, d-1$, reduces to the original scheme (5.13).
- (ii) In the case $d = 2$ or $d = 3$, if $\mathfrak{F}^m$ satisfies (5.12), and if $c_i^m = 0$ for $i = 1, \dots, d-1$, then (5.19) provides a stability estimate for (5.18).

- (iii) Choosing $\delta_i^m(\vec{q}_k^m) = 1$ and $c_i^m(\vec{q}_k^m) = 0$ for $i = 1, \dots, d-1$, it follows intuitively from (5.19) that tangential motion of $\vec{q}_k^m$ in the direction of $\vec{\tau}_i^m(\vec{q}_k^m)$ will be suppressed if $\alpha_i^m(\vec{q}_k^m)$ is large. Conversely, it is also clear from (5.18b) that choosing $\delta_i^m(\vec{q}_k^m) = 0$ and $\alpha_i^m(\vec{q}_k^m) > 0$ allows us to fix the tangential motion. These observations form an ansatz to control tangential movement in the discrete evolution of geometric flows. In particular, in Barrett et al. (2008d) the following strategies have been proposed and employed.

- (S1) $\alpha_i^m = \alpha \in \mathbb{R}_{\geq 0}$, $\delta_i^m = 1$, $c_i^m = 0$;
 (S2) $\alpha_i^m = \alpha \in \mathbb{R}_{> 0}$, $\delta_i^m = \delta \in \mathbb{R}_{> 0}$,
 $c_i^m(\vec{q}_k^m) = \frac{1}{\Delta t_m} (\vec{z}_k^m - \vec{q}_k^m) \cdot \vec{\tau}_i^m(\vec{q}_k^m)$, $k = 1, \dots, K$;
 (S3) $\alpha_i^m = 1$, $\delta_i^m = 0$,
 $c_i^m(\vec{q}_k^m) = \frac{1}{\Delta t_m} (\vec{z}_k^m - \vec{q}_k^m) \cdot \vec{\tau}_i^m(\vec{q}_k^m)$, $k = 1, \dots, K$;

for $i = 1, \dots, d-1$, where $\vec{z}_k^m$ is the average of the neighbouring nodes of $\vec{q}_k^m$. The effect of these strategies can be summarized as follows. With increasing $\alpha > 0$, (S1) leads to smaller $|\beta_i^{m+1}|$, $i = 1 \rightarrow d-1$, and hence to less tangential motion, see (5.18c). Strategy (S2), on the other hand, is intended to induce a tangential movement towards the ‘‘barycentres’’ $\vec{z}_k^m$. Lastly, (S3) completely fixes the tangential motion, so that after the time step, each vertex $\vec{X}^{m+1}(\vec{q}_k^m)$ has the same tangential components as $\vec{z}_k^m$.

- (iv) Similarly to §5.3, a semidiscrete variant of the scheme (5.18) can also be considered. It will satisfy the appropriate analogue of Theorem 5.3(i), as well as Theorem 5.3(ii) when the approximated flow is volume preserving.

Remark 5.10.

- (i) In place of (5.13) and (5.18) it is possible to consider two closely related variants, where in (5.13) and (5.18) the terms $\vec{v}^m$ are replaced by $\frac{\vec{\omega}^m}{|\vec{\omega}^m|}$. On recalling (3.5) this is a minor change to the original schemes, where at each vertex $\vec{\omega}^m$ is now normalized. For these variants all the results in Theorem 5.5 and Theorem 5.8 still hold true, as well as most of the results in Remark 5.6(i) and Remark 5.9. The only property in the latter two remarks that no longer holds is the volume preservation. As can be seen from the proof of Theorem 5.3(ii), volume conservation requires $\vec{v}^m$ to be present in (5.13) and (5.18), and it is for this reason that in general we prefer these schemes in their original form.
- (ii) In the case of mean curvature flow, when $\mathfrak{F}^m(\chi) = \chi$, the solution $\vec{X}^{m+1} \in \underline{V}(\Gamma^m)$ to (5.18) for the strategy (S1) from Remark 5.9(iii) satisfies

$$\begin{aligned} \frac{1}{\Delta t_m} \left\langle \left[\left(\vec{X}^{m+1} - \text{id} \right) \cdot \vec{\omega}^m \right] \vec{\omega}^m + \alpha \sum_{i=1}^{d-1} \left[\left(\vec{X}^{m+1} - \text{id} \right) \cdot \vec{\tau}_i^m \right] \vec{\tau}_i^m, \vec{\eta} \right\rangle_{\Gamma^m}^h \\ + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m). \end{aligned} \quad (5.22)$$

A closely related approximation is obtained by normalizing $\vec{\omega}^m$ in (5.22) to yield

$$\begin{aligned} \frac{1}{\Delta t_m} \left\langle \left[\left(\vec{X}^{m+1} - \text{id} \right) \cdot \vec{\omega}^m \right] \frac{\vec{\omega}^m}{|\vec{\omega}^m|^2} + \alpha \sum_{i=1}^{d-1} \left[\left(\vec{X}^{m+1} - \text{id} \right) \cdot \vec{\tau}_i^m \right] \vec{\tau}_i^m, \vec{\eta} \right\rangle_{\Gamma^m}^h \\ + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m), \end{aligned} \quad (5.23)$$

and this corresponds to the variant of (5.18) discussed in (i). On introducing $\underline{Q}_\theta^m \in \underline{V}(\Gamma^m)$, for $\theta \in \mathbb{R}_{\geq 0}$, with

$$\underline{Q}_\theta^m(\vec{q}_k^m) = \theta \underline{\text{Id}} + (1 - \theta) \frac{\vec{\omega}^m(\vec{q}_k^m) \otimes \vec{\omega}^m(\vec{q}_k^m)}{|\vec{\omega}^m(\vec{q}_k^m)|^2}, \quad k = 1, \dots, K, \quad (5.24)$$

it immediately follows from the fact that $\left\{ \frac{\vec{\omega}^m(\vec{q}_k^m)}{|\vec{\omega}^m(\vec{q}_k^m)|}, \vec{\tau}_1^m(\vec{q}_k^m), \dots, \vec{\tau}_{d-1}^m(\vec{q}_k^m) \right\}$ is an orthonormal basis, that for every $k = 1, \dots, K$ and for every $\vec{z} \in \mathbb{R}^d$

$$\begin{aligned} [\vec{z} \cdot \vec{\omega}^m(\vec{q}_k^m)] \frac{\vec{\omega}^m(\vec{q}_k^m)}{|\vec{\omega}^m(\vec{q}_k^m)|^2} + \alpha \sum_{i=1}^{d-1} [\vec{z} \cdot \vec{\tau}_i^m(\vec{q}_k^m)] \vec{\tau}_i^m(\vec{q}_k^m) \\ = (1 - \alpha) \vec{z} \cdot \vec{\omega}^m(\vec{q}_k^m) \frac{\vec{\omega}^m(\vec{q}_k^m)}{|\vec{\omega}^m(\vec{q}_k^m)|^2} + \alpha \vec{z} = \underline{Q}_\alpha^m(\vec{q}_k^m) \vec{z}. \end{aligned}$$

Hence, for $\alpha = \theta$, (5.23) is equivalent to

$$\left\langle \underline{Q}_\theta^m \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \vec{\eta} \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m). \quad (5.25)$$

Clearly, $\theta = 1$ collapses to (4.33) with mass lumping, while $\theta = 0$ is (4.12) with normalized $\vec{\omega}^m$, recall (i). For $\theta \in (0, 1)$ we obtain some interpolation between the two, with the tangential motion as described in (S1) from Remark 5.9(iii) for $\alpha = \theta$. We also observe that the main idea in Elliott and Fritz (2017), for the case $d = 2$, is to introduce $\theta \underline{\text{Id}} + (1 - \theta) \vec{\nu}^m \otimes \vec{\nu}^m$ into the first term in (4.37), similarly to how (5.25) relates to (4.33).

Remark 5.11 (Discrete linear systems). *It is a simple matter to adapt the definitions and techniques in §4.3 in order to derive the discrete linear systems that need to be solved at each time level for the approximations (5.4), (5.13) and (5.18). The most efficient way is employing a sparse direct solution method such as UMFPACK, see Davis (2004).*

5.6 Alternative parametric methods

An alternative parametric finite element approximation of surface diffusion is given in Bänsch et al. (2005). Their scheme is based on a discretization of the formulation

$$\vec{\mathcal{V}} = \mathcal{V} \vec{\nu}, \quad \mathcal{V} = -\Delta_s \kappa, \quad \kappa = \vec{\kappa} \cdot \vec{\nu}, \quad \vec{\kappa} = \Delta_s \vec{\text{id}}, \quad \text{on } \Gamma(t),$$

in contrast to (5.3). Compared to (5.4) there are two more variables, and as the surface always moves in a direction collinear to the normal, the surface meshes will in general deteriorate.

We refer also to Bänsch et al. (2004), where, on assuming a sufficiently smooth solution, an error analysis is presented for a semidiscrete finite element approximation by continuous piecewise polynomials of degree $k \geq 1$ for a graph formulation of surface diffusion. A semidiscrete finite element approximation of axisymmetric surface diffusion by continuous piecewise linears in a graph formulation has been considered in Coleman et al. (1996). The corresponding error analysis, on assuming a sufficiently smooth solution, is presented in Deckelnick et al. (2003). In addition, a parametric finite element approximation of axisymmetric surface diffusion has been considered in Barrett et al. (2019b).

6 Anisotropic flows

6.1 Derivation of the governing equations

In many interface problems the energy density is directionally dependent. This can result, for example, from a material's directional dependence of a physical property. This appears, for example, in a crystal where the energy of an interface depends on how its direction is related to the crystal lattice orientations. A typical anisotropic surface energy has the form

$$|\Gamma|_\gamma = \int_\Gamma \gamma(\vec{\nu}) \, d\mathcal{H}^{d-1}, \quad (6.1)$$

where Γ is a closed orientable C^1 -hypersurface in $\mathbb{R}^d$, $d \geq 2$, with a unit normal field $\vec{\nu}$, and $\gamma : \mathbb{S}^{d-1} \rightarrow \mathbb{R}_{>0}$ is a given anisotropic energy density. It is mathematically convenient, to extend γ to a function on $\mathbb{R}^d$. In particular, denoting the extension again with γ , we assume that it is absolutely homogeneous of degree one, i.e.

$$\gamma(\lambda \vec{p}) = |\lambda| \gamma(\vec{p}) \quad \forall \vec{p} \in \mathbb{R}^d, \lambda \in \mathbb{R}.$$

Assuming from now on that $\gamma \in C^2(\mathbb{R}^d \setminus \{\vec{0}\})$, we can differentiate this identity with respect to λ to obtain

$$\gamma'(\vec{p}) \cdot \vec{p} = \gamma(\vec{p}) \quad \forall \vec{p} \in \mathbb{R}^d \setminus \{\vec{0}\}, \quad (6.2)$$

where γ' is the gradient of γ . In the isotropic case, $\gamma(\vec{p}) = |\vec{p}|$, and so $\gamma'(\vec{p}) = \frac{\vec{p}}{|\vec{p}|}$. We refer to Taylor et al. (1992); Bellettini et al. (1999); Giga (2006) for more details on anisotropic energies in materials science and geometry.

Lemma 6.1. *Let $(\Gamma(t))_{t \in [0, T]}$ be a C^2 -evolving closed orientable hypersurface with normal vector field $\vec{\nu}$. Then we have the anisotropic version of (4.1)*

$$\frac{d}{dt} |\Gamma(t)|_\gamma = - \langle \kappa_\gamma, \mathcal{V} \rangle_{\Gamma(t)},$$

where $\kappa_\gamma = -\nabla_s \cdot \vec{\nu}_\gamma$ is the weighted mean curvature and $\vec{\nu}_\gamma = \gamma'(\vec{\nu})$ is the Cahn–Hoffmann vector, the anisotropic version of Lemma 2.13(i).

Proof. It follows from the transport theorem, Theorem 2.32, on noting (6.1), (6.2), Lemma 2.37(ii), Theorem 2.21 and Lemma 2.7(i), that

$$\begin{aligned} \frac{d}{dt} |\Gamma(t)|_\gamma &= \frac{d}{dt} \langle 1, \gamma(\vec{\nu}) \rangle_{\Gamma(t)} = \langle 1, \partial_t^\square \gamma(\vec{\nu}) - \gamma(\vec{\nu}) \mathcal{V} \kappa \rangle_{\Gamma(t)} \\ &= \langle 1, \gamma'(\vec{\nu}) \cdot \partial_t^\square \vec{\nu} - \gamma'(\vec{\nu}) \cdot \vec{\nu} \mathcal{V} \kappa \rangle_{\Gamma(t)} \\ &= \langle 1, -\gamma'(\vec{\nu}) \cdot \nabla_s \mathcal{V} + \nabla_s \cdot (\gamma'(\vec{\nu}) \mathcal{V}) \rangle_{\Gamma(t)} \\ &= \langle \nabla_s \cdot \gamma'(\vec{\nu}), \mathcal{V} \rangle_{\Gamma(t)} = -\langle \kappa_\gamma, \mathcal{V} \rangle_{\Gamma(t)}. \end{aligned}$$

□

We can hence define anisotropic versions of mean curvature flow and surface diffusion as

$$(a) \quad \mathcal{V} = \beta(\vec{\nu}) \kappa_\gamma \quad \text{and} \quad (b) \quad \mathcal{V} = -\nabla_s \cdot (\beta(\vec{\nu}) \nabla_s \kappa_\gamma), \quad (6.3)$$

where $\beta : \mathbb{S}^{d-1} \rightarrow \mathbb{R}_{>0}$ is a smooth kinetic coefficient. We refer to Taylor et al. (1992); Cahn and Taylor (1994); Taylor and Cahn (1994); Giga (2006) for a derivation and more information about these evolution laws.

For anisotropic mean curvature flow we obtain from Lemma 6.1 and (6.3) that

$$\frac{d}{dt} |\Gamma(t)|_\gamma = -\langle \kappa_\gamma, \mathcal{V} \rangle_{\Gamma(t)} = -\langle \beta(\vec{\nu}), \kappa_\gamma^2 \rangle_{\Gamma(t)} \leq 0, \quad (6.4)$$

and for anisotropic surface diffusion it holds with the help of Lemma 2.7(i), Definition 2.5(ii) and the divergence theorem, Theorem 2.21, that

$$\frac{d}{dt} |\Gamma(t)|_\gamma = -\langle \kappa_\gamma, \mathcal{V} \rangle_{\Gamma(t)} = -\langle \beta(\vec{\nu}), |\nabla_s \kappa_\gamma|^2 \rangle_{\Gamma(t)} \leq 0. \quad (6.5)$$

Of course, also for the surface energy $|\Gamma|_\gamma$, an isoperimetric problem can be formulated. Here one wants to find the shape, which minimizes $|\Gamma|_\gamma$ under all shapes with a given enclosed volume. In order to do so, one defines the dual function

$$\gamma^*(\vec{q}) = \sup_{\vec{p} \in \mathbb{R}^d \setminus \{\vec{0}\}} \frac{\vec{p} \cdot \vec{q}}{\gamma(\vec{p})} \quad \forall \vec{q} \in \mathbb{R}^d.$$

Then the solution of the isoperimetric problem is, up to a scaling, the Wulff shape

$$\mathcal{W} = \{\vec{q} \in \mathbb{R}^d : \gamma^*(\vec{q}) \leq 1\}.$$

This is the 1-ball of γ^* and we also define the 1-ball of γ

$$\mathcal{F} = \{\vec{p} \in \mathbb{R}^d : \gamma(\vec{p}) \leq 1\},$$

which is called Frank diagram. We refer to Figure 3 for examples. Also surface energies for which the Frank diagram or the Wulff shape have flat parts, edges and corners are of interest. These are called crystalline surface energies, and we will be able to approximate these also in a stable manner.



Figure 3: Frank diagram and Wulff shape in $\mathbb{R}^2$ for the l^1 -norm, $\gamma(\vec{p}) = \sum_{i=1}^2 |p_i|$, left, and for the weighted norm $\gamma(\vec{p}) = (\vec{p} \cdot \underline{G} \vec{p})^{\frac{1}{2}}$, $\underline{G} = \frac{1}{4} \begin{pmatrix} 4 & 0 \\ 0 & 1 \end{pmatrix}$, right.

6.2 Suitable weak formulations

Coming up with stable discretizations is a very difficult task as the flows

$$\mathcal{V} = \beta(\vec{\nu}) \kappa_\gamma \quad \text{and} \quad \mathcal{V} = -\nabla_s \cdot (\beta(\vec{\nu}) \nabla_s \kappa_\gamma) \quad \text{on } \Gamma(t)$$

are even more nonlinear than their isotropic counterparts. A major difficulty is that an analogue of the identity

$$\vec{\kappa} = \kappa \vec{\nu} = \Delta_s \text{id} \quad \text{on } \Gamma(t), \quad (6.6)$$

recall Lemma 2.13(ii), is no longer true in general. However, in many practical situations the present authors were able to come up with an anisotropic version of (6.6).

The main observation is that (6.6) remains true if we replace the standard Euclidean inner product in $\mathbb{R}^d$ by an inner product

$$(\vec{u}, \vec{v})_{\tilde{G}} = \vec{u} \cdot \tilde{G} \vec{v} \quad \forall \vec{u}, \vec{v} \in \mathbb{R}^d, \quad (6.7)$$

where $\tilde{G} \in \mathbb{R}^{d \times d}$ is symmetric and positive definite. One only has to replace the mean curvature vector $\vec{\kappa}$ and the Laplace–Beltrami operator Δ_s by versions which are appropriate for this new inner product. In fact, one just has to consider the canonical Laplace–Beltrami operator on $\Gamma(t)$ with respect to the Riemannian metric given by the new inner product. However, the surface energy density related to the new inner product needs to be identified. It can be shown, see Barrett et al. (2008c, Lemma 2.1), that

$$\gamma(\vec{\nu}) = \sqrt{\vec{\nu} \cdot \underline{G} \vec{\nu}} \quad (6.8)$$

leads to $\tilde{G} = [\det \underline{G}]^{\frac{1}{d-1}} \underline{G}^{-1}$ and a weighted mean curvature κ_γ for which we have a relationship similar to that in the isotropic case, recall (6.6). In fact, it is shown that

$$\kappa_\gamma \vec{\nu} = \gamma(\vec{\nu}) \tilde{G} \Delta_s^{\tilde{G}} \text{id} \quad \text{on } \Gamma(t),$$

see Barrett et al. (2008c, (2.33), (2.37)), where $\Delta_s^{\tilde{G}} = \nabla_s^{\tilde{G}} \cdot \nabla_s^{\tilde{G}}$ is the Laplace–Beltrami operator induced by the inner product (6.6) with $\nabla_s^{\tilde{G}} \cdot$ and $\nabla_s^{\tilde{G}}$ the associated tangential divergence and tangential gradient, respectively. A suitable generalized divergence theorem on manifolds then allows one to introduce a weak formulation of $\gamma(\vec{\nu}) \tilde{G} \Delta_s^{\tilde{G}} \text{id}$.

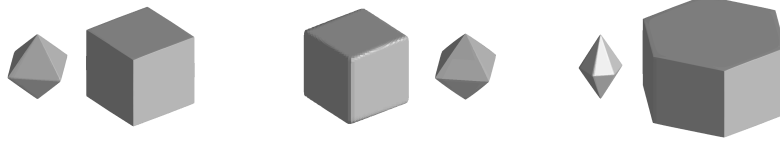


Figure 4: Frank diagram and Wulff shape in $\mathbb{R}^3$ for a regularized l^1 -norm, $\gamma(\vec{p}) = \sum_{\ell=1}^3 [\varepsilon^2 |\vec{p}|^2 + p_\ell^2(1 - \varepsilon^2)]^{\frac{1}{2}}$, $\varepsilon = 0.01$, left, a cubic anisotropy, $\gamma(\vec{p}) = [\sum_{\ell=1}^3 [\varepsilon^2 |\vec{p}|^2 + p_\ell^2(1 - \varepsilon^2)]^{\frac{r}{2}}]^{\frac{1}{r}}$, $\varepsilon = 0.01$, $r = 30$, middle, and a hexagonal anisotropy, $\gamma(\vec{p}) = \sum_{\ell=1}^4 [\vec{p} \cdot \underline{R}_\ell^\top \text{diag}(1, \varepsilon^2, \varepsilon^2) \underline{R}_\ell \vec{p}]^{\frac{1}{2}}$, $\varepsilon = 0.01$, right. Here $\underline{R}_\ell$, $\ell = 1, \dots, 4$ are suitable rotation matrices.

Unfortunately, simple anisotropies of the form (6.8) only lead to ellipsoidal Wulff shapes as in the bottom row of Figure 3, and of course we would like to handle more general situations.

We now consider a larger class of surface energy densities, which are given as suitable norms of the ellipsoidal anisotropies. In particular, we choose

$$\gamma(\vec{p}) = \left(\sum_{\ell=1}^L [\gamma_\ell(\vec{p})]^r \right)^{\frac{1}{r}}, \quad \gamma_\ell(\vec{p}) = \sqrt{\vec{p} \cdot \underline{G}_\ell \vec{p}}, \quad \ell = 1, \dots, L, \quad (6.9)$$

so that

$$\gamma'(\vec{p}) = [\gamma(\vec{p})]^{1-r} \sum_{\ell=1}^L [\gamma_\ell(\vec{p})]^{r-1} \gamma'_\ell(\vec{p}).$$

Here $r \in [1, \infty)$ and $\underline{G}_\ell \in \mathbb{R}^{d \times d}$, $\ell = 1, \dots, L$, are symmetric and positive definite. It turns out that most energies of relevance can be approximated by the above class of energies. In particular, hexagonal and cubic anisotropies can be modelled with appropriate choices of r , L and $\{\underline{G}_\ell\}_{\ell=1}^L$, see Figure 4. We remark that in the planar case, $d = 2$, from a modelling point of view, there is no benefit in choosing $r > 1$. Moreover, the choice $r = 1$ has the advantage that it leads to linear schemes, i.e. a linear system of equations needs to be solved at each time level.

Most of the surface calculus discussed in Section 2 can be repeated in the context of the energies discussed above. We obtain for example, see Barrett et al. (2008c, Theorem 2.1), that for a C^2 -hypersurface Γ it holds that

$$\kappa_\gamma \vec{\nu} = \sum_{\ell=1}^L \gamma_\ell(\vec{\nu}) \underline{\tilde{G}}_\ell \nabla_s^{\tilde{G}_\ell} \cdot \left[\left[\frac{\gamma_\ell(\vec{\nu})}{\gamma(\vec{\nu})} \right]^{r-1} \nabla_s^{\tilde{G}_\ell} \text{id} \right] \quad \text{on } \Gamma, \quad (6.10)$$

where $\underline{\tilde{G}}_\ell = [\det \underline{G}_\ell]^{\frac{1}{d-1}} \underline{G}_\ell^{-1}$, $\ell = 1, \dots, L$, and $\nabla_s^{\tilde{G}_\ell}$, $(\nabla_s^{\tilde{G}_\ell} \cdot)$ are defined as follows. Let $\Gamma \subset \mathbb{R}^d$ be a C^1 -hypersurface and let $\vec{p} \in \Gamma$. Let $\{\vec{\tau}_1, \dots, \vec{\tau}_{d-1}\}$ be an orthonormal basis of $T_{\vec{p}}\Gamma$ with respect to the inner product $(\cdot, \cdot)_{\tilde{G}_\ell}$ on $\mathbb{R}^d$ induced by $\underline{\tilde{G}}_\ell$, recall (6.7). Let

$f : \Gamma \rightarrow \mathbb{R}$, $\vec{f} : \Gamma \rightarrow \mathbb{R}^d$ be C^1 -functions. The anisotropic surface gradient of f , the anisotropic surface divergence of $\vec{f}$ and the anisotropic surface Jacobian of $\vec{f}$ at the point $\vec{p} \in \Gamma$ are defined as

$$(\nabla_s^{\tilde{G}_\ell} f)(\vec{p}) = \sum_{i=1}^{d-1} (\partial_{\vec{\tau}_i} f)(\vec{p}) \vec{\tau}_i, \quad (6.11a)$$

$$(\nabla_s^{\tilde{G}_\ell} \cdot \vec{f})(\vec{p}) = \sum_{i=1}^{d-1} \tilde{\underline{G}}_\ell \vec{\tau}_i \cdot (\partial_{\vec{\tau}_i} \vec{f})(\vec{p}), \quad (6.11b)$$

$$(\nabla_s^{\tilde{G}_\ell} \vec{f})(\vec{p}) = \sum_{i=1}^{d-1} (\partial_{\vec{\tau}_i} \vec{f})(\vec{p}) \otimes \tilde{\underline{G}}_\ell \vec{\tau}_i. \quad (6.11c)$$

The definitions (6.11) are anisotropic versions of Definition 2.5(ii)–(iv) in the case $n = d - 1$. If, in addition, $\vec{g} \in C^1(\Gamma)$, we also define

$$\left(\nabla_s^{\tilde{G}_\ell} \vec{f}, \nabla_s^{\tilde{G}_\ell} \vec{g} \right)_{\tilde{G}_\ell}(\vec{p}) = \sum_{i=1}^{d-1} \left((\partial_{\vec{\tau}_i} \vec{f})(\vec{p}), (\partial_{\vec{\tau}_i} \vec{g})(\vec{p}) \right)_{\tilde{G}_\ell}.$$

Using a generalised divergence theorem, see Barrett et al. (2008c, Lemma 2.8), we can obtain the following weak formulations of the anisotropic flows (6.3) in the case that the anisotropic energy density γ is of the form (6.9). Given a closed hypersurface $\Gamma(0)$, find an evolving hypersurface $(\Gamma(t))_{t \in [0, T]}$ with a global parameterization and induced velocity field $\vec{\mathcal{V}}$, and $\varkappa_\gamma \in L^2(\mathcal{G}_T)$ as follows. For almost all $t \in (0, T)$, find $\vec{\mathcal{V}}(\cdot, t) \in [L^2(\Gamma(t))]^d$ and $\varkappa_\gamma(\cdot, t) \in L^2(\Gamma(t))$, respectively $H^1(\Gamma(t))$, such that

$$\left\langle \vec{\mathcal{V}}, \chi \vec{\nu} \right\rangle_{\Gamma(t)} = \begin{cases} \langle \beta(\vec{\nu}) \varkappa_\gamma, \chi \rangle_{\Gamma(t)} & \forall \chi \in L^2(\Gamma(t)) \\ \langle \beta(\vec{\nu}) \nabla_s \varkappa_\gamma, \nabla_s \chi \rangle_{\Gamma(t)} & \forall \chi \in H^1(\Gamma(t)) \end{cases}, \quad (6.12a)$$

$$\langle \varkappa_\gamma \vec{\nu}, \vec{\eta} \rangle_{\Gamma(t)} + \left\langle \nabla_s^{\tilde{G}} \text{id}, \nabla_s^{\tilde{G}} \vec{\eta} \right\rangle_{\Gamma(t), \gamma} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d, \quad (6.12b)$$

where

$$\left\langle \nabla_s^{\tilde{G}} \vec{\chi}, \nabla_s^{\tilde{G}} \vec{\eta} \right\rangle_{\Gamma(t), \gamma} = \sum_{\ell=1}^L \int_{\Gamma(t)} \left[\frac{\gamma_\ell(\vec{\nu})}{\gamma(\vec{\nu})} \right]^{r-1} (\nabla_s^{\tilde{G}_\ell} \vec{\chi}, \nabla_s^{\tilde{G}_\ell} \vec{\eta})_{\tilde{G}_\ell} \gamma_\ell(\vec{\nu}) \, d\mathcal{H}^{d-1} \quad (6.13)$$

for all $\vec{\chi}, \vec{\eta} \in [H^1(\Gamma(t))]^d$. In the above weak formulations only derivatives up to first order appear, and hence once again the equations can be discretized with the help of continuous piecewise linear finite elements.

6.3 Finite element approximation

The weak formulations (6.12) can be used to formulate finite element approximations of (6.3). Discretizing the velocity and the geometry, similarly as in (4.6) for isotropic mean

curvature flow, we recall the following finite element approximations from Barrett et al. (2008b,c).

Let the closed polyhedral hypersurface Γ^0 be an approximation of $\Gamma(0)$. Then, for $m = 0, \dots, M-1$, find $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$, for $\vec{X}^{m+1} \in \underline{V}(\Gamma^m)$, with unit normal $\vec{\nu}^{m+1}$, and $\kappa_\gamma^{m+1} \in V(\Gamma^m)$ such that

$$\left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \chi \vec{\nu}^m \right\rangle_{\Gamma^m}^h = \begin{cases} \langle \beta(\vec{\nu}^m) \kappa_\gamma^{m+1}, \chi \rangle_{\Gamma^m}^h \\ \langle \beta(\vec{\nu}^m) \nabla_s \kappa_\gamma^{m+1}, \nabla_s \chi \rangle_{\Gamma^m} \end{cases} \quad \forall \chi \in V(\Gamma^m), \quad (6.14a)$$

$$\langle \kappa_\gamma^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h + \left\langle \nabla_s^{\tilde{G}_\ell} \vec{X}^{m+1}, \nabla_s^{\tilde{G}_\ell} \vec{\eta} \right\rangle_{\Gamma^m, \gamma} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m). \quad (6.14b)$$

In the above, we have used the notation

$$\begin{aligned} & \left\langle \nabla_s^{\tilde{G}_\ell} \vec{X}^{m+1}, \nabla_s^{\tilde{G}_\ell} \vec{\eta} \right\rangle_{\Gamma^m, \gamma} \\ &= \sum_{\ell=1}^L \int_{\Gamma^m} \left[\frac{\gamma_\ell(\vec{\nu}^{m+1} \circ \vec{X}^{m+1})}{\gamma(\vec{\nu}^{m+1} \circ \vec{X}^{m+1})} \right]^{r-1} (\nabla_s^{\tilde{G}_\ell} \vec{X}^{m+1}, \nabla_s^{\tilde{G}_\ell} \vec{\eta})_{\tilde{G}_\ell} \gamma_\ell(\vec{\nu}^m) \, d\mathcal{H}^{d-1}, \end{aligned}$$

i.e. a discrete analogue of (6.13).

Remark 6.2 (Curves in the plane). *On using the notation from §3.1.2, and similarly to (4.13), the systems (6.14) simplify considerably in the case $d = 2$, i.e. for the evolution of curves in the plane, recall also Barrett et al. (2008c, (3.5)). In particular, we can reformulate (6.14) as follows. Let $\vec{X}^0 \in \underline{V}^h(\mathbb{I})$ be such that $\Gamma^0 = \vec{X}^0(\mathbb{I})$ is a polygonal approximation of $\Gamma(0)$. Then, for $m = 0, \dots, M-1$, find $(\vec{X}^{m+1}, \kappa_\gamma^{m+1}) \in \underline{V}^h(\mathbb{I}) \times V^h(\mathbb{I})$ such that*

$$-\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\Delta t_m}, \chi [\vec{X}_\rho^m]^\perp \right\rangle_{\mathbb{I}}^h = \begin{cases} \left\langle \beta \left(-\frac{[\vec{X}_\rho^m]^\perp}{|\vec{X}_\rho^m|} \right) \kappa_\gamma^{m+1}, \chi [\vec{X}_\rho^m] \right\rangle_{\mathbb{I}}^h \\ \left\langle \beta \left(-\frac{[\vec{X}_\rho^m]^\perp}{|\vec{X}_\rho^m|} \right) (\kappa_\gamma^{m+1})_\rho, \chi_\rho |\vec{X}_\rho^m|^{-1} \right\rangle_{\mathbb{I}} \end{cases}, \quad (6.15a)$$

$$-\left\langle \kappa_\gamma^{m+1} [\vec{X}_\rho^m]^\perp, \vec{\eta} \right\rangle_{\mathbb{I}}^h + \sum_{\ell=1}^L \left\langle \left[\frac{\gamma_\ell([\vec{X}_\rho^{m+1}]^\perp)}{\gamma([\vec{X}_\rho^{m+1}]^\perp)} \right]^{r-1} \frac{\underline{G}_\ell [\vec{X}_\rho^{m+1}]^\perp}{\gamma_\ell([\vec{X}_\rho^m]^\perp)}, \vec{\eta}_\rho^\perp \right\rangle_{\mathbb{I}} = 0 \quad (6.15b)$$

for all $\chi \in V^h(\mathbb{I})$ and $\vec{\eta} \in \underline{V}^h(\mathbb{I})$.

For $r = 1$ in (6.9) the systems (6.14) do not depend on $\vec{\nu}^{m+1}$, and so they reduce to linear systems for the unknowns $\vec{X}^{m+1}$ and κ_γ^{m+1} . For these discrete systems we have the following existence and uniqueness result, which can be shown by generalizing the proofs of the corresponding isotropic cases, see Theorems 4.3 and 5.1.

Theorem 6.3. *Let Γ^m satisfy Assumption 3.24(i), and let γ be of the form (6.9) with $r = 1$. Then there exists a unique solution $(\vec{X}^{m+1}, \kappa_\gamma^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to the systems (6.14).*

Proof. The two results can be shown as in the proofs of Theorem 4.3 and Theorem 5.1, see also Barrett et al. (2008c, Theorem 3.1). $\square$

Remark 6.4. *For the nonlinear discretizations with $r > 1$, neither existence nor uniqueness results are known. However, in practice there are no difficulties in finding solutions to the nonlinear systems (6.14), and the employed iterative solvers always converged.*

The main property of the schemes (6.14) are that they can be shown to be stable. This enables one to compute solutions for strongly anisotropic, nearly crystalline anisotropies. Something which is difficult with other schemes in the literature. The main insight is that a local inequality for the anisotropic energy is true, which is similar to the isotropic version stated in Lemma 3.15 for $d = 3$. In fact, we have the following result.

Lemma 6.5. *Let $d = 3$ and let $\Gamma^h = \bigcup_{j=1}^J \bar{\sigma}_j$ be a polyhedral hypersurface, with unit normal $\vec{\nu}^h$, in $\mathbb{R}^d$. Then we have for $j = 1, \dots, J$ and $\ell = 1, \dots, L$ that*

$$\frac{1}{2} \int_{\sigma_j} \gamma_\ell(\vec{\nu}^h) |\nabla_s^{\tilde{G}_\ell} \vec{X}|_{\tilde{G}_\ell}^2 d\mathcal{H}^2 \geq \int_{\vec{X}(\sigma_j)} \gamma_\ell(\vec{\nu}_{\vec{X}}^h) d\mathcal{H}^2 \quad \forall \vec{X} \in \underline{V}(\Gamma^h),$$

with equality for $\vec{X} = \text{id}|_{\Gamma^h} \in \underline{V}(\Gamma^h)$. Here $\vec{\nu}_{\vec{X}}^h$ is the unit normal on the polyhedral hypersurface $\vec{X}(\Gamma^h)$ and $|\cdot|_{\tilde{G}_\ell}^2 = (\cdot, \cdot)_{\tilde{G}_\ell}$.

Proof. See Barrett et al. (2008c, Lemma 3.1). $\square$

Lemma 6.6. *Let γ be of the form (6.9) and let $d = 2$ or $d = 3$. Let $\Gamma^h = \bigcup_{j=1}^J \bar{\sigma}_j$ be a polyhedral hypersurface, with unit normal $\vec{\nu}^h$, in $\mathbb{R}^d$. Let γ be of the form (6.9) and let $\vec{X} \in \underline{V}(\Gamma^h)$. Then it holds that*

$$\left\langle \nabla_s^{\tilde{G}} \vec{X}, \nabla_s^{\tilde{G}} (\vec{X} - \text{id}) \right\rangle_{\Gamma^h, \gamma} \geq |\vec{X}(\Gamma^h)|_\gamma - |\Gamma^h|_\gamma,$$

where $|\Gamma^h|_\gamma = \langle 1, \gamma(\vec{\nu}^h) \rangle_{\Gamma^h}$.

Proof. The proof for $d = 3$ hinges on Lemma 6.5 and can be found in Barrett et al. (2008c, Theorem 3.2). On recalling Remark 6.2, the result for $d = 2$, and $r = 1$, can be shown by using ideas similar to (3.13) in the proof of Lemma 3.17, see Barrett et al. (2008b, Theorem 2.5). It can easily be extended to the case $r \geq 1$, on using the techniques in Barrett et al. (2008c, Theorem 3.2). $\square$

Theorem 6.7. *Let γ be of the form (6.9) and let $d = 2$ or $d = 3$. Let $(\vec{X}^{m+1}, \kappa_\gamma^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ be a solution of (6.14). Then it holds that*

$$|\Gamma^{m+1}|_\gamma + \Delta t_m \left\{ \begin{aligned} &\langle \beta(\vec{\nu}^m) \kappa_\gamma^{m+1}, \kappa_\gamma^{m+1} \rangle_{\Gamma^m}^h \\ &\langle \beta(\vec{\nu}^m) \nabla_s \kappa_\gamma^{m+1}, \nabla_s \kappa_\gamma^{m+1} \rangle_{\Gamma^m} \end{aligned} \right\} \leq |\Gamma^m|_\gamma, \quad (6.16)$$

where we recall (6.1).

Proof. Similarly to the proof of Theorem 4.4, we can choose $\chi = \kappa_\gamma^{m+1} \in V(\Gamma^m)$ in (6.14a) and $\vec{\eta} = \frac{1}{\Delta t_m} (\vec{X}^{m+1} - \text{id}_{|\Gamma^m}) \in \underline{V}(\Gamma^m)$ in (6.14b), and then combine with Lemma 6.6, in order to obtain the desired results. $\square$

The inequalities (6.16) are the discrete analogues of (6.4) and (6.5), respectively, and anisotropic analogues of Theorems 4.4 and 5.2, respectively.

6.4 Solution method and discrete systems

In comparison to the isotropic case the assembly of the matrices is only slightly more complicated. In addition to the matrices in §4.3, we define $M_{\Gamma^m, \beta}, A_{\Gamma^m, \beta} \in \mathbb{R}^{K \times K}$ with entries

$$[M_{\Gamma^m, \beta}]_{kl} = \langle \beta(\vec{\nu}^m) \phi_k^{\Gamma^m}, \phi_l^{\Gamma^m} \rangle_{\Gamma^m}^h, \quad [A_{\Gamma^m, \beta}]_{kl} = \langle \beta(\vec{\nu}^m) \nabla_s \phi_k^{\Gamma^m}, \nabla_s \phi_l^{\Gamma^m} \rangle_{\Gamma^m}.$$

Moreover, given a $\vec{v} \in \underline{V}_c(\Gamma^m)$, we introduce $\underline{A}_{\Gamma^m, \gamma}(\vec{v}) \in (\mathbb{R}^{d \times d})^{K \times K}$ with entries

$$[\underline{A}_{\Gamma^m, \gamma}(\vec{v})]_{kl} = \sum_{\ell=1}^L \left\langle \left[\frac{\gamma_\ell(\vec{v})}{\gamma(\vec{v})} \right]^{r-1} \gamma_\ell(\vec{\nu}^m) \nabla_s^{\tilde{G}_\ell} \phi_k^{\Gamma^m}, \nabla_s^{\tilde{G}_\ell} \phi_l^{\Gamma^m} \right\rangle_{\Gamma^m} \tilde{G}_\ell,$$

where we have noted (6.13) and (6.7). Assembling these matrices is straightforward, since assembling e.g. $\left(\left\langle \nabla_s^{\tilde{G}_\ell} \phi_k^{\Gamma^m}, \nabla_s^{\tilde{G}_\ell} \phi_l^{\Gamma^m} \right\rangle_{\Gamma^m} \right)_{k,l=1}^K$ is very similar to assembling A_m in (4.10).

Using the notation from (4.11), we can then formulate (6.14) as: Find $(\delta \vec{X}^{m+1}, \kappa_\gamma^{m+1}) \in (\mathbb{R}^d)^K \times \mathbb{R}^K$ such that

$$\begin{pmatrix} \Delta t_m \begin{pmatrix} M_{\Gamma^m, \beta} & -\vec{N}_{\Gamma^m}^\top \\ A_{\Gamma^m, \beta} & \underline{A}_{\Gamma^m, \gamma}(\vec{v}^{m+1}) \end{pmatrix} \end{pmatrix} \begin{pmatrix} \kappa_\gamma^{m+1} \\ \delta \vec{X}^{m+1} \end{pmatrix} = \begin{pmatrix} 0 \\ -\underline{A}_{\Gamma^m, \gamma}(\vec{v}^{m+1}) \vec{X}^m \end{pmatrix}, \quad (6.17)$$

where we have used the notation $\vec{v}^{m+1} = \vec{\nu}^{m+1} \circ \vec{X}^{m+1}$, and where we recall that $\delta \vec{X}^{m+1}$ is the vector of coefficients with respect to the standard basis for $\vec{X}^{m+1} - \text{id}_{|\Gamma^m} \in \underline{V}(\Gamma^m)$.

If γ is of the form (6.9) with $r = 1$, then the system (6.17) does not depend on $\vec{v}^{m+1}$ and so is linear. Hence it can be solved analogously to (4.11), i.e. either with a sparse direct solver or with the help of a Schur complement approach and a preconditioned conjugate gradient solver, see Barrett et al. (2008c, §4) for details.

If $r > 1$, on the other hand, then the nonlinear system (6.17) can be solved with a lagged fixed-point type iteration, where each iterate is obtained by solving a linear system of the form (6.17), with $\vec{v}^{m+1}$ replaced by a given quantity $\vec{v}^{m+1, i}$. We note that in practice such an iteration always converges, and refer to Barrett et al. (2008c, §4) for further details.

6.5 Volume conservation for semidiscrete schemes

For the semidiscrete continuous-in-time variants of (6.14) it is straightforward to prove the obvious anisotropic analogues of Theorem 4.6(i) and Theorem 5.3(i), as well as Theorem 5.3(ii) in the case of anisotropic surface diffusion.

Remark 6.8 (Tangential motion). *In the anisotropic situation the tangential motion induced by the semidiscrete analogue of (6.14b) will no longer lead to surfaces satisfying Definition 3.20. In particular, Theorem 4.6(ii) will in general not hold. In the planar case, and if γ is of the form (6.9) with $L = 1$ and $r = 1$, then equidistribution with respect to γ can be shown, see Barrett et al. (2008b, Remark 2.7). However, the fully discrete schemes (6.14), for any γ of the form (6.9) and for $d = 2$ and $d = 3$, exhibit good quality meshes in practice, without coalescence that could lead to a breakdown of the schemes. See, for example, the numerical simulations in Barrett et al. (2008c, §5).*

6.6 Alternative numerical approaches

For the case $d = 2$ a numerical scheme for anisotropic mean curvature flow has been proposed in Dziuk (1999a), and an error estimate for a semidiscrete continuous-in-time variant is shown, on assuming that the approximated solution is sufficiently smooth.

Moreover, and still for $d = 2$, fully implicit fully discrete schemes, similar to (4.28), for anisotropic evolution equations are considered in Barrett et al. (2011).

The extension of the methods discussed in this section to anisotropic evolution laws of surface clusters and surfaces with boundary has been discussed in Barrett et al. (2008b, 2010a,d).

For parametric methods for anisotropic curvature driven flows in higher codimension we refer to Pozzi (2007, 2008); Barrett et al. (2010b).

We refer also to Deckelnick and Dziuk (1999), where, on assuming a sufficiently smooth solution, an error analysis is presented for a semidiscrete finite element approximation by continuous piecewise linears of a graph formulation of anisotropic mean curvature flow. We refer to Deckelnick et al. (2005b) for the corresponding error analysis for a fully discrete finite element approximation of a graph formulation of anisotropic surface diffusion.

We also refer to Deckelnick et al. (2005a) for the approximation of anisotropic mean curvature flow in the context of level set and phase field methods. For the former we mention Clarenz et al. (2005); Burger et al. (2007), while for the latter we refer to Caginalp and Lin (1987); Garcke et al. (1999); Beneš (2003); Gräßer et al. (2013) and the present authors' work in Barrett et al. (2013b, 2014a) on stable approximations of anisotropic mean curvature flow and anisotropic surface diffusion.

Finally we mention that for strongly anisotropic surface energies, some authors propose a curvature energy regularization, which leads to higher order flows with similarities to Willmore flow, see Burger (2005); Haußer and Voigt (2005); Torabi et al. (2009).

7 Coupling bulk equations to geometric equations on the surface and applications to crystal growth

We now consider how curvature driven interface evolutions can involve quantities defined in the bulk regions surrounding the interface.

7.1 The Mullins–Sekerka problem

Let us start with one of the simplest problems that couple geometric equations on the interface to equations in the bulk. Let $\Omega \subset \mathbb{R}^d$, $d \geq 2$, be a domain with a Lipschitz boundary $\partial\Omega$, which is separated by an interface into two different phases. The interface is at each time t assumed to be a closed C^2 -hypersurface $\Gamma(t) \subset \Omega$. We adopt the notation in §2.4, recall Figure 1. and assume that two phases occupy regions $\Omega_-(t)$ and $\Omega_+(t) = \Omega \setminus \overline{\Omega_-(t)}$ with $\Gamma(t) = \partial\Omega_-(t)$, and with $\vec{\nu}$ denoting the outer unit normal to $\Omega_-(t)$ on $\Gamma(t)$. Then the Mullins–Sekerka problem is given as follows. Given $\Gamma(0)$, find $u : \Omega \times [0, T] \rightarrow \mathbb{R}$ and the evolving interface $(\Gamma(t))_{t \in [0, T]}$ such that for all $t \in (0, T]$ the following conditions hold

$$-\Delta u = 0 \quad \text{in } \Omega_-(t), \quad -\Delta u = 0 \quad \text{in } \Omega_+(t), \quad (7.1a)$$

$$u = \varkappa \quad \text{on } \Gamma(t), \quad [\partial_{\vec{\nu}} u]_-^+ = -\mathcal{V} \quad \text{on } \Gamma(t), \quad (7.1b)$$

$$\partial_{\vec{\nu}_\Omega} u = 0 \quad \text{on } \partial\Omega, \quad (7.1c)$$

where we have recalled the notation (2.13) and $\vec{\nu}_\Omega$ is the outer unit normal to Ω on $\partial\Omega$.

7.1.1 Weak formulation of the Mullins–Sekerka problem

A finite element approximation of the Mullins–Sekerka problem needs a suitable weak formulation, which is given as follows. Given a closed hypersurface $\Gamma(0) \subset \Omega$, we seek an evolving hypersurface $(\Gamma(t))_{t \in [0, T]}$ that separates Ω into $\Omega_-(t)$ and $\Omega_+(t)$, with a global parameterization and induced velocity field $\vec{\mathcal{V}}$, and $\varkappa \in L^2(\mathcal{G}_T)$ as well as $u : \Omega \times [0, T] \rightarrow \mathbb{R}$ as follows. For almost all $t \in (0, T)$, find $(u(\cdot, t), \vec{\mathcal{V}}(\cdot, t), \varkappa(\cdot, t)) \in H^1(\Omega) \times [L^2(\Gamma(t))]^d \times L^2(\Gamma(t))$ such that

$$(\nabla u, \nabla \phi) = \left\langle \vec{\mathcal{V}}, \phi \vec{\nu} \right\rangle_{\Gamma(t)} \quad \forall \phi \in H^1(\Omega), \quad (7.2a)$$

$$\langle u, \chi \rangle_{\Gamma(t)} = \langle \varkappa, \chi \rangle_{\Gamma(t)} \quad \forall \chi \in L^2(\Gamma(t)), \quad (7.2b)$$

$$\langle \varkappa \vec{\nu}, \vec{\eta} \rangle_{\Gamma(t)} + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d. \quad (7.2c)$$

Here $(\cdot, \cdot) = \langle \cdot, \cdot \rangle_\Omega$ is the L^2 -inner product on Ω . It is easy to show that a sufficiently smooth solution to (7.2) solves (7.1). To this end, we observe that it follows from (7.2a)

and Remark 2.36, on using a density argument, that

$$\begin{aligned} \langle \mathcal{V}, \phi \rangle_{\Gamma(t)} &= \left\langle \vec{\mathcal{V}}, \phi \vec{\nu} \right\rangle_{\Gamma(t)} = (\nabla u, \nabla \phi) \\ &= - \int_{\Omega_-(t) \cup \Omega_+(t)} \phi \Delta u \, d\mathcal{L}^d + \langle \partial_{\vec{\nu}_\Omega} u, \phi \rangle_{\partial\Omega} - \langle [\partial_{\vec{\nu}} u]_-^+, \phi \rangle_{\Gamma(t)} \\ &\quad \forall \phi \in H^1(\Omega). \end{aligned} \quad (7.3)$$

Now the fundamental lemma of the calculus of variations, together with (7.3), yields that (7.1a), (7.1c) and the second condition in (7.1b) hold. Similarly, it follows from (7.2b) and (7.2c), on recalling Remark 2.22(iv), that the first condition in (7.1b) is also satisfied.

Remark 7.1. *For a sufficiently smooth weak solution of (7.2), we can formally prove the following results.*

- (i) *The Mullins–Sekerka problem decreases the surface area of the interface. This follows from the transport theorem, Theorem 2.32, (7.2b) with $\chi = \mathcal{V}$ and (7.2a) with $\phi = u$, as*

$$\frac{d}{dt} |\Gamma(t)| = - \langle \mathcal{K}, \mathcal{V} \rangle_{\Gamma(t)} = - \langle u, \mathcal{V} \rangle_{\Gamma(t)} = - \left\langle \vec{\mathcal{V}}, u \vec{\nu} \right\rangle_{\Gamma(t)} = - |\nabla u|_\Omega^2 \leq 0.$$

- (ii) *The Mullins–Sekerka problem preserves the volume $\mathcal{L}^d(\Omega_-(t))$, and hence $\mathcal{L}^d(\Omega_+(t))$, as the transport theorem, Theorem 2.33, yields that*

$$\frac{d}{dt} \mathcal{L}^d(\Omega_-(t)) = \langle \mathcal{V}, 1 \rangle_{\Gamma(t)} = \left\langle \vec{\mathcal{V}}, \vec{\nu} \right\rangle_{\Gamma(t)} = (\nabla u, \nabla 1) = 0,$$

where we have chosen $\phi = 1$ in (7.2a).

Remark 7.2. *Given the hypersurface $\Gamma(t) \subset \Omega$, and hence its normal $\vec{\nu}(t)$ and curvature $\mathcal{K}(t)$, we can solve (7.1a), (7.1c) and the first equation in (7.1b) to obtain a bulk function $u(t)$ that depends on $\mathcal{K}(t)$. Defining now*

$$\mathfrak{F}(\mathcal{K}) = - [\partial_{\vec{\nu}} u]_-^+,$$

we obtain that

$$\langle \mathfrak{F}(\mathcal{K}), \mathcal{K} \rangle_{\Gamma(t)} = - \langle [\partial_{\vec{\nu}} u]_-^+, \mathcal{K} \rangle_{\Gamma(t)} = - \langle [\partial_{\vec{\nu}} u]_-^+, u \rangle_{\Gamma(t)} = |\nabla u|_\Omega^2 \geq 0,$$

where we have observed the first equation in (7.1b), and the choice $\phi = u$ in (7.3), on noting (7.1a) and (7.1c). Therefore, the Mullins–Sekerka problem (7.1) can be written in the general form (5.9) satisfying (5.10).

7.1.2 An unfitted finite element approximation of the Mullins–Sekerka problem

In addition to the discretization of the evolving hypersurface, we need a discretization of the domain Ω . For simplicity we assume that Ω is a polyhedral domain. Although a generalization to a curved domain Ω is possible using suitable boundary approximations, see Ciarlet (1978). For all $m \geq 0$, let $\mathcal{T}^m$ be a regular partitioning of Ω into disjoint open simplices, so that $\bar{\Omega} = \cup_{o \in \mathcal{T}^m} \bar{o}$, see Ciarlet (1978) for a definition of regular partitioning and further details about finite elements. Note that we allow for time-dependent bulk triangulations. Associated with $\mathcal{T}^m$ is the finite element space

$$S^m = \{\chi \in C(\bar{\Omega}) : \chi|_o \text{ is affine } \forall o \in \mathcal{T}^m\} \subset H^1(\Omega). \quad (7.4)$$

Let K_{S^m} be the number of nodes of $\mathcal{T}^m$ and let $\{\vec{p}_k^m\}_{k=1}^{K_{S^m}}$ be the coordinates of these nodes. Let $\{\phi_k^{S^m}\}_{k=1}^{K_{S^m}}$ be the standard basis functions for S^m . We introduce $I^m : C(\bar{\Omega}) \rightarrow S^m$, the interpolation operator, such that $(I^m \eta)(\vec{p}_k^m) = \eta(\vec{p}_k^m)$ for $k = 1, \dots, K_{S^m}$. A discrete semi-inner product on $C(\bar{\Omega})$ is then defined by

$$(\eta_1, \eta_2)_m^h = (I^m[\eta_1 \eta_2], 1) \quad \forall \eta_1, \eta_2 \in C(\bar{\Omega}),$$

with the induced seminorm given by $|\eta|_{\Omega, m} = [(\eta, \eta)_m^h]^{\frac{1}{2}}$ for $\eta \in C(\bar{\Omega})$.

We can now introduce the finite element approximation of the Mullins–Sekerka problem from Barrett et al. (2010c), based on the weak formulation (7.2), as follows. Let the closed polyhedral hypersurface Γ^0 be an approximation of $\Gamma(0)$ and recall the time interval partitioning (4.5). Then, for $m = 0, \dots, M-1$, find $(U^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) \in S^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that

$$(\nabla U^{m+1}, \nabla \varphi) = \left\langle \pi_{\Gamma^m} \left[\frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m} \cdot \vec{\omega}^m \right], \varphi \right\rangle_{\Gamma^m} \quad \forall \varphi \in S^m, \quad (7.5a)$$

$$\langle \kappa^{m+1}, \chi \rangle_{\Gamma^m}^h = \langle U^{m+1}, \chi \rangle_{\Gamma^m} \quad \forall \chi \in V(\Gamma^m), \quad (7.5b)$$

$$\langle \kappa^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (7.5c)$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$. In the above we have recalled (3.3).

Remark 7.3 (Implementation). *The approximation (7.5) is called unfitted because the surface mesh is totally independent of the bulk mesh, and is not fitted to the bulk mesh in the sense that the surface mesh does not consist of faces of the bulk mesh, see Barrett and Elliott (1982). As a consequence, special quadrature rules need to be employed in order to calculate the right hand sides in (7.5a) and (7.5b). Here the most challenging aspect is to compute intersections $\sigma^m \cap o^m$ between an arbitrary element $\sigma^m \subset \Gamma^m$ and an element $o^m \in \mathcal{T}^m$ of the bulk mesh. An algorithm that describes how these intersections can be calculated is given in Barrett et al. (2010c, p. 6284), see also Figures 4 and 5 in Barrett et al. (2010c).*

Before stating our next result, we need an assumption on the compatibility between bulk and surface mesh.

Assumption 7.4. *Let Γ^m and $\mathcal{T}^m$ be such that*

$$\dim \left\{ \int_{\Gamma^m} \varphi \vec{\omega}^m d\mathcal{H}^{d-1} : \varphi \in S^m \right\} = d.$$

Theorem 7.5. *Let Γ^m and $\mathcal{T}^m$ satisfy Assumption 7.4. Then there exists a unique solution $(U^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) \in S^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to (7.5). In addition, if $d = 2$ or $d = 3$, then a solution to (7.5) satisfies the stability estimate*

$$|\Gamma^{m+1}| + \Delta t_m |\nabla U^{m+1}|_\Omega^2 \leq |\Gamma^m|.$$

Proof. Existence follows from uniqueness and hence we consider the homogeneous linear system. Find $(U, \vec{X}, \kappa) \in S^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that

$$\Delta t_m (\nabla U, \nabla \varphi) - \left\langle \pi_{\Gamma^m}[\vec{X} \cdot \vec{\omega}^m], \varphi \right\rangle_{\Gamma^m} = 0 \quad \forall \varphi \in S^m, \quad (7.6a)$$

$$\langle \kappa, \chi \rangle_{\Gamma^m}^h - \langle U, \chi \rangle_{\Gamma^m} = 0 \quad \forall \chi \in V(\Gamma^m), \quad (7.6b)$$

$$\langle \kappa \vec{\omega}^m, \vec{\eta} \rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m), \quad (7.6c)$$

where we have noted (3.5) in (7.6c). Choosing $\varphi = U$ in (7.6a), $\chi = \pi_{\Gamma^m}[\vec{X} \cdot \vec{\omega}^m]$ in (7.6b) and $\vec{\eta} = \vec{X}$ in (7.6c) gives

$$\Delta t_m |\nabla U|_\Omega^2 + \left| \nabla_s \vec{X} \right|_{\Gamma^m}^2 = 0.$$

We hence obtain that U is constant in Ω and that $\vec{X}$ is constant on Γ^m . Now (7.6a) and Assumption 7.4 yield that $\vec{X} = \vec{0}$. Moreover, it follows from (7.6b) that $\kappa = U$ is constant on Γ^m . Hence we can proceed as in the proof of Theorem 5.1 to show that $\kappa = U = 0$, and so we obtain uniqueness.

It remains to prove the stability bound. Here we choose $\varphi = U^{m+1}$ in (7.5a), $\chi = \pi_{\Gamma^m}[(\vec{X}^{m+1} - \text{id}) \cdot \vec{\omega}^m]$ in (7.5b) and $\vec{\eta} = \vec{X}^{m+1} - \text{id}_{\Gamma^m}$ in (7.5c) and obtain

$$\Delta t_m |\nabla U^{m+1}|_\Omega^2 + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s (\vec{X}^{m+1} - \text{id}) \right\rangle_{\Gamma^m} = 0.$$

Now Lemma 3.17 yields the claim. $\square$

Remark 7.6 (Semidiscrete scheme). *We note that the above stability bound is a discrete analogue of Remark 7.1(i). However, the fully discrete scheme (7.5) will in general not satisfy an exact discrete analogue of the volume conservation property Remark 7.1(ii). That is because choosing $\varphi = 1$ in (7.5a) only leads to*

$$\begin{aligned} 0 &= \left\langle \pi_{\Gamma^m} \left[(\vec{X}^{m+1} - \text{id}) \cdot \vec{\omega}^m \right], 1 \right\rangle_{\Gamma^m} = \left\langle \vec{X}^{m+1} - \text{id}, \vec{\omega}^m \right\rangle_{\Gamma^m}^h \\ &= \left\langle \vec{X}^{m+1} - \text{id}, \vec{\nu}^m \right\rangle_{\Gamma^m}^h = \left\langle \vec{X}^{m+1} - \text{id}, \vec{\nu}^m \right\rangle_{\Gamma^m}, \end{aligned} \quad (7.7)$$

where we have noted (3.5) and (3.6). In general, the terms in (7.7) do not equal the discrete volume change $\mathcal{L}^d(\Omega_-^{m+1}) - \mathcal{L}^d(\Omega_-^m)$, where Ω_-^m denotes the interior of Γ^m . However, on recalling Remark 5.4(ii) it is possible to prove an exact discrete analogue of Remark 7.1(ii) for a semidiscrete version of the scheme (7.5). Moreover, this semidiscrete scheme will satisfy the mesh property Theorem 5.3(iii).

Remark 7.7 (Discrete linear systems). *On recalling the notation from §4.3, we can formulate the linear systems of equations to be solved at each time level for (7.5) as follows. Find $(U^{m+1}, \kappa^{m+1}, \delta \vec{X}^{m+1}) \in \mathbb{R}^{K_{sm}} \times \mathbb{R}^K \times (\mathbb{R}^d)^K$ such that*

$$\begin{pmatrix} A_\Omega & 0 & -\frac{1}{\Delta t_m} \vec{N}_{\Omega, \Gamma^m}^\top \\ -M_{\Gamma^m, \Omega} & M_{\Gamma^m} & 0 \\ 0 & \vec{N}_{\Gamma^m} & \underline{A}_{\Gamma^m} \end{pmatrix} \begin{pmatrix} U^{m+1} \\ \kappa^{m+1} \\ \delta \vec{X}^{m+1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -\underline{A}_{\Gamma^m} \vec{X}^m \end{pmatrix}, \quad (7.8)$$

where we use a similar abuse of notation as in (4.11). The definitions of the matrices in (7.8) are either given in (4.10), or they follow directly from (7.5), see also Barrett et al. (2010c, §4.1) for details. In practice, the linear system (7.8) can either be solved with a sparse direct solution method like UMFPACK, see Davis (2004), or by first using a Schur complement approach and then use a (preconditioned) conjugate gradient solver. Once again, we refer to Barrett et al. (2010c, §4.1) for more details.

7.2 The Stefan problem with a (kinetic) Gibbs–Thomson law

In general crystal growth phenomena involve more complex models, in comparison to the above Mullins–Sekerka model. The overall model is the Stefan problem with a Gibbs–Thomson law and kinetic undercooling with anisotropic surface energy (6.1) taken into account. It is given as follows with the same notation and conventions as for (7.1).

Given $\Gamma(0)$ and, if $\vartheta > 0$, $u_0 : \Omega \rightarrow \mathbb{R}$, find $u : \Omega \times [0, T] \rightarrow \mathbb{R}$ and the evolving interface $(\Gamma(t))_{t \in [0, T]}$ such that $\vartheta u(\cdot, 0) = \vartheta u_0$ and for all $t \in (0, T]$ the following conditions hold

$$\vartheta \partial_t u - \mathcal{K}_- \Delta u = f \quad \text{in } \Omega_-(t), \quad \vartheta \partial_t u - \mathcal{K}_+ \Delta u = f \quad \text{in } \Omega_+(t), \quad (7.9a)$$

$$\frac{\rho \mathcal{V}}{\beta(\vec{\nu})} = \alpha \kappa_\gamma - a u \quad \text{on } \Gamma(t), \quad [\mathcal{K} \partial_{\vec{\nu}} u]_-^+ = -\lambda \mathcal{V} \quad \text{on } \Gamma(t), \quad (7.9b)$$

$$\partial_{\vec{\nu}_\Omega} u = 0 \quad \text{on } \partial_N \Omega, \quad u = u_D \quad \text{on } \partial_D \Omega, \quad (7.9c)$$

where $[\mathcal{K} \partial_{\vec{\nu}} u]_-^+$ is defined similarly to (2.13), and $\partial \Omega = \overline{\partial_N \Omega} \cup \overline{\partial_D \Omega}$ with $\partial_N \Omega \cap \partial_D \Omega = \emptyset$. In the above system u denotes deviation from the melting temperature at a planar interface, f describes heat sources, $\vartheta \in \mathbb{R}_{\geq 0}$ is the volumetric heat capacity, and $\mathcal{K}(\cdot, t) = \mathcal{K}_+ \mathcal{X}_{\Omega_+(t)} + \mathcal{K}_- \mathcal{X}_{\Omega_-(t)}$, with $\mathcal{K}_\pm \in \mathbb{R}_{>0}$, is the phase-dependent thermal conductivity, recall (2.11). Moreover, $\lambda \in \mathbb{R}_{>0}$ is the latent heat per unit volume, $\alpha \in \mathbb{R}_{>0}$ is an interfacial energy density per surface area, $\rho \in \mathbb{R}_{\geq 0}$ is a kinetic coefficient and $a \in \mathbb{R}_{>0}$ is a coefficient having the dimension entropy/volume. In addition, as in §6.1, $\beta : \mathbb{S}^{d-1} \rightarrow \mathbb{R}_{>0}$ is a dimensionless mobility function, which allows one to describe the dependence of the mobility on the

local orientation of the interface. Clearly, on choosing $\vartheta = \rho = 0$, $\mathcal{K} = a = \alpha = \lambda = 1$ and $\partial\Omega = \partial_N\Omega$ then (7.9) in the isotropic case collapses to (7.1).

In order to state the weak form of (7.9), we introduce the function spaces

$$S_0 = \{\phi \in H^1(\Omega) : \phi = 0 \text{ on } \partial_D\Omega\} \text{ and } S_D = \{\phi \in H^1(\Omega) : \phi = u_D \text{ on } \partial_D\Omega\}, \quad (7.10)$$

where we assume for simplicity from now on that $u_D \in \mathbb{R}$, with $u_D = 0$ in the case $\partial_N\Omega = \partial\Omega$. Now a weak formulation of (7.9) for an anisotropic surface energy density of the form (6.9) can be obtained by generalizing the weak formulation of the Mullins–Sekerka problem, (7.2), as follows.

Given a closed hypersurface $\Gamma(0) \subset \Omega$ and, if $\vartheta > 0$, $u_0 \in L^2(\Omega)$, we seek an evolving hypersurface $(\Gamma(t))_{t \in [0, T]}$ that separates Ω into $\Omega_-(t)$ and $\Omega_+(t)$, with a global parameterization and induced velocity field $\vec{\mathcal{V}}$, and $\varkappa \in L^2(\mathcal{G}_T)$ as well as $u \in H^1(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega))$ with $\vartheta u(\cdot, 0) = \vartheta u_0$ as follows. For almost all $t \in (0, T)$, find $(u(\cdot, t), \vec{\mathcal{V}}(\cdot, t), \varkappa(\cdot, t)) \in S_D \times [L^2(\Gamma(t))]^d \times L^2(\Gamma(t))$ such that

$$\vartheta (\partial_t u, \phi) + (\mathcal{K} \nabla u, \nabla \phi) - (f, \phi) = \lambda \left\langle \vec{\mathcal{V}}, \phi \vec{\nu} \right\rangle_{\Gamma(t)} \quad \forall \phi \in S_0, \quad (7.11a)$$

$$\rho \left\langle \frac{\vec{\mathcal{V}}}{\beta(\vec{\nu})}, \chi \vec{\nu} \right\rangle_{\Gamma(t)} = \langle \alpha \varkappa_\gamma - a u, \chi \rangle_{\Gamma(t)} \quad \forall \chi \in L^2(\Gamma(t)), \quad (7.11b)$$

$$\langle \varkappa_\gamma \vec{\nu}, \vec{\eta} \rangle_{\Gamma(t)} + \left\langle \nabla_s^{\tilde{G}} \text{id}, \nabla_s^{\tilde{G}} \vec{\eta} \right\rangle_{\Gamma(t), \gamma} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d, \quad (7.11c)$$

where we have adopted the notation (6.13).

We can establish the following formal a priori bound for a sufficiently smooth solution of (7.11). Choosing $\phi = u - u_D$ in (7.11a), $\chi = \frac{\lambda}{a} \vec{\mathcal{V}} \cdot \vec{\nu}$ in (7.11b) and $\vec{\eta} = \frac{\alpha\lambda}{a} \vec{\mathcal{V}}$ in (7.11c) we obtain, on noting the transport theorem, Theorem 2.33, and Lemma 6.1 that

$$\begin{aligned} & \frac{d}{dt} \left(\frac{\vartheta}{2} |u - u_D|_\Omega^2 + \frac{\alpha\lambda}{a} |\Gamma(t)|_\gamma + \lambda u_D \mathcal{L}^d(\Omega_-(t)) \right) \\ & + (\mathcal{K} \nabla u, \nabla u) + \frac{\lambda\rho}{a} \langle \beta(\vec{\nu}), \mathcal{V}^2 \rangle_{\Gamma(t)} = (f, u - u_D). \end{aligned} \quad (7.12)$$

We now introduce the finite element approximations of S_0 and S_D . On recalling (7.4) and (7.10), we set

$$S_0^m = S^m \cap S_0 \quad \text{and} \quad S_D^m = S^m \cap S_D. \quad (7.13)$$

Then a finite element approximation of (7.11) from Barrett et al. (2010c), combining the ideas introduced for mean curvature flow in Section 4, for anisotropic flows in Section 6 and for the Mullins–Sekerka problem above, is given as follows. Let the closed polyhedral hypersurface Γ^0 be an approximation of $\Gamma(0)$, and, if $\vartheta > 0$, let $U^0 \in S_D^0$ be an approximation of u_0 , e.g. $U^0 = I^0 u_0$ if $u_0 \in C(\bar{\Omega})$. Then, for $m = 0, \dots, M-1$, find

$(U^{m+1}, \vec{X}^{m+1}, \kappa_\gamma^{m+1}) \in S_D^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that

$$\begin{aligned} \vartheta \left(\frac{U^{m+1} - U^m}{\Delta t_m}, \varphi \right)_m^h + (\mathcal{K} \nabla U^{m+1}, \nabla \varphi) - \lambda \left\langle \pi_{\Gamma^m} \left[\frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m} \cdot \vec{\omega}^m \right], \varphi \right\rangle_{\Gamma^m} \\ = (f^{m+1}, \varphi)_m^h \quad \forall \varphi \in S_0^m, \end{aligned} \quad (7.14a)$$

$$\begin{aligned} \rho \left\langle [\beta(\vec{\nu}^m)]^{-1} \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \chi \vec{\omega}^m \right\rangle_{\Gamma^m}^h - \alpha \langle \kappa_\gamma^{m+1}, \chi \rangle_{\Gamma^m}^h + a \langle U^{m+1}, \chi \rangle_{\Gamma^m} = 0 \\ \forall \chi \in V(\Gamma^m), \end{aligned} \quad (7.14b)$$

$$\langle \kappa_\gamma^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h + \langle \nabla_s^{\tilde{G}} \vec{X}^{m+1}, \nabla_s^{\tilde{G}} \vec{\eta} \rangle_{\Gamma^m, \gamma} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (7.14c)$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$. In the above, we have introduced $f^{m+1} = f(\cdot, t_{m+1})$, where we assume for convenience that $f(\cdot, t) \in C(\bar{\Omega})$ for all $t \in [0, T]$. Moreover, we have recalled (3.3) and observe that using $\vec{\omega}^m$ in (7.14b), and not $\vec{\nu}^m$, is necessary in order to be able to prove existence, uniqueness and stability results for (7.14), see the proof of Theorem 7.9 below.

Remark 7.8 (Implementation). *Compared to the computational challenges discussed in Remark 7.3 for (7.5), the only new difficulty in (7.14) is the term $(\mathcal{K} \nabla U^{m+1}, \nabla \varphi)$. In order to compute this in the case $\mathcal{K}_+ \neq \mathcal{K}_-$, it is necessary to calculate $\mathcal{L}^d(o \cap \Omega_-^m)$ for every $o \in \mathcal{T}^m$, where Ω_-^m denotes the interior of Γ^m . This can be done as described in Barrett et al. (2013a, Remark 4.2), but turns out to be computationally expensive due to the unfitted nature of the finite element approximation. Alternatively, suitable numerical approximations of the integral $(\mathcal{K} \nabla U^{m+1}, \nabla \varphi)$ can be introduced, similarly to what we present in §7.3 and Section 8, below. The case of phase-dependent forcings $f_\pm$ in (7.9a) can be dealt with similarly, on introducing a suitable analogue of $(f^{m+1}, \varphi)_m^h$ in (7.14a).*

On defining

$$\mathcal{E}^m(U, \vec{X}) = \frac{\vartheta}{2} |U - u_D|_{\Omega, m}^2 + \frac{\alpha \lambda}{a} |\vec{X}(\Gamma^m)|_\gamma$$

for $U \in C(\bar{\Omega})$ and $\vec{X} \in \underline{V}(\Gamma^m)$, we have the following results.

Theorem 7.9. *Let Γ^m and $\mathcal{T}^m$ satisfy Assumption 3.24(ii) and Assumption 7.4, and let $U^m \in C(\bar{\Omega})$. Let γ be of the form (6.9) with $r = 1$. Then there exists a unique solution $(U^{m+1}, \vec{X}^{m+1}, \kappa_\gamma^{m+1}) \in S_D^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to (7.14). Moreover, if $d = 2$ or $d = 3$ and if γ is of the form (6.9) with $r \in [1, \infty)$, then a solution to (7.14) satisfies*

$$\begin{aligned} \mathcal{E}^m(U^{m+1}, \vec{X}^{m+1}) + \lambda u_D \left\langle \vec{X}^{m+1} - \text{id}, \vec{\nu}^m \right\rangle_{\Gamma^m} + \frac{\vartheta}{2} |U^{m+1} - U^m|_{\Omega, m}^2 \\ + \Delta t_m (\mathcal{K} \nabla U^{m+1}, \nabla U^{m+1}) + \Delta t_m \frac{\lambda \rho}{a} \left(\left| [\beta(\vec{\nu}^m)]^{-\frac{1}{2}} \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m} \cdot \vec{\omega}^m \right|_{\Gamma^m}^h \right)^2 \\ \leq \mathcal{E}^m(U^m, \text{id}) + \Delta t_m (f^{m+1}, U^{m+1} - u_D)_m^h. \end{aligned} \quad (7.15)$$

Proof. The existence and uniqueness proof for $r = 1$ proceeds analogously to the proof of Theorem 7.5. In particular, if $(U, \vec{X}, \kappa_\gamma) \in S_0^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ denotes a solution to the homogeneous analogue of (7.14), similarly to (7.6), then choosing $\varphi = U$, $\chi = \frac{\lambda}{a} \pi_{\Gamma^m} [\vec{X} \cdot \vec{\omega}^m]$ and $\vec{\eta} = \frac{\alpha\lambda}{a} \vec{X}$ yields

$$\begin{aligned} & \vartheta |U|_{\Omega, m}^2 + \Delta t_m (\mathcal{K} \nabla U, \nabla U) + \frac{\lambda \rho}{\Delta t_m a} \left(\left| [\beta(\vec{\nu}^m)]^{-\frac{1}{2}} \vec{X} \cdot \vec{\omega}^m \right|_{\Gamma^m}^h \right)^2 \\ & + \frac{\alpha \lambda}{a} \left\langle \nabla_s^{\tilde{G}} \vec{X}, \nabla_s^{\tilde{G}} \vec{X} \right\rangle_{\Gamma^m, \gamma} = 0, \end{aligned}$$

which implies that U is constant in Ω , with $U = 0$ if $\vartheta > 0$ or $S_0^m \neq S^m$, and that $\vec{X}$ is constant on Γ^m , since all the involved physical parameters are nonnegative, with $\mathcal{K}$, α , a and λ being positive. As in the proof of Theorem 7.5 we can then infer from Assumption 7.4 that $\vec{X} = \vec{0}$. This implies that $\kappa_\gamma = \frac{a}{\alpha} U$ is constant on Γ^m and so we can proceed as in the proof of Theorem 7.5 to show that $\kappa_\gamma = U = 0$. Overall this proves existence of a unique solution $(U^{m+1}, \vec{X}^{m+1}, \kappa_\gamma^{m+1}) \in S_D^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to (7.14).

It remains to establish (7.15). Choosing $\varphi = U^{m+1} - u_D$ in (7.14a), $\chi = \frac{\lambda}{a} \pi_{\Gamma^m} [(\vec{X}^{m+1} - \vec{\text{id}}_{|\Gamma^m}) \cdot \vec{\omega}^m]$ in (7.14b) and $\vec{\eta} = \frac{\alpha\lambda}{a} (\vec{X}^{m+1} - \vec{\text{id}}_{|\Gamma^m})$ in (7.14c) yields that

$$\begin{aligned} & \vartheta (U^{m+1} - U^m, U^{m+1} - u_D)_m^h + \Delta t_m (\mathcal{K} \nabla U^{m+1}, \nabla U^{m+1}) \\ & + \frac{\alpha \lambda}{a} \left\langle \nabla_s^{\tilde{G}} \vec{X}^{m+1}, \nabla_s^{\tilde{G}} (\vec{X}^{m+1} - \vec{\text{id}}) \right\rangle_{\Gamma^m, \gamma} \\ & + \Delta t_m \frac{\lambda \rho}{a} \left(\left| [\beta(\vec{\nu}^m)]^{-\frac{1}{2}} \frac{\vec{X}^{m+1} - \vec{\text{id}}}{\Delta t_m} \cdot \vec{\omega}^m \right|_{\Gamma^m}^h \right)^2 \\ & = -\lambda u_D \left\langle \vec{X}^{m+1} - \vec{\text{id}}, \vec{\omega}^m \right\rangle_{\Gamma^m}^h + \Delta t_m (f^{m+1}, U^{m+1} - u_D)_m^h \end{aligned}$$

and hence (7.15) follows immediately from Lemma 6.6 and (3.6). $\square$

Remark 7.10 (Semidiscrete scheme). *We note that (7.15) closely mimics the corresponding continuous energy law (7.12). The reason why it is not an exact discrete analogue of (7.12) has been discussed in Remark 7.6 already. However, on recalling Remark 5.4(ii) it is possible to prove an exact discrete analogue of (7.12) for a semidiscrete version of the scheme (7.14), see also Barrett et al. (2010c, Remark 3.5). In addition, this semidiscrete scheme will feature the tangential motion discussed in Remark 6.8.*

Remark 7.11 (Discrete systems). *It is a simple matter to combine the techniques in Remark 7.7 and §6.4 in order to derive the discrete systems that need to be solved at each time level for (7.14). If γ is of the form (6.9) with $r = 1$, then the systems are linear and can hence it can be solved analogously to Remark 7.7, i.e. either with a sparse direct solver or with the help of a Schur complement approach and a preconditioned conjugate gradient solver. If $r > 1$, on the other hand, then the systems are nonlinear and can be solved with a lagged fixed-point type iteration. We refer to Barrett et al. (2010c, §4) for further details.*

7.3 One-sided free boundary problems

In this section we consider the situation where diffusion is restricted to one phase. We hence study one-sided versions of the Mullins–Sekerka or Stefan problems. This is, for example, relevant for snow crystal growth, where diffusion can be restricted to the gas phase. In this case we only find the unknown u in one-phase, which occupies at time t a domain $\Omega_+(t)$. Once again, for simplicity of the presentation, we always assume that the region $\Omega_-(t) = \Omega \setminus \overline{\Omega_+(t)}$ is compactly contained in Ω . The problem now reads as follows. Given $\Gamma(0)$ and, if $\vartheta > 0$, $u_0 : \Omega_+(0) \rightarrow \mathbb{R}$, find the evolving interface $(\Gamma(t))_{t \in [0, T]}$ and $u(\cdot, t) : \Omega_+(t) \rightarrow \mathbb{R}$, $t \in [0, T]$, such that $\vartheta u(\cdot, 0) = \vartheta u_0(\cdot)$ and for all $t \in (0, T]$ the following conditions hold

$$\vartheta \partial_t u - \mathcal{K}_+ \Delta u = f \quad \text{in } \Omega_+(t), \quad u = u_D \quad \text{on } \partial\Omega, \quad (7.16a)$$

$$\frac{\rho \mathcal{V}}{\beta(\vec{\nu})} = \alpha \kappa_\gamma - a u \quad \text{and} \quad \mathcal{K}_+ \partial_{\vec{\nu}} u = -\lambda \mathcal{V} \quad \text{on } \Gamma(t), \quad (7.16b)$$

where the given data satisfies the same conditions as in (7.9). For snow crystal growth $-u$ is a suitably scaled concentration with $-u_D$ being the scaled supersaturation, see Libbrecht (2005); Barrett et al. (2012a, 2013a).

As we wish to model snow crystal growth, we now state a relevant hexagonal surface energy. Let $d = 3$ and $l_\varepsilon(\vec{p}) = [\varepsilon^2 |\vec{p}|^2 + p_1^2 (1 - \varepsilon^2)]^{\frac{1}{2}}$ for $\varepsilon > 0$. We then introduce the rotation matrices

$$\underline{R}_1(\theta) = \begin{pmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \underline{R}_2(\theta) = \begin{pmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{pmatrix}.$$

Then setting

$$\gamma(\vec{p}) = l_\varepsilon(\underline{R}_2(\frac{\pi}{2})\vec{p}) + \frac{1}{\sqrt{3}} \sum_{\ell=1}^3 l_\varepsilon(\underline{R}_1(\theta_0 + \frac{\ell\pi}{3})\vec{p}),$$

where $\theta_0 \in [0, \frac{\pi}{3})$ rotates the anisotropy in the $x_1 - x_2$ plane, defines a density of the form (6.9), with $r = 1$ and $L = 4$, that approximates a crystalline surface energy density with a regular hexagonal prism as its Wulff shape, where each face of the Wulff shape has the same distance to the origin.

We recall from Barrett et al. (2013a) an unfitted finite element approximation of the above one-sided problem, following ideas of Barrett and Elliott (1982). Given an approximation of the interface Γ^m , we let Ω_+^m denote the exterior of Γ^m and let Ω_-^m denote the interior of Γ^m , so that $\Gamma^m = \partial\Omega_-^m = \overline{\Omega_-^m} \cap \overline{\Omega_+^m}$. We now introduce the appropriate discrete trial and test function spaces. To this end, let $\Omega_+^{m,h}$ be an approximation to Ω_+^m and set $\Omega_-^{m,h} = \Omega \setminus \overline{\Omega_+^{m,h}}$. We stress that $\Omega_+^{m,h}$ need not necessarily be a union of elements from $\mathcal{T}^m$. Then we define, on recalling (7.4) and (7.13), the finite element spaces

$$\begin{aligned} S_+^m &= \left\{ \chi \in S^m : \chi(\vec{p}_k^n) = 0 \text{ if } \text{supp } \phi_k^{S^m} \subset \overline{\Omega_-^{m,h}}, k = 1, \dots, K_{S^m} \right\}, \\ S_{0,+}^m &= S_0^m \cap S_+^m, \quad S_{D,+}^m = S_D^m \cap S_+^m. \end{aligned} \quad (7.17)$$

Our finite element approximation of (7.16) is then given as follows. Let the closed polyhedral hypersurface Γ^0 be an approximation of $\Gamma(0)$, and, if $\vartheta > 0$, let $U^0 \in S_D^0$ be an approximation of u_0 , e.g. $U^0 = I^0 u_0$ if $u_0 \in C(\bar{\Omega})$ is an extension of the given $u_0 \in C(\bar{\Omega}_+(0))$. Then, for $m = 0, \dots, M-1$, find $(U^{m+1}, \vec{X}^{m+1}, \kappa_\gamma^{m+1}) \in S_{D,+}^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that

$$\begin{aligned} & \vartheta \left(\frac{U^{m+1} - U^m}{\Delta t_m}, \varphi \right)_{m,+}^h + \mathcal{K}_+ (\nabla U^{m+1}, \nabla \varphi)_{m,+} \\ & - \lambda \left\langle \pi_{\Gamma^m} \left[\frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m} \cdot \vec{\omega}^m \right], \varphi \right\rangle_{\Gamma^m} = (f^{m+1}, \varphi)_{m,+}^h \quad \forall \varphi \in S_{0,+}^m, \end{aligned} \quad (7.18a)$$

$$\begin{aligned} & \rho \left\langle [\beta(\vec{\nu}^m)]^{-1} \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \chi \vec{\omega}^m \right\rangle_{\Gamma^m}^h - \alpha \langle \kappa_\gamma^{m+1}, \chi \rangle_{\Gamma^m}^h + a \langle U^{m+1}, \chi \rangle_{\Gamma^m} = 0 \\ & \quad \forall \chi \in V(\Gamma^m), \end{aligned} \quad (7.18b)$$

$$\langle \kappa_\gamma^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h + \langle \nabla_s^{\tilde{G}} \vec{X}^{m+1}, \nabla_s^{\tilde{G}} \vec{\eta} \rangle_{\Gamma^m, \gamma} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (7.18c)$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$. Here we define for all $\chi, \varphi \in S^m$

$$\begin{aligned} (\nabla \chi, \nabla \varphi)_{m,+} &= \int_{\Omega_+^{m,h}} \nabla \chi \cdot \nabla \varphi \, d\mathcal{L}^d \\ &= \sum_{o \in \mathcal{T}^m} \frac{\mathcal{L}^d(o \cap \Omega_+^{m,h})}{\mathcal{L}^d(o)} \int_o \nabla \chi \cdot \nabla \varphi \, d\mathcal{L}^d \end{aligned} \quad (7.19)$$

and, in a similar fashion,

$$(\chi, \varphi)_{m,+}^h = \sum_{o \in \mathcal{T}^m} \frac{\mathcal{L}^d(o \cap \Omega_+^{m,h})}{\mathcal{L}^d(o)} \int_o I^m[\chi \varphi] \, d\mathcal{L}^d.$$

It follows immediately from (7.17) and (7.19) that

$$(\nabla \varphi, \nabla \varphi)_{m,+} > 0 \quad \forall \varphi \in S_{0,+}^m \setminus \{0\}.$$

Remark 7.12.

- (i) We note that for $\vartheta > 0$ the approximation (7.18) is only meaningful when the discrete solid region does not shrink, see Barrett et al. (2013a, Remark 3.1). In practice this technical constraint is not very restrictive, since in most physically relevant applications the solid region grows.
- (ii) Existence and uniqueness for $r = 1$, as well as stability for $r \in [1, \infty)$, can be shown for (7.18) under appropriate assumptions, see Barrett et al. (2013a, Theorems 3.1 and 3.2) for the proofs for the case $r = 1$. We note that the stability proof in Barrett et al. (2013a, Theorem 3.2), for $d = 2$ and $d = 3$, immediately carries over to the case $r > 1$, on recalling Lemma 6.6.

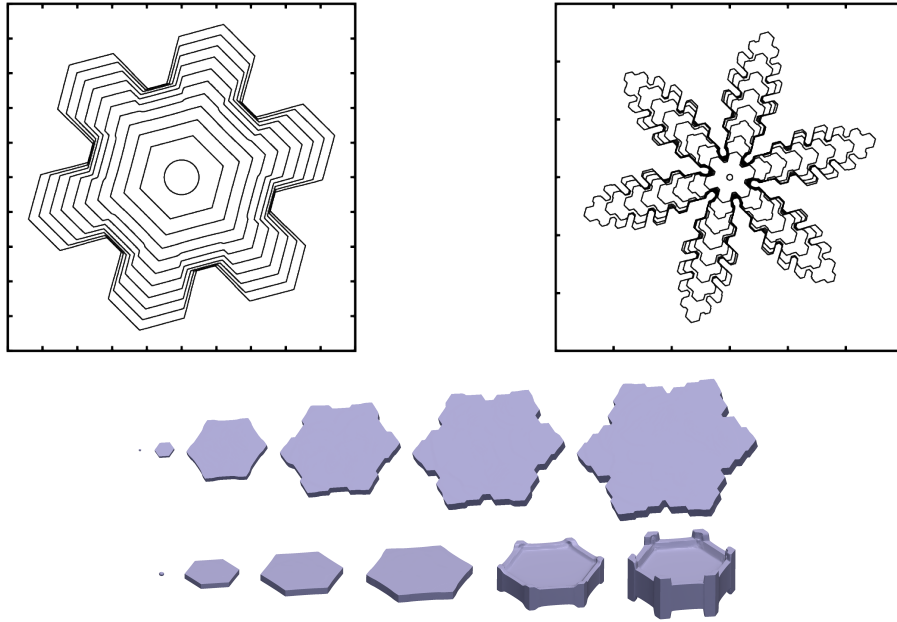


Figure 5: Visualizations of the numerical experiments from Barrett et al. (2013a, Fig. 12), above, Barrett et al. (2013a, Fig. 22), middle, and Barrett et al. (2013a, Fig. 27 (left)), below. The 2D solutions are shown at times $t = 0, 0.5, \dots, 5$ (left) and $t = 0, 5, \dots, 40$ (right). The snapshots for the 3D simulations are taken at times $t = 0, 5, 50, 100, 150, 200$ (middle) and $t = 0, 10, \dots, 50$ (below).

- (iii) *The main new computational challenge in implementing the scheme (7.18), compared to (7.14) with $\mathcal{K}_+ = \mathcal{K}_-$, is the determination of $S_{0,+}^m$ and the calculation of the terms involving $(\cdot, \cdot)_{m,+}$ and $(\cdot, \cdot)_{m,+}^h$ at each time step. Clearly, the involved difficulty crucially depends on the choice of $\Omega_+^{m,h}$ as an approximation to Ω_+^m . A thorough discussion of possible choices can be found in Barrett et al. (2013a, §4.1).*

We present two numerical snow crystal growth simulations based on the scheme (7.18) with a hexagonal surface energy density γ , and with a time-dependent mobility β , in Figure 5.

7.4 Alternative numerical approaches

Other authors who numerically studied crystal growth with the help of a front tracking type method are Roosen and Taylor (1991); Yokoyama (1993); Almgren (1993); Schmidt (1993, 1996, 1998); Juric and Tryggvason (1996); Bänsch and Schmidt (2000). A level set method for crystal growth was studied in Sethian and Strain (1992). In the context of phase field approximations, we refer to Kobayashi (1993); Wheeler et al. (1993); Karma and Rappel (1998); Debierre et al. (2003); Nestler (2005), as well as to the works by the present authors Barrett et al. (2013b, 2014a,b). Solidification phenomena can also be described with the help of cellular automata and we refer to Reiter (2005); Libbrecht

(2008); Gravner and Griffeath (2009) for details.

8 Two-phase flow

We now study free boundary problems appearing in fluid flow. Here we consider two immiscible fluids that are separated by an interface, which moves in time with a velocity given by that of the fluid. We start with the simplest situation in which the evolution in the two phases is given by Stokes flow. For the discretization of the evolving hypersurface we consider the parametric finite element approximation introduced above. The good mesh properties are particularly helpful in two-phase flow as the mesh, which is moved by the fluid velocity, can change quite drastically. Many other approaches, using a surface mesh, have problems in such situations due the mesh deteriorating. This is not the case, in most situations, for the approach stated below. Moreover, on using a simple XFEM pressure space enrichment, we obtain exact volume conservation for the two phase regions. Furthermore, our fully discrete finite element approximation can be shown to be unconditionally stable. A common feature in two-phase flow is that nonphysical velocities appear in numerical approximations. If surface tension effects are taken into account, a jump discontinuity in the pressure results, and this poses serious challenges for the numerical method. This can lead to nonphysical velocities. These so-called spurious velocities are typically avoided by the XFEM approach discussed in this section.

8.1 Two-phase Stokes flow

In this section we consider the flow of viscous, incompressible, immiscible two fluid systems in a low Reynolds regime, i.e. we can neglect inertia terms. The governing equations for the velocity $\vec{u}$ and the pressure p are given by the momentum equation and conservation of mass, i.e.

$$-\mu_{\pm} \Delta \vec{u} + \nabla p = \vec{f}, \quad \nabla \cdot \vec{u} = 0 \quad \text{in } \Omega_{\pm}(t), \quad (8.1)$$

where $\vec{f}$ is a possible forcing, and $\Omega_+(t)$ and $\Omega_-(t)$ are the time dependent regions occupied by the two fluid phases as in Figure 1 in §2.4, where $\Omega \subset \mathbb{R}^d$ is again a fixed domain, with $d \geq 2$. As usual, we let $\vec{\nu}$ denote the outer unit normal to $\Omega_-(t)$ on $\Gamma(t) = \partial\Omega_-(t)$. We consider the case in which the viscosity of the two fluids can be different and introduce $\mu(\cdot, t) = \mu_+ \chi_{\Omega_+(t)} + \mu_- \chi_{\Omega_-(t)}$, with $\mu_{\pm} \in \mathbb{R}_{>0}$ denoting the fluid viscosities, recall (2.11). We now define the conditions that have to hold on the interface. Therefore, we introduce the stress tensor

$$\underline{\sigma} = \mu (\nabla \vec{u} + (\nabla \vec{u})^T) - p \underline{\text{Id}} = 2\mu \underline{D}(\vec{u}) - p \underline{\text{Id}}, \quad (8.2)$$

where $\underline{D}(\vec{u}) = \frac{1}{2} (\nabla \vec{u} + (\nabla \vec{u})^T)$ is the rate of deformation tensor. Using the fact that the velocity is divergence free, we can rewrite (8.1) as

$$-\nabla \cdot \underline{\sigma} = \vec{f}, \quad \nabla \cdot \vec{u} = 0 \quad \text{in } \Omega_{\pm}(t).$$

On the moving interface, we require

$$[\vec{u}]_{-}^{+} = \vec{0}, \quad [\underline{\sigma} \vec{\nu}]_{-}^{+} = -\gamma_0 \kappa \vec{\nu}, \quad \mathcal{V} = \vec{u} \cdot \vec{\nu} \quad \text{on } \Gamma(t),$$

where $\gamma_0 \in \mathbb{R}_{>0}$ represents surface tension. To close the system we prescribe initial data $\Gamma(0)$ and the boundary condition $\vec{u} = \vec{0}$ on $\partial\Omega$. Overall, we can rewrite the total system as follows. Given $\Gamma(0)$, find $\vec{u} : \Omega \times [0, T] \rightarrow \mathbb{R}^d$, $p : \Omega \times [0, T] \rightarrow \mathbb{R}$ and the evolving interface $(\Gamma(t))_{t \in [0, T]}$ such that for all $t \in (0, T]$ the following conditions hold

$$-2\mu \nabla \cdot \underline{D}(\vec{u}) + \nabla p = \vec{f}, \quad \nabla \cdot \vec{u} = 0 \quad \text{in } \Omega_{\pm}(t), \quad \vec{u} = \vec{0} \quad \text{on } \partial\Omega, \quad (8.3a)$$

$$[\vec{u}]_{-}^{+} = \vec{0}, \quad [(2\mu \underline{D}(\vec{u}) - p \underline{\text{Id}}) \vec{\nu}]_{-}^{+} = -\gamma_0 \kappa \vec{\nu}, \quad \mathcal{V} = \vec{u} \cdot \vec{\nu} \quad \text{on } \Gamma(t). \quad (8.3b)$$

A finite element approximation of (8.3) needs a suitable weak formulation. Here a choice has to be made regarding the tangential velocity $\vec{\mathcal{V}}_T$, recall Definition 2.25(iii), which will have important repercussions on the discrete level. Given our results derived in the previous sections, see e.g. Section 4, it is natural to not fix $\vec{\mathcal{V}}_T$ explicitly and to use the formulations

$$\vec{\mathcal{V}} \cdot \vec{\nu} = \vec{u} \cdot \vec{\nu} \quad \text{and} \quad \kappa \vec{\nu} = \Delta_s \vec{\text{id}} \quad \text{on } \Gamma(t), \quad (8.4)$$

compare with (4.3). An alternative approach would let $\vec{\mathcal{V}}_T$ be given by the fluid flow, and so use the formulations

$$\vec{\mathcal{V}} = \vec{u} \quad \text{and} \quad \kappa \vec{\nu} = \Delta_s \vec{\text{id}} \quad \text{on } \Gamma(t),$$

compare with (4.32). We will consider this alternative approach in §8.1.4. However, our main focus is on the formulation (8.4), which will lead to good mesh properties for the discrete schemes.

We begin with the following simple generalization of Remark 2.36

$$\begin{aligned} & - \int_{\Omega_{-}(t) \cup \Omega_{+}(t)} (\nabla \cdot \underline{\mathcal{G}}) \cdot \vec{\xi} \, d\mathcal{L}^d \\ & = 2 \left(\mu \underline{D}(\vec{u}), \underline{D}(\vec{\xi}) \right) - \left(p, \nabla \cdot \vec{\xi} \right) + \left\langle [\underline{\mathcal{G}} \vec{\nu}]_{-}^{+}, \vec{\xi} \right\rangle_{\Gamma(t)} \quad \forall \vec{\xi} \in [H_0^1(\Omega)]^d, \end{aligned} \quad (8.5)$$

where we have noted for symmetric matrices $\underline{A} \in \mathbb{R}^{d \times d}$ that $\underline{A} : \underline{B} = \underline{A} : \frac{1}{2}(\underline{B} + \underline{B}^T)$ for all $\underline{B} \in \mathbb{R}^{d \times d}$. Now (8.5) leads to the following weak formulation of (8.3), using the formulations (8.4). Given a closed hypersurface $\Gamma(0) \subset \Omega$, we seek an evolving hypersurface $(\Gamma(t))_{t \in [0, T]}$ that separates Ω into $\Omega_{-}(t)$ and $\Omega_{+}(t)$, with a global parameterization and induced velocity field $\vec{\mathcal{V}}$, and $\kappa \in L^2(\mathcal{G}_T)$ as well as $\vec{u} : \Omega \times [0, T] \rightarrow \mathbb{R}^d$ and $p : \Omega \times [0, T] \rightarrow \mathbb{R}$ as follows. For almost all $t \in (0, T)$, find $(\vec{u}(\cdot, t), p(\cdot, t), \vec{\mathcal{V}}(\cdot, t), \kappa(\cdot, t)) \in [H_0^1(\Omega)]^d \times L^2(\Omega) \times [L^2(\Gamma(t))]^d \times L^2(\Gamma(t))$ such that

$$2 \left(\mu \underline{D}(\vec{u}), \underline{D}(\vec{\xi}) \right) - \left(p, \nabla \cdot \vec{\xi} \right) = \left(\vec{f}, \vec{\xi} \right) + \gamma_0 \left\langle \kappa \vec{\nu}, \vec{\xi} \right\rangle_{\Gamma(t)} \quad \forall \vec{\xi} \in [H_0^1(\Omega)]^d, \quad (8.6a)$$

$$(\nabla \cdot \vec{u}, \varphi) = 0 \quad \forall \varphi \in L^2(\Omega), \quad (8.6b)$$

$$\left\langle \vec{\mathcal{V}} \cdot \vec{\nu}, \chi \right\rangle_{\Gamma(t)} = \left\langle \vec{u} \cdot \vec{\nu}, \chi \right\rangle_{\Gamma(t)} \quad \forall \chi \in L^2(\Gamma(t)), \quad (8.6c)$$

$$\left\langle \kappa \vec{\nu}, \vec{\eta} \right\rangle_{\Gamma(t)} + \left\langle \nabla_s \vec{\text{id}}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d. \quad (8.6d)$$

Remark 8.1. *For a sufficiently smooth weak solution of (8.6), we can formally prove the following results.*

- (i) *The two-phase Stokes flow, in the absence of external forcings, decreases the surface area of the interface. This follows from the transport theorem, Theorem 2.32, (8.6c) with $\chi = \kappa$, (8.6a) with $\xi = \vec{u}$ and (8.6b) with $\varphi = p$, as one then obtains the energy identity*

$$\begin{aligned} \gamma_0 \frac{d}{dt} |\Gamma(t)| &= -\gamma_0 \left\langle \kappa \vec{v}, \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} = -\gamma_0 \left\langle \kappa \vec{v}, \vec{u} \right\rangle_{\Gamma(t)} \\ &= -2 (\mu \underline{D}(\vec{u}), \underline{D}(\vec{u})) + \left(\vec{f}, \vec{u} \right). \end{aligned} \quad (8.7)$$

- (ii) *The two-phase Stokes flow preserves $\mathcal{L}^d(\Omega_{\pm}(t))$, as the transport theorem, Theorem 2.33, (8.6c) with $\chi = 1$, the divergence theorem and (8.6b) with $\varphi = \mathcal{X}_{\Omega_{-}(t)}$ yield that*

$$\frac{d}{dt} \mathcal{L}^d(\Omega_{-}(t)) = \left\langle \vec{\mathcal{V}}, \vec{v} \right\rangle_{\Gamma(t)} = \langle \vec{u}, \vec{v} \rangle_{\Gamma(t)} = (\nabla \cdot \vec{u}, \mathcal{X}_{\Omega_{-}(t)}) = 0. \quad (8.8)$$

Remark 8.2. *In the case $\vec{f} = \vec{0}$ the evolution (8.6) decreases the surface area of the interface $\Gamma(t)$, recall (8.7), and can be written in the general form (5.9) satisfying (5.10). This can be seen as follows. For a given interface $\Gamma(t)$, with normal $\vec{v}(t)$ and curvature $\kappa(t)$, we solve (8.6a), (8.6b) for $(\vec{u}(\cdot, t), p(\cdot, t)) \in [H_0^1(\Omega)]^d \times L^2(\Omega)$ and set*

$$\mathfrak{F}(\kappa) = \vec{u} \cdot \vec{v}.$$

We then compute, similarly to (8.7),

$$\langle \mathfrak{F}(\kappa), \kappa \rangle_{\Gamma(t)} = \langle \vec{u} \cdot \vec{v}, \kappa \rangle_{\Gamma(t)} = \frac{2}{\gamma_0} (\mu \underline{D}(\vec{u}), \underline{D}(\vec{u})) \geq 0. \quad (8.9)$$

8.1.1 Finite element approximation

In order to approximate the velocity and pressure on $\mathcal{T}^m$, recall the assumptions and notation above (7.4), we introduce finite element spaces $\mathbb{U}^m \subset [H_0^1(\Omega)]^d$ and $\mathbb{P}^m \subset L^2(\Omega)$. We require also the space $\widehat{\mathbb{P}}^m = \mathbb{P}^m \cap \widehat{\mathbb{P}}$, where $\widehat{\mathbb{P}} = \{\varphi \in L^2(\Omega) : (\varphi, 1) = 0\}$. The velocity/pressure finite element spaces $(\mathbb{U}^m, \mathbb{P}^m)$ satisfy the LBB inf-sup condition if there exists a $C \in \mathbb{R}_{>0}$ independent of $h^m = \max_{o \in \mathcal{T}^m} \{\text{diam}(o)\}$, such that

$$\inf_{\varphi \in \widehat{\mathbb{P}}^m} \sup_{\vec{\xi} \in \mathbb{U}^m} \frac{(\varphi, \nabla \cdot \vec{\xi})}{|\varphi|_{\Omega} \|\vec{\xi}\|_{1,\Omega}} \geq C > 0, \quad (8.10)$$

where $\|\cdot\|_{1,\Omega}^2 = |\cdot|_{\Omega}^2 + |\nabla \cdot \cdot|_{\Omega}^2$ defines the H^1 -norm on Ω , see e.g. Girault and Raviart (1986, p. 114).

Next we introduce a generalization of (7.4) to

$$\mathcal{S}_k^m = \{\chi \in C(\bar{\Omega}) : \chi|_o \in \mathcal{P}_k(o) \quad \forall o \in \mathcal{T}^m\} \subset H^1(\Omega), \quad (8.11)$$

where, for $k \in \mathbb{N}$, $\mathcal{P}_k(o)$ denotes the space of polynomials of degree k on o . In addition, we denote by $\mathcal{S}_0^m$ the space of piecewise constant functions on $\mathcal{T}^m$. Then, for example, we may choose the lowest order Taylor–Hood element P2-P1, the P2-P0 element, or the P2-(P1+P0) element on setting $\mathbb{U}^m = [\mathcal{S}_2^m]^d \cap \mathbb{U}$, and $\mathbb{P}^m = \mathcal{S}_1^m, \mathcal{S}_0^m$ or $\mathcal{S}_1^m + \mathcal{S}_0^m$, respectively. It is well-known that the P2-P1 element satisfies the LBB condition (8.10) for $d = 2$ and $d = 3$, where the latter requires the weak constraint that all simplices have a vertex in Ω , see Boffi (1997). While the other two choices, P2-P0 and P2-(P1+P0), satisfy it for $d = 2$.

Moreover, as in earlier sections, we approximate the interface at time t_m by a polyhedral surface Γ^m with the same notation. Similarly to §7.3, let Ω_+^m denote the exterior of Γ^m and Ω_-^m the interior of Γ^m , so that $\Gamma^m = \partial\Omega_-^m = \bar{\Omega}_-^m \cap \bar{\Omega}_+^m$. For simplicity we assume that the unit normal $\vec{\nu}^m$ on Γ^m points into Ω_+^m . Due to the phase-dependent viscosity, $\mu_{\pm}$, we now subdivide the elements of the bulk mesh $\mathcal{T}^m$ into exterior, interior and interfacial elements as follows. Let

$$\mathcal{T}_{\pm}^m = \{o \in \mathcal{T}^m : o \subset \Omega_{\pm}^m\}, \quad \mathcal{T}_{\Gamma^m}^m = \{o \in \mathcal{T}^m : o \cap \Gamma^m \neq \emptyset\}. \quad (8.12)$$

The disjoint partition $\mathcal{T}^m = \mathcal{T}_-^m \cup \mathcal{T}_+^m \cup \mathcal{T}_{\Gamma^m}^m$ can easily be found e.g. with the Algorithm 4.1 in Barrett et al. (2013a).

Similarly to §7.3, we use an unfitted finite element approximation of (8.6). We define the discrete viscosity $\mu^m \in \mathcal{S}_0^m$, for $m \geq 0$, as

$$\mu_{|o}^m = \begin{cases} \mu_- & o \in \mathcal{T}_-^m, \\ \mu_+ & o \in \mathcal{T}_+^m, \\ \frac{1}{2}(\mu_- + \mu_+) & o \in \mathcal{T}_{\Gamma^m}^m. \end{cases} \quad (8.13)$$

Then the unfitted finite element approximation of (8.6) from Barrett et al. (2013c) is given as follows. Let the closed polyhedral hypersurface Γ^0 be an approximation of $\Gamma(0)$ and recall the time interval partitioning (4.5). Then, for $m = 0, \dots, M-1$, find $(\vec{U}^{m+1}, P^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) \in \mathbb{U}^m \times \hat{\mathbb{P}}^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that

$$2 \left(\mu^m \underline{D}(\vec{U}^{m+1}), \underline{D}(\vec{\xi}) \right) - \left(P^{m+1}, \nabla \cdot \vec{\xi} \right) = \left(\vec{f}^{m+1}, \vec{\xi} \right) + \gamma_0 \left\langle \kappa^{m+1} \vec{\nu}^m, \vec{\xi} \right\rangle_{\Gamma^m} \quad \forall \vec{\xi} \in \mathbb{U}^m, \quad (8.14a)$$

$$\left(\nabla \cdot \vec{U}^{m+1}, \varphi \right) = 0 \quad \forall \varphi \in \hat{\mathbb{P}}^m, \quad (8.14b)$$

$$\left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m} \cdot \vec{\nu}^m, \chi \right\rangle_{\Gamma^m}^h = \left\langle \vec{U}^{m+1} \cdot \vec{\nu}^m, \chi \right\rangle_{\Gamma^m} \quad \forall \chi \in V(\Gamma^m), \quad (8.14c)$$

$$\left\langle \kappa^{m+1} \vec{\nu}^m, \vec{\eta} \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (8.14d)$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$. Here, with the help of the interpolation operator $\vec{I}_2^m : [C(\bar{\Omega})]^d \rightarrow [\mathcal{S}_2^m]^d$, the natural generalization of $I^m : C(\bar{\Omega}) \rightarrow S^m$, we define $\vec{f}^{m+1} = \vec{I}_2^m \vec{f}(\cdot, t_{m+1})$.

We note that the scheme (8.14) is linear in the unknowns $(\vec{U}^{m+1}, P^{m+1}, \vec{X}^{m+1}, \kappa^{m+1})$. For the mathematical analysis of (8.14) it is convenient to introduce a reduced version. Given $\mathbb{U}^m$ and $\mathbb{P}^m$, we define

$$\mathbb{U}_0^m = \{\vec{U} \in \mathbb{U}^m : (\nabla \cdot \vec{U}, \varphi) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}}^m\}. \quad (8.15)$$

Then the discrete pressure can be eliminated from (8.14) to yield the following reduced variant. For $m = 0, \dots, M-1$, find $(\vec{U}^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) \in \mathbb{U}_0^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that

$$2 \left(\mu^m \underline{D}(\vec{U}^{m+1}), \underline{D}(\vec{\xi}) \right) = \left(\vec{f}^{m+1}, \vec{\xi} \right) + \gamma_0 \left\langle \kappa^{m+1} \vec{\nu}^m, \vec{\xi} \right\rangle_{\Gamma^m} \quad \forall \vec{\xi} \in \mathbb{U}_0^m, \quad (8.16a)$$

$$\left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m} \cdot \vec{\nu}^m, \chi \right\rangle_{\Gamma^m}^h = \left\langle \vec{U}^{m+1} \cdot \vec{\nu}^m, \chi \right\rangle_{\Gamma^m} \quad \forall \chi \in V(\Gamma^m), \quad (8.16b)$$

$$\left\langle \kappa^{m+1} \vec{\nu}^m, \vec{\eta} \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (8.16c)$$

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

We now show existence, uniqueness and stability results for the two schemes (8.16) and (8.14).

Theorem 8.3.

- (i) Let Γ^m satisfy Assumption 3.24. Then there exists a unique solution $(\vec{U}^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) \in \mathbb{U}_0^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to (8.16).
- (ii) If $(\vec{U}^{m+1}, P^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) \in \mathbb{U}^m \times \widehat{\mathbb{P}}^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ solves (8.14), then $(\vec{U}^{m+1}, \vec{X}^{m+1}, \kappa^{m+1})$ is a solution to (8.16).
- (iii) Let $(\mathbb{U}^m, \widehat{\mathbb{P}}^m)$ satisfy the LBB condition (8.10) and let Γ^m satisfy Assumption 3.24. Then there exists a unique solution $(\vec{U}^{m+1}, P^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) \in \mathbb{U}^m \times \widehat{\mathbb{P}}^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to (8.14).

Proof. (i) Existence follows from uniqueness and hence we consider the homogeneous linear system. Find $(\vec{U}, \vec{X}, \kappa) \in \mathbb{U}_0^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that

$$2 \left(\mu^m \underline{D}(\vec{U}), \underline{D}(\vec{\xi}) \right) = \gamma_0 \left\langle \kappa \vec{\nu}^m, \vec{\xi} \right\rangle_{\Gamma^m} \quad \forall \vec{\xi} \in \mathbb{U}_0^m, \quad (8.17a)$$

$$\left\langle \vec{X} \cdot \vec{\nu}^m, \chi \right\rangle_{\Gamma^m}^h = \Delta t_m \left\langle \vec{U} \cdot \vec{\nu}^m, \chi \right\rangle_{\Gamma^m} \quad \forall \chi \in V(\Gamma^m), \quad (8.17b)$$

$$\left\langle \kappa \vec{\nu}^m, \vec{\eta} \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m). \quad (8.17c)$$

We now need to show that the zero solution is the only possible solution. Choosing $\vec{\xi} = \Delta t_m \vec{U}$ in (8.17a), $\chi = \gamma_0 \kappa$ in (8.17b) and $\vec{\eta} = \gamma_0 \vec{X}$ in (8.17c), we obtain

$$2 \Delta t_m \left(\mu^m \underline{D}(\vec{U}), \underline{D}(\vec{U}) \right) + \gamma_0 \left| \nabla_s \vec{X} \right|_{\Gamma^m}^2 = 0.$$

Now Korn's inequality, see e.g. Zeidler (1988, §62.15), yields $\vec{U} = \vec{0}$. Hence it follows from (8.17b), (8.17c) and the proof of Lemma 3.26 that $\vec{X} = \vec{0}$ and $\kappa = 0$.

(ii) The claim follows trivially from (8.14b) and the definition of $\mathbb{U}_0^m$.

(iii) Upon considering the homogeneous system, for $(\vec{U}, P, \vec{X}, \kappa) \in \mathbb{U}^m \times \widehat{\mathbb{P}}^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ it follows immediately from (ii) and (i) that $\vec{U} = \vec{0}$, $\vec{X} = \vec{0}$ and $\kappa = 0$. Then the LBB inf-sup condition (8.10) yields that $P = 0$. $\square$

Theorem 8.4. *Let $d = 2$ or $d = 3$. Let $(\vec{U}^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) \in \mathbb{U}_0^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ be a solution to (8.16), or let $(\vec{U}^{m+1}, P^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) \in \mathbb{U}^m \times \widehat{\mathbb{P}}^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ be a solution to (8.14). Then it holds that*

$$\gamma_0 |\Gamma^{m+1}| + 2 \Delta t_m \left(\mu^m \underline{D}(\vec{U}^{m+1}), \underline{D}(\vec{U}^{m+1}) \right) \leq \gamma_0 |\Gamma^m| + \Delta t_m \left(\vec{f}^{m+1}, \vec{U}^{m+1} \right). \quad (8.18)$$

Proof. It follows from Theorem 8.3(ii) that we only need to consider (8.16). Choosing $\vec{\xi} = \vec{U}^{m+1} \in \mathbb{U}_0^m$ in (8.16a), $\chi = \gamma_0 \kappa^{m+1}$ in (8.16b) and $\vec{\eta} = \gamma_0 (\vec{X}^{m+1} - \text{id}|_{\Gamma^m})$ in (8.16c) yields that

$$\begin{aligned} 2 \Delta t_m \left(\mu^m \underline{D}(\vec{U}^{m+1}), \underline{D}(\vec{U}^{m+1}) \right) + \gamma_0 \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s (\vec{X}^{m+1} - \text{id}) \right\rangle_{\Gamma^m} \\ = \Delta t_m \left(\vec{f}^{m+1}, \vec{U}^{m+1} \right). \end{aligned}$$

Hence (8.18) follows immediately, on recalling Lemma 3.17. $\square$

Remark 8.5.

- (i) *The stability bound (8.18) is a natural fully discrete analogue of (8.7).*
- (ii) *In the case $\vec{f} = \vec{0}$, it is possible to derive the stability bound (8.18) with the help of the general strategy from §5.4, on recalling (8.9). To this end, for a given Γ^m and $\kappa \in V(\Gamma^m)$, we determine $\vec{U} \in \mathbb{U}_0^m$ as the unique solution to*

$$2 \left(\mu^m \underline{D}(\vec{U}), \underline{D}(\vec{\xi}) \right) = \gamma_0 \left\langle \kappa \vec{\nu}^m, \vec{\xi} \right\rangle_{\Gamma^m} \quad \forall \vec{\xi} \in \mathbb{U}_0^m. \quad (8.19)$$

We then define $\mathfrak{F}^m(\kappa) \in V(\Gamma^m)$ such that $\langle \mathfrak{F}^m(\kappa), \chi \rangle_{\Gamma^m}^h = \left\langle \vec{U}, \chi \vec{\nu}^m \right\rangle_{\Gamma^m}^h$ for all $\chi \in V(\Gamma^m)$. Choosing $\vec{\xi} = \vec{U}$ in (8.19) we obtain that

$$\langle \mathfrak{F}^m(\kappa), \kappa \rangle_{\Gamma^m}^h = \frac{2}{\gamma_0} \left(\mu^m \underline{D}(\vec{U}), \underline{D}(\vec{U}) \right) \geq 0 \quad \forall \kappa \in V(\Gamma^m).$$

Now Theorem 5.5(ii) implies the desired stability result.

- (iii) The scheme (8.14) leads to well-behaved meshes for Γ^m , $m = 1, \dots, M$, which follows as in §4.6 by considering a semidiscrete version, see Barrett et al. (2013c, Remark 3). In particular, we obtain equidistribution in two space dimensions and conformal polyhedral hypersurfaces in three space dimensions.

Remark 8.6 (Discrete linear systems). We recall the notations and definitions from Remark 7.7. Moreover, as is standard practice for the solution of linear systems arising from discretizations of (Navier–)Stokes equations, we avoid the complications of the constrained pressure space $\hat{\mathbb{P}}^m$ by considering an overdetermined linear system with $\mathbb{P}^m$ instead. Introducing the obvious abuse of notation, the linear system (8.14), with $\hat{\mathbb{P}}^m$ replaced by $\mathbb{P}^m$, can be formulated as: Find $(\vec{U}^{m+1}, P^{m+1}, \kappa^{m+1}, \delta \vec{X}^{m+1}) \in (\mathbb{R}^d)^{K_{\mathbb{U}^m}} \times \mathbb{R}^{K_{\mathbb{P}^m}} \times \mathbb{R}^K \times (\mathbb{R}^d)^K$ such that

$$\begin{pmatrix} \underline{B}_\Omega & \vec{C}_\Omega & -\gamma_0 \vec{N}_{\Gamma^m, \Omega} & 0 \\ \vec{C}_\Omega^\top & 0 & 0 & 0 \\ \vec{N}_{\Gamma^m, \Omega}^\top & 0 & 0 & -\frac{1}{\Delta t_m} \vec{N}_{\Gamma^m}^\top \\ 0 & 0 & \vec{N}_{\Gamma^m} & \underline{A}_{\Gamma^m} \end{pmatrix} \begin{pmatrix} \vec{U}^{m+1} \\ P^{m+1} \\ \kappa^{m+1} \\ \delta \vec{X}^{m+1} \end{pmatrix} = \begin{pmatrix} \underline{M}_\Omega \vec{f}^{m+1} \\ 0 \\ 0 \\ -\underline{A}_{\Gamma^m} \vec{X}^m \end{pmatrix}, \quad (8.20)$$

where $K_{\mathbb{U}^m}$ and $K_{\mathbb{P}^m}$ denote the degrees of freedom for the finite element spaces $\mathbb{U}^m$ and $\mathbb{P}^m$, respectively. The definitions of the matrices in (8.20) are either given in (4.10), or they follow directly from (8.14), see also Barrett et al. (2015a, §5) for details.

The overdetermined linear system (8.20) can either be solved directly, with the help of a sparse QR factorization method such as SPQR, see Davis (2011). Or it can be solved with the help of a Schur complement approach that eliminates $(\kappa^{m+1}, \delta \vec{X}^{m+1})$ from (8.20), and then uses an iterative solver for the remaining system in $(\vec{U}^{m+1}, P^{m+1})$. This approach has the advantage that for the reduced system well-known solution methods for finite element discretizations for the standard (Navier–)Stokes equations may be employed. In particular, we let

$$\Xi_{\Gamma^m} = \begin{pmatrix} 0 & -\frac{1}{\Delta t_m} \vec{N}_{\Gamma^m}^\top \\ \vec{N}_{\Gamma^m} & \underline{A}_{\Gamma^m} \end{pmatrix}$$

and recall from Lemma 3.26 that if Assumption 3.24 holds, then the matrix Ξ_{Γ^m} is non-singular. On defining $\underline{T}_\Omega = (\vec{N}_{\Gamma^m, \Omega} \ 0) \Xi_{\Gamma^m}^{-1} \begin{pmatrix} \vec{N}_{\Gamma^m, \Omega}^\top \\ 0 \end{pmatrix}$, we can reduce (8.20) to

$$\begin{pmatrix} \vec{B}_\Omega + \gamma_0 \underline{T}_\Omega & \vec{C}_\Omega \\ \vec{C}_\Omega^\top & 0 \end{pmatrix} \begin{pmatrix} \vec{U}^{m+1} \\ P^{m+1} \end{pmatrix} = \begin{pmatrix} \underline{M}_\Omega \vec{f}^{m+1} - \gamma_0 (\vec{N}_{\Gamma^m, \Omega} \ 0) \Xi_{\Gamma^m}^{-1} \begin{pmatrix} 0 \\ \underline{A}_{\Gamma^m} \vec{X}^m \end{pmatrix} \\ 0 \end{pmatrix} \quad (8.21)$$

and $\begin{pmatrix} \kappa^{m+1} \\ \delta \vec{X}^{m+1} \end{pmatrix} = \Xi_{\Gamma^m}^{-1} \begin{pmatrix} -\vec{N}_{\Gamma^m, \Omega}^\top \vec{U}^{m+1} \\ -\underline{A}_{\Gamma^m} \vec{X}^m \end{pmatrix}$. The linear system (8.21) can be solved, for example, with preconditioned GMRES iterative solvers for standard (Navier–)Stokes discretizations, see e.g. Elman et al. (2005) for some examples. For particular preconditioners for (8.21) and further details on possible solution procedures, we refer to Barrett et al. (2015a, §5).

8.1.2 Semidiscrete finite element approximation

In this section we introduce a continuous-in-time semidiscrete variant of (8.14). Similarly to (7.4) and (8.11), for a fixed regular partitioning $\mathcal{T}^h$ of Ω , with $\overline{\Omega} = \cup_{o \in \mathcal{T}^h} \overline{o}$, we introduce the finite element spaces

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

As before, we let $\mathcal{S}_0^h$ denote the space of piecewise constant functions on $\mathcal{T}^h$. Let $\mathbb{U}^h \subset [H_0^1(\Omega)]^d$ and $\mathbb{P}^h(t) \subset L^2(\Omega)$ be the finite element spaces for the semidiscrete velocity and pressure approximations, and set $\widehat{\mathbb{P}}^h(t) = \mathbb{P}^h(t) \cap \widehat{\mathbb{P}}$. Note that while $\mathbb{U}^h$ is fixed, for later developments we allow a time-dependent discrete pressure space $\mathbb{P}^h(t)$, see §8.1.3 below. In addition, we use the notation of §3.4 for evolving polyhedral surfaces, the corresponding finite element spaces, and discrete time derivatives. In addition, we define

$$\widehat{\mathbb{P}}_T^h = \left\{ \varphi \in L^2(0, T; L^2(\Omega)) : \varphi(t) \in \widehat{\mathbb{P}}^h(t) \quad \forall t \in (0, T] \right\}. \quad (8.22)$$

Given $\Gamma^h(t)$, we denote by $\Omega_+^h(t)$ the exterior of $\Gamma^h(t)$ and by $\Omega_-^h(t)$ the interior of $\Gamma^h(t)$, so that $\Gamma^h(t) = \partial\Omega_-^h(t) = \overline{\Omega_-^h(t)} \cap \overline{\Omega_+^h(t)}$. The elements of the bulk mesh $\mathcal{T}^h$ are partitioned into interior, exterior and interfacial elements precisely as in (8.12), and the discrete viscosity $\mu^h(t) \in \mathcal{S}_0^h$ is defined as the natural semidiscrete analogue of (8.13).

Then we can formulate the semidiscrete analogue of (8.14) as follows. Given the closed polyhedral hypersurface $\Gamma^h(0)$, find an evolving polyhedral hypersurface $\mathcal{G}_T^h$ with induced velocity $\vec{\mathcal{V}}^h \in \underline{V}(\mathcal{G}_T^h)$, $\kappa^h \in V(\mathcal{G}_T^h)$, $\vec{U}^h \in L^2(0, T; \mathbb{U}^h)$ and $P^h \in \widehat{\mathbb{P}}_T^h$ as follows. For all $t \in (0, T]$, find $(\vec{U}^h(\cdot, t), P^h(\cdot, t), \vec{\mathcal{V}}^h(\cdot, t), \kappa^h(\cdot, t)) \in \mathbb{U}^h \times \widehat{\mathbb{P}}^h(t) \times \underline{V}(\Gamma^h(t)) \times V(\Gamma^h(t))$ such that

$$2 \left(\mu^h \underline{D}(\vec{U}^h), \underline{D}(\vec{\xi}) \right) - \left(P^h, \nabla \cdot \vec{\xi} \right) = \left(\vec{f}^h, \vec{\xi} \right) + \gamma_0 \left\langle \kappa^h \vec{\nu}^h, \vec{\xi} \right\rangle_{\Gamma^h(t)} \quad \forall \vec{\xi} \in \mathbb{U}^h, \quad (8.23a)$$

$$\left(\nabla \cdot \vec{U}^h, \varphi \right) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}}^h(t), \quad (8.23b)$$

$$\left\langle \vec{\mathcal{V}}^h \cdot \vec{\nu}^h, \chi \right\rangle_{\Gamma^h(t)}^h = \left\langle \vec{U}^h \cdot \vec{\nu}^h, \chi \right\rangle_{\Gamma^h(t)} \quad \forall \chi \in V(\Gamma^h(t)), \quad (8.23c)$$

$$\left\langle \kappa^h \vec{\nu}^h, \vec{\eta} \right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h(t)), \quad (8.23d)$$

where $\vec{f}^h$ is the natural semidiscrete analogue of the fully discrete forcings $\vec{f}^{m+1}$, $m = 0, \dots, M-1$.

Theorem 8.7. *Let $(\mathcal{G}_T^h, \kappa^h, \vec{U}^h, P^h)$ be a solution of (8.23).*

(i) *It holds that*

$$\gamma_0 \frac{d}{dt} |\Gamma^h(t)| + 2 \left(\mu^h \underline{D}(\vec{U}^h), \underline{D}(\vec{U}^h) \right) = \left(\vec{f}^h, \vec{U}^h \right).$$

(ii) If $\mathcal{X}_{\Omega_-^h(t)} \in \mathbb{P}^h(t)$, then it holds that

$$\frac{d}{dt} \mathcal{L}^d(\Omega_-^h(t)) = 0.$$

(iii) For any $t \in (0, T]$, it holds that $\Gamma^h(t)$ is a conformal polyhedral surface. In particular, for $d = 2$, any two neighbouring elements of the curve $\Gamma^h(t)$ either have equal length, or they are parallel.

Proof. (i) Similarly to the proof of Theorem 4.6(i), choosing $\vec{\xi} = \vec{U}^h(\cdot, t) \in \mathbb{U}^h$, $\varphi = P^h(\cdot, t) \in \widehat{\mathbb{P}}^h(t)$, $\chi = \kappa^h(\cdot, t) \in V(\Gamma^h(t))$, $\vec{\eta} = \vec{\mathcal{V}}^h(\cdot, t) \in \underline{V}(\Gamma^h(t))$ in (8.23) gives

$$\begin{aligned} \gamma_0 \frac{d}{dt} |\Gamma^h(t)| &= \gamma_0 \left\langle \nabla_s \text{id}, \nabla_s \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)} = -\gamma_0 \left\langle \vec{\mathcal{V}}^h, \kappa^h \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h \\ &= -\gamma_0 \left\langle \vec{U}^h, \kappa^h \vec{\nu}^h \right\rangle_{\Gamma^h(t)} = \left(\vec{f}^h, \vec{U}^h \right) - 2 \left(\mu^h \underline{D}(\vec{U}^h), \underline{D}(\vec{U}^h) \right), \end{aligned}$$

which is the claim.

(ii) Similarly to the proof of Theorem 5.3(ii), choosing $\chi = 1$ in (8.23c) and $\varphi = \mathcal{X}_{\Omega_-^h(t)} - \frac{\mathcal{L}^d(\Omega_-^h(t))}{\mathcal{L}^d(\Omega)} \in \widehat{\mathbb{P}}^h(t)$ in (8.23b) yields, on using the divergence theorem, that

$$\begin{aligned} \frac{d}{dt} \mathcal{L}^d(\Omega_-^h(t)) &= \left\langle \vec{\mathcal{V}}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h = \left\langle \vec{U}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)} = \left(\nabla \cdot \vec{U}^h, \mathcal{X}_{\Omega_-^h(t)} \right) \\ &= \left(\nabla \cdot \vec{U}^h, \mathcal{X}_{\Omega_-^h(t)} - \frac{\mathcal{L}^d(\Omega_-^h(t))}{\mathcal{L}^d(\Omega)} \right) = 0, \end{aligned}$$

in a discrete analogue to (8.8).

(iii) This follows directly from Definition 3.20 and Theorem 3.22. $\square$

8.1.3 XFEM _{Γ} for conservation of the phase volumes

Conservation of the total mass, equivalent to the conservation of $\mathcal{L}^d(\Omega_-(t))$, (8.8), is clearly a desirable property on the discrete level. We have seen in Theorem 8.7(ii) that the semidiscrete scheme (8.23) conserves $\mathcal{L}^d(\Omega_-^h(t))$ only if the time-dependent discrete pressure spaces $\mathbb{P}^h(t)$ contain the characteristic function of the discrete inner phase $\mathcal{X}_{\Omega_-^h(t)}$ for all $t \in [0, T]$. Hence, for the fully discrete approximation (8.14) it was suggested in Barrett et al. (2013c, §3.4) to extend the pressure space $\mathbb{P}^m$ by one single basis function, namely $\mathcal{X}_{\Omega_-^m}$. There, we referred to this as the XFEM _{Γ} approach, because the extra contributions to (8.14a) and (8.14b) coming from $\mathcal{X}_{\Omega_-^m} - \frac{\mathcal{L}^d(\Omega_-^m)}{\mathcal{L}^d(\Omega)} \in \widehat{\mathbb{P}}^m$ can be written in terms of integrals over Γ^m , on noting from the divergence theorem that

$$\left(\nabla \cdot \vec{\xi}, \mathcal{X}_{\Omega_-^m} - \frac{\mathcal{L}^d(\Omega_-^m)}{\mathcal{L}^d(\Omega)} \right) = \left(\nabla \cdot \vec{\xi}, \mathcal{X}_{\Omega_-^m} \right) = \left\langle \vec{\nu}^m, \vec{\xi} \right\rangle_{\Gamma^m} \quad \forall \vec{\xi} \in \mathbb{U}^m. \quad (8.24)$$

For the fully discrete approximation (8.14), even with the XFEM $_{\Gamma}$ pressure space extension, it is not possible to show that the total mass is conserved. However, we observe that combining (8.24), with $\vec{\xi} = \vec{U}^{m+1}$, (8.14b) and (8.14c) leads to

$$\left\langle \vec{X}^{m+1} - \text{id}, \vec{\nu}^m \right\rangle_{\Gamma^m} = 0,$$

which means that in practice this fully discrete approximation conserves the volume of the two phases well, see also Remark 5.4(ii).

Moreover, it turns out that the XFEM $_{\Gamma}$ approach avoids spurious velocities. To make this precise, we state the following theorem.

Theorem 8.8.

- (i) Let $d = 2$ or $d = 3$. Let $(\vec{U}^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) \in \mathbb{U}^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ be a solution to (8.16) with $\vec{f}^{m+1} = \vec{0}$. If $\vec{X}^{m+1} = \text{id}|_{\Gamma^m}$, then $\vec{U}^{m+1} = \vec{0}$.
- (ii) Let $\mathcal{X}_{\Omega_-^m} \in \mathbb{P}^m$, let Γ^m satisfy Assumption 3.24, and let Γ^m be a polyhedral surface with constant discrete mean curvature, i.e. there exists a constant $\bar{\kappa} \in \mathbb{R}$ such that

$$\bar{\kappa} \langle \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m} + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m).$$

Then Γ^m is a conformal polyhedral surface, recall Definition 3.20, and $(\vec{U}^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) = (\vec{0}, \vec{X}^m, \bar{\kappa}) \in \mathbb{U}_0^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ is the unique solution to (8.16) with $\vec{f}^{m+1} = \vec{0}$.

- (iii) Let the assumptions in (ii) hold and let $(\mathbb{U}^m, \widehat{\mathbb{P}}^m)$ satisfy the LBB condition (8.10). Then Γ^m is a conformal polyhedral surface, and $(\vec{U}^{m+1}, P^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) = (\vec{0}, -\gamma_0 \bar{\kappa} [\mathcal{X}_{\Omega_-^m} - \frac{\mathcal{L}^d(\Omega_-^m)}{\mathcal{L}^d(\Omega)}], \text{id}|_{\Gamma^m}, \bar{\kappa}) \in \mathbb{U}^m \times \widehat{\mathbb{P}}^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ is the unique solution to (8.14) with $\vec{f}^{m+1} = \vec{0}$.

Proof. (i) It follows from Theorem 8.4 that the solution fulfills (8.18) with Γ^{m+1} replaced by Γ^m and $\vec{f}^{m+1} = \vec{0}$. Hence we obtain $(\mu^m \underline{D}(\vec{U}^{m+1}), \underline{D}(\vec{U}^{m+1})) = 0$, and so Korn's inequality implies $\vec{U}^{m+1} = \vec{0}$.

(ii) It immediately follows from (3.6) that Γ^m is a conformal polyhedral surface. Theorem 8.3(i) implies that in order to establish the remaining result, we only need to show that $(\vec{U}^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) = (\vec{0}, \text{id}|_{\Gamma^m}, \bar{\kappa})$ is a solution to (8.16) with $\vec{f}^{m+1} = \vec{0}$. But this follows immediately from $\bar{\kappa} \langle \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m} = \langle \bar{\kappa} \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h$ for all $\vec{\eta} \in \underline{V}(\Gamma^m)$, and

$$\left\langle \vec{\nu}^m, \vec{\xi} \right\rangle_{\Gamma^m} = \left(\nabla \cdot \vec{\xi}, \mathcal{X}_{\Omega_-^m} - \frac{\mathcal{L}^d(\Omega_-^m)}{\mathcal{L}^d(\Omega)} \right) = 0 \quad \forall \vec{\xi} \in \mathbb{U}_0^m,$$

where we have recalled (8.24) and (8.15).

(iii) On recalling Theorem 8.3(iii), the proof is analogous to the proof of (ii). It holds

that

$$\begin{aligned} & \gamma_0 \left\langle \kappa^{m+1} \vec{\nu}^m, \vec{\xi} \right\rangle_{\Gamma^m} + \left(P^{m+1}, \nabla \cdot \vec{\xi} \right) \\ &= \gamma_0 \bar{\kappa} \left\langle \vec{\nu}^m, \vec{\xi} \right\rangle_{\Gamma^m} - \gamma_0 \bar{\kappa} \left(\mathcal{X}_{\Omega_-^m} - \frac{\mathcal{L}^d(\Omega_-^m)}{\mathcal{L}^d(\Omega)}, \nabla \cdot \vec{\xi} \right) = 0 \quad \forall \vec{\xi} \in \mathbb{U}^m, \end{aligned}$$

and this proves the claim. $\square$

Remark 8.9. *It follows from Theorem 8.8 that, independently of the choice of $\mu_{\pm}$, no spurious velocities appear for discrete stationary solutions, $\Gamma^{m+1} = \Gamma^m$. Moreover, for the XFEM $_{\Gamma}$ approach it holds that polyhedral surfaces with constant discrete mean curvature are discrete stationary solutions. In particular, spherical bubbles can be approximated by such polyhedral surfaces, and so our method admits a stationary solution with zero velocity in these situations. This is not the case for many other discretizations and is one of the reasons for spurious velocities in simple situations like a spherical bubble.*

8.1.4 Approximations based on the fluidic tangential velocity

Let us briefly discuss an alternative approximation of two-phase Stokes flow, that is based on a weak formulation of (8.3a) and

$$[\vec{u}]_-^+ = \vec{0}, \quad [(2\mu \underline{D}(\vec{u}) - p \underline{\text{Id}}) \vec{\nu}]_-^+ = -\gamma_0 \vec{\kappa}, \quad \vec{\kappa} = \Delta_s \vec{\text{id}}, \quad \vec{\mathcal{V}} = \vec{u} \quad \text{on } \Gamma(t)$$

as opposed to (8.3) with (8.4). The semidiscrete finite element approximation, in line with (8.23), then features the equations

$$2 \left(\mu^h \underline{D}(\vec{U}^h), \underline{D}(\vec{\xi}) \right) - \left(P^h, \nabla \cdot \vec{\xi} \right) = \left(\vec{f}^h, \vec{\xi} \right) + \gamma_0 \left\langle \vec{\kappa}^h, \vec{\xi} \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\xi} \in \mathbb{U}^h, \quad (8.25a)$$

$$\left(\nabla \cdot \vec{U}^h, \varphi \right) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}}^h(t), \quad (8.25b)$$

$$\left\langle \vec{\mathcal{V}}^h, \vec{\chi} \right\rangle_{\Gamma^h(t)}^h = \left\langle \vec{U}^h, \vec{\chi} \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\chi} \in \underline{V}(\Gamma^h(t)), \quad (8.25c)$$

$$\left\langle \vec{\kappa}^h, \vec{\eta} \right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s \vec{\text{id}}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h(t)), \quad (8.25d)$$

for $(\vec{U}^h(\cdot, t), P^h(\cdot, t), \vec{\mathcal{V}}^h(\cdot, t), \vec{\kappa}^h(\cdot, t)) \in \mathbb{U}^h \times \widehat{\mathbb{P}}^h(t) \times \underline{V}(\Gamma^h(t)) \times \underline{V}(\Gamma^h(t))$. We note that a variant of (8.25) without numerical integration can also be considered, see Barrett et al. (2013c, §3.6) for details on the fully discrete case. It is a simple matter to prove that solutions to (8.25) satisfy the stability result Theorem 8.7(i). However, since $\vec{\nu}^h(\cdot, t)$ is not a valid test function in (8.25c), it is not possible to prove the volume conservation result in Theorem 8.7(ii) for a solution of (8.25), even if $\mathcal{X}_{\Omega_-^h(t)} \in \mathbb{P}^h(t)$. However, on choosing $\vec{\chi} = \vec{\omega}^h(\cdot, t) \in \underline{V}(\Gamma^h(t))$ in (8.25c), it follows from Theorem 3.31 and (3.6) that

$$\frac{d}{dt} \mathcal{L}^d(\Omega_-^h(t)) = \left\langle \vec{\mathcal{V}}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h = \left\langle \vec{\mathcal{V}}^h, \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h = \left\langle \vec{U}^h, \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h. \quad (8.26)$$

Hence, by enforcing the needed condition

$$\left\langle \vec{U}^h, \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h = 0$$

directly, together with a suitable Lagrange multiplier $P_{\text{sing}}^h(t) \in \mathbb{R}$, we can introduce the following semidiscrete approximation of two-phase Stokes flow that satisfies Theorem 8.7(i), (ii). Note that in order for (8.26) to hold, it is crucial to employ numerical integration on $\Gamma^h(t)$ throughout.

Given the closed polyhedral hypersurface $\Gamma^h(0)$, find an evolving polyhedral hypersurface $\mathcal{G}_T^h$ with induced velocity $\vec{\mathcal{V}}^h \in \underline{V}(\mathcal{G}_T^h)$, $\vec{\kappa}^h \in \underline{V}(\mathcal{G}_T^h)$, $\vec{U}^h \in L^2(0, T; \mathbb{U}^h)$, $P^h \in \widehat{\mathbb{P}}_T^h$ and $P_{\text{sing}}^h \in L^2(0, T; \mathbb{R})$ as follows. For all $t \in (0, T]$, find $(\vec{U}^h(\cdot, t), P^h(\cdot, t), P_{\text{sing}}^h(t), \vec{\mathcal{V}}^h(\cdot, t), \vec{\kappa}^h(\cdot, t)) \in \mathbb{U}^h \times \widehat{\mathbb{P}}^h(t) \times \mathbb{R} \times \underline{V}(\Gamma^h(t)) \times \underline{V}(\Gamma^h(t))$ such that

$$\begin{aligned} 2 \left(\mu^h \underline{D}(\vec{U}^h), \underline{D}(\vec{\xi}) \right) - \left(P^h, \nabla \cdot \vec{\xi} \right) - P_{\text{sing}}^h \left\langle \vec{\omega}^h, \vec{\xi} \right\rangle_{\Gamma^h(t)}^h \\ = \left(\vec{f}^h, \vec{\xi} \right) + \gamma_0 \left\langle \vec{\kappa}^h, \vec{\xi} \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\xi} \in \mathbb{U}^h, \end{aligned} \quad (8.27a)$$

$$\left(\nabla \cdot \vec{U}^h, \varphi \right) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}}^h(t) \quad \text{and} \quad \left\langle \vec{U}^h, \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h = 0, \quad (8.27b)$$

$$\left\langle \vec{\mathcal{V}}^h, \vec{\chi} \right\rangle_{\Gamma^h(t)}^h = \left\langle \vec{U}^h, \vec{\chi} \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\chi} \in \underline{V}(\Gamma^h(t)), \quad (8.27c)$$

$$\left\langle \vec{\kappa}^h, \vec{\eta} \right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h(t)). \quad (8.27d)$$

We note that in terms of pressure space enrichment, the above procedure may be viewed as a virtual element method, see e.g. Beirão da Veiga et al. (2013).

8.2 Two-phase Navier–Stokes flow

In Barrett et al. (2015a) the present authors extended the approximation (8.14) to two-phase Navier–Stokes flow, which is given by the model (8.3) with the first equation in (8.3a) replaced by

$$\rho(\partial_t \vec{u} + (\vec{u} \cdot \nabla) \vec{u}) - 2\mu \nabla \cdot \underline{D}(\vec{u}) + \nabla p = \vec{f} \quad \text{in } \Omega_{\pm}(t),$$

where $\rho(\cdot, t) = \rho_+ \chi_{\Omega_+(t)} + \rho_- \chi_{\Omega_-(t)}$, with $\rho_{\pm} \in \mathbb{R}_{\geq 0}$ denoting the two fluid densities, and with the additional initial condition $\rho(\cdot, 0) \vec{u}(\cdot, 0) = \rho(\cdot, 0) \vec{u}_0$ in Ω . The treatment of the interface evolution, and its coupling to the quantities in the bulk, remains unchanged, and for the approximation of the fluid flow in the bulk standard techniques for the finite element approximation of one-phase Navier–Stokes flow can be employed, see e.g. Temam (2001). In the following, we recall the fully discrete approximation from Barrett et al. (2015a), which is based on the weak formulation of two-phase Navier–Stokes flow defined by (8.6) with the additional terms

$$\frac{1}{2} \frac{d}{dt} \left(\rho \vec{u}, \vec{\xi} \right) + \frac{1}{2} \left(\rho \partial_t \vec{u}, \vec{\xi} \right) + \frac{1}{2} \left(\rho, [(\vec{u} \cdot \nabla) \vec{u}] \cdot \vec{\xi} - [(\vec{u} \cdot \nabla) \vec{\xi}] \cdot \vec{u} \right) \quad (8.28)$$

on the left hand side of (8.6a), recall Barrett et al. (2015a, (3.9)).

Let $\rho^m \in \mathcal{S}_0^m$ be defined analogously to (8.13), for $m \geq 0$, and set $\rho^{-1} = \rho^0$. In addition we define the standard projection operator $I_0^m : L^1(\Omega) \rightarrow \mathcal{S}_0^m$, such that $(I_0^m \eta)|_o = \frac{1}{\mathcal{L}^d(o)} \int_o \eta \, d\mathcal{L}^d$ for all $o \in \mathcal{T}^m$. In this section, we consider the partitioning $t_m = m \Delta t$, $m = 0, \dots, M$, of $[0, T]$ into uniform time steps $\Delta t = \frac{T}{M}$. Uniform time steps are required in order to be able to introduce a consistent fully discrete approximation of the time derivative terms in (8.28). Let the closed polyhedral hypersurface Γ^0 be an approximation of $\Gamma(0)$, and let $\vec{U}^0 \in \mathbb{U}^0$ be an approximation to $\vec{u}_0$. Then, for $m = 0, \dots, M-1$, find $(\vec{U}^{m+1}, P^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) \in \mathbb{U}^m \times \hat{\mathbb{P}}^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that

$$\begin{aligned} & \frac{1}{2} \left(\frac{\rho^m \vec{U}^{m+1} - (I_0^m \rho^{m-1}) \vec{I}_2^m \vec{U}^m}{\Delta t} + (I_0^m \rho^{m-1}) \frac{\vec{U}^{m+1} - \vec{I}_2^m \vec{U}^m}{\Delta t}, \vec{\xi} \right) \\ & + \frac{1}{2} \left(\rho^m, [(\vec{I}_2^m \vec{U}^m \cdot \nabla) \vec{U}^{m+1}] \cdot \vec{\xi} - [(\vec{I}_2^m \vec{U}^m \cdot \nabla) \vec{\xi}] \cdot \vec{U}^{m+1} \right) \\ & + 2 \left(\mu^m \underline{D}(\vec{U}^{m+1}), \underline{D}(\vec{\xi}) \right) - \left(P^{m+1}, \nabla \cdot \vec{\xi} \right) = \left(\vec{f}^{m+1}, \vec{\xi} \right) + \gamma_0 \left\langle \kappa^{m+1} \vec{\nu}^m, \vec{\xi} \right\rangle_{\Gamma^m} \\ & \quad \forall \vec{\xi} \in \mathbb{U}^m, \end{aligned} \quad (8.29a)$$

$$(\nabla \cdot \vec{U}^{m+1}, \varphi) = 0 \quad \forall \varphi \in \hat{\mathbb{P}}^m, \quad (8.29b)$$

$$\left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t} \cdot \vec{\nu}^m, \chi \right\rangle_{\Gamma^m}^h = \left\langle \vec{U}^{m+1} \cdot \vec{\nu}^m, \chi \right\rangle_{\Gamma^m} \quad \forall \chi \in V(\Gamma^m), \quad (8.29c)$$

$$\left\langle \kappa^{m+1} \vec{\nu}^m, \vec{\eta} \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m), \quad (8.29d)$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$. Clearly, in the case $\rho_- = \rho_+ = 0$, the approximation (8.29) collapses to the scheme (8.14), with uniform time steps, for two-phase Stokes flow.

Theorem 8.10.

- (i) Let $(\mathbb{U}^m, \hat{\mathbb{P}}^m)$ satisfy the LBB condition (8.10), let Γ^m satisfy Assumption 3.24 and let $\vec{U}^m \in [C(\bar{\Omega})]^d$. Then there exists a unique solution $(\vec{U}^{m+1}, P^{m+1}, \vec{X}^{m+1}, \kappa^{m+1}) \in \mathbb{U}^m \times \hat{\mathbb{P}}^m \times \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to (8.29).
- (ii) Let $d = 2$ or $d = 3$. Then a solution to (8.29) satisfies

$$\begin{aligned} & \frac{1}{2} \left(\rho^m, |\vec{U}^{m+1}|^2 \right) + \gamma_0 |\Gamma^{m+1}| + \frac{1}{2} \left(I_0^m \rho^{m-1}, |\vec{U}^{m+1} - \vec{I}_2^m \vec{U}^m|^2 \right) \\ & + 2 \Delta t \left(\mu^m \underline{D}(\vec{U}^{m+1}), \underline{D}(\vec{U}^{m+1}) \right) \\ & \leq \frac{1}{2} \left(I_0^m \rho^{m-1}, |\vec{I}_2^m \vec{U}^m|^2 \right) + \gamma_0 |\Gamma^m| + \Delta t \left(\vec{f}^{m+1}, \vec{U}^{m+1} \right). \end{aligned} \quad (8.30)$$

Proof. (i) The result can be shown as in the proof of Theorem 8.3.

(ii) We choose $\vec{\xi} = \vec{U}^{m+1}$ in (8.29a), $\varphi = P^{m+1}$ in (8.29b), $\chi = \gamma_0 \kappa^{m+1}$ in (8.29c) and

$\vec{\eta} = \gamma_0 (\vec{X}^{m+1} - \text{id}|_{\Gamma^m})$ in (8.29d) to obtain

$$\begin{aligned} & \frac{1}{2} \left(\rho^m \vec{U}^{m+1}, \vec{U}^{m+1} \right) + \frac{1}{2} \left((I_0^m \rho^{m-1}) (\vec{U}^{m+1} - \vec{I}_2^m \vec{U}^m), \vec{U}^{m+1} - \vec{I}_2^m \vec{U}^m \right) \\ & + 2 \Delta t \left(\mu^m \underline{D}(\vec{U}^{m+1}), \underline{D}(\vec{U}^{m+1}) \right) + \gamma_0 \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s (\vec{X}^{m+1} - \text{id}) \right\rangle_{\Gamma^m} \\ & = \frac{1}{2} \left((I_0^m \rho^{m-1}) \vec{I}_2^m \vec{U}^m, \vec{I}_2^m \vec{U}^m \right) + \Delta t \left(\vec{f}^{m+1}, \vec{U}^{m+1} \right). \end{aligned}$$

Hence (8.30) follows immediately, on recalling Lemma 3.17. $\square$

Remark 8.11.

(i) If $d = 2$ or $d = 3$ then, on assuming that

$$\left(I_0^m \rho^{m-1}, |\vec{I}_2^m \vec{U}^m|^2 \right) \leq \left(\rho^{m-1}, |\vec{U}^m|^2 \right) \quad \text{for } m = 1, \dots, M-1,$$

we can prove an unconditional stability bound for the scheme (8.29), see Barrett et al. (2015a, Theorem 4.2). The condition is always satisfied if no bulk mesh coarsening in time is performed.

(ii) If

$$\mathcal{X}_{\Omega_-^m} \in \mathbb{P}^m \quad \text{for } m = 0, \dots, M-1,$$

then a semidiscrete continuous-in-time version of (8.29) conserves the volume of the two phase exactly, which follows from the direct discrete analogue of Remark 8.1(ii), as discussed previously in §8.1.3.

- (iii) The scheme (8.29) leads to well-behaved meshes, which follows as usual by considering a semidiscrete version, see §4.6. In particular, we obtain equidistribution in two space dimensions and conformal polyhedral hypersurfaces in three space dimensions.
- (iv) It is a simple manner to extend the scheme (8.29), and hence (8.14), to more general boundary conditions than $\vec{u} = \vec{0}$ on $\partial\Omega$ for the fluid flow. Apart from this no-slip condition, also free-slip and stress-free boundary conditions, as well as their inhomogeneous analogues, may be considered. See Barrett et al. (2013c, 2015a, 2016a) for details.
- (v) The discrete linear systems arising from (8.29) can be solved as described in Remark 8.6.

In Figure 6 we show some numerical results for a generalization of the scheme (8.29) to include, for example, free-slip boundary conditions on parts of the boundary $\partial\Omega$ and gravitational forces $\vec{f} = \rho \vec{f}_1$. In Figure 6 we show the interface of a rising bubble together with a visualization of the fluid flow for three different simulations from Barrett et al. (2015a). The two 2D simulations have a density values $10 \rho_- = \rho_+ = 10^3$ and $10^3 \rho_- = \rho_+ = 10^3$, respectively, while the 3D simulation has $10 \rho_- = \rho_+ = 10^3$. As the density of the inner fluid is chosen smaller than the density of the outer fluid in each case, the bubble rises in the presence of gravity.

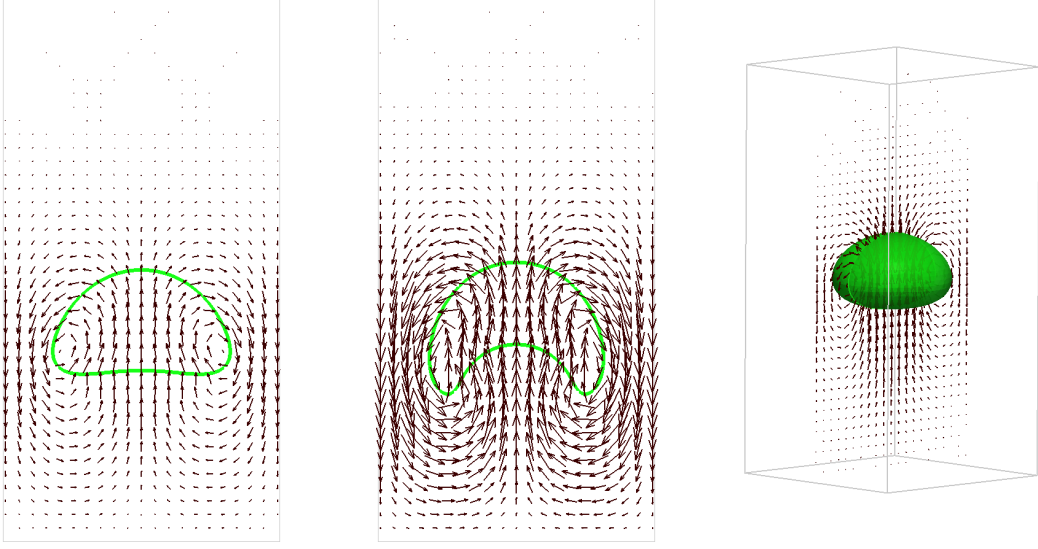


Figure 6: Visualization of the numerical results for the rising droplet experiments shown in Figures 3, 7 and 11 in Barrett et al. (2015a). Each plot shows the interface Γ^m and the velocity $\vec{U}^m$ at time $t = 1.5$. For the 3D experiment, the fluid velocity is only visualized within a 2D cut through Ω .

8.3 Alternative numerical approaches

Numerical methods based on interface tracking methods using an indicator function to describe the interface are also popular methods to numerically solve two-phase flow problems. The volume of fluid (VOF) method uses a characteristic function of one of the phases to evolve the interface and has been used by Hirt and Nichols (1981) and Renardy and Renardy (2002). Another interface tracking method is the level set method, which uses a level set function to track the interface. We refer to Sussman et al. (1994) and to Groß and Reusken (2007) and the references therein for details. Phase field methods, which are also called diffuse interface methods in this context, have been studied numerically by Kim et al. (2004); Kay et al. (2008); Grün and Klingbeil (2014); Garcke et al. (2016). Other parametric methods, which use a polyhedral mesh to directly represent the interface, are discussed in Unverdi and Tryggvason (1992); Bänsch (2001); Tryggvason et al. (2001); Ganesan et al. (2007); Agnese and Nürnberg (2016, 2019).

It is possible to generalize the approximation (8.29) to the case when surfactants are present. Then the surface tension γ_0 depends on the local concentration of surface active agents on the moving interface. The cases of insoluble and soluble surfactants have been considered by the authors in Barrett et al. (2015b) and Barrett et al. (2015c), respectively. Other approaches to two phase flow with surfactants are discussed in James and Lowengrub (2004); Groß and Reusken (2007); Ganesan and Tobiska (2012); Aland et al. (2017) and the references therein.

9 Willmore flow

9.1 Derivation of the flow

Willmore flow is the L^2 -gradient flow of the Willmore energy

$$E(\Gamma) = \frac{1}{2} \int_{\Gamma} \kappa^2 \, d\mathcal{H}^{d-1},$$

for a sufficiently smooth hypersurface Γ in $\mathbb{R}^d$, $d \geq 2$. We remark that in the case $d = 2$ this evolution law is often called elastic flow. In order to derive Willmore flow, we need the first variation of $E(\Gamma)$, which is given in the following lemma. Here we make use of the notations and conventions introduced in §2.4.

Lemma 9.1. *Let $\mathcal{G}_T$ be a closed C^4 -evolving orientable hypersurface. Then it holds that*

$$\frac{d}{dt} E(\Gamma(t)) = \langle \Delta_s \kappa + \kappa |\nabla_s \vec{\nu}|^2 - \frac{1}{2} \kappa^3, \mathcal{V} \rangle_{\Gamma(t)}.$$

Proof. Using Theorem 2.32, Lemma 2.39(ii) and Remark 2.22(i), we compute

$$\begin{aligned} \frac{d}{dt} E(\Gamma(t)) &= \langle \kappa, \partial_t^\square \kappa - \frac{1}{2} \kappa^2 \mathcal{V} \rangle_{\Gamma(t)} = \langle \kappa, \Delta_s \mathcal{V} + \mathcal{V} |\nabla_s \vec{\nu}|^2 - \frac{1}{2} \kappa^2 \mathcal{V} \rangle_{\Gamma(t)} \\ &= \langle \Delta_s \kappa + \kappa |\nabla_s \vec{\nu}|^2 - \frac{1}{2} \kappa^3, \mathcal{V} \rangle_{\Gamma(t)}, \end{aligned} \quad (9.1)$$

where we have used the fact that $\Gamma(t)$ has no boundary. $\square$

Hence we obtain that an evolving hypersurface $(\Gamma(t))_{t \in [0, T]}$, with

$$\mathcal{V} = -\Delta_s \kappa - \kappa |\nabla_s \vec{\nu}|^2 + \frac{1}{2} \kappa^3 \quad \text{on } \Gamma(t), \quad (9.2)$$

most efficiently decreases the Willmore energy, and this evolution law is called Willmore flow. Therefore, (9.2) is the L^2 -gradient flow of the Willmore energy.

9.2 A finite element approximation of Willmore flow

We begin with finite element approximations of Willmore flow from Barrett et al. (2007a, 2008d) or in the spirit of those papers. They are based on the following formulation of Willmore flow

$$\vec{\mathcal{V}} \cdot \vec{\nu} = -\Delta_s \kappa - \kappa |\nabla_s \vec{\nu}|^2 + \frac{1}{2} \kappa^3, \quad \kappa \vec{\nu} = \Delta_s \text{id} \quad \text{on } \Gamma(t). \quad (9.3)$$

Comparing (5.3) with (9.3), we note that once a suitable approximation of $|\nabla_s \vec{\nu}|^2$ is given, then it is a simple matter to extend the techniques in Section 5 in order to derive finite element approximations for Willmore flow. For $d = 2$, $|\nabla_s \vec{\nu}|^2$ collapses to κ^2 , recall Lemma 2.12(iv), and so we can consider the scheme in Barrett et al. (2007a, §2.3). In general, we rely on one of the approximations in (3.21) to obtain a discrete approximation of the

Weingarten map $\nabla_s \vec{\nu}$. Hence, we introduce the following finite element approximations for this formulation of Willmore flow. Let the closed polyhedral hypersurface Γ^0 be an approximation to $\Gamma(0)$, and let $\kappa_{\Gamma^0}^0 \in V(\Gamma^0)$ be an approximation to its mean curvature. We also recall the time interval partitioning (4.5). Then, for $m = 0, \dots, M-1$, first find $\underline{W}^{m+1} \in \underline{V}(\Gamma^m)$, or $\underline{W}^{m+1} \in \underline{V}_c(\Gamma^m)$, as an approximation of the Weingarten map on Γ^m , and then find $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that

$$\begin{aligned} \left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \chi \vec{\nu}^m \right\rangle_{\Gamma^m}^h &= \langle \nabla_s \kappa^{m+1}, \nabla_s \chi \rangle_{\Gamma^m} - \frac{1}{2} \langle (\kappa_{\Gamma^m}^m)^2 \kappa^{m+1}, \chi \rangle_{\Gamma^m}^h \\ &= - \langle \kappa_{\Gamma^m}^m |\underline{W}^{m+1}|^2, \chi \rangle_{\Gamma^m}^h \quad \forall \chi \in V(\Gamma^m), \end{aligned} \quad (9.4a)$$

$$\langle \kappa^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h + \langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (9.4b)$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$ and $\kappa_{\Gamma^{m+1}}^{m+1} = \kappa^{m+1} \circ (\vec{X}^{m+1})^{-1} \in V(\Gamma^{m+1})$. For the definition of $\underline{W}^{m+1}$ we may, for example, choose one of the formulations (3.21), based on Γ^m and possibly $\kappa_{\Gamma^m}^m$ or $\vec{\kappa}^m = \vec{\pi}_{\Gamma^m}[\kappa_{\Gamma^m}^m \vec{\omega}^m]$.

Theorem 9.2. *Let Γ^m satisfy Assumption 3.24(i), let $\kappa_{\Gamma^m}^m \in V(\Gamma^m)$ and $\underline{W}^{m+1} \in \underline{V}(\Gamma^m)$, or $\underline{W}^{m+1} \in \underline{V}_c(\Gamma^m)$, be given. Then there exists a unique solution $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ to (9.4).*

Proof. The desired result follows similarly to the proof of Theorem 5.1. $\square$

Remark 9.3.

- (i) *Similarly to §5.3, a semidiscrete variant of the scheme (9.4) can also be considered, and it will satisfy Theorem 5.3(iii).*
- (ii) *Similarly to §5.5, one can consider a variant of the scheme (9.4) with reduced or induced tangential motion.*
- (iii) *The discrete linear systems arising at each time level of (9.4) are very similar to the ones induced by (5.4). They can be solved, for example, with the help of a sparse factorization package such as UMFPACK, see Davis (2004).*

9.3 A stable approximation of Willmore flow

Unfortunately, it does not seem possible to prove a stability result for the fully discrete approximation (9.4) of (9.3). However, the important paper Dziuk (2008) introduced a stable semidiscrete finite element approximation of Willmore flow. The discretization is based on an alternative formulation of the first variation of the Willmore energy, which leads to a weak formulation of Willmore flow. In order to derive the weak formulation, we prove the following result, which is inspired by Dziuk (2008, Lemma 3).

Lemma 9.4. *Let $\mathcal{G}_T$ be a closed C^3 -evolving orientable hypersurface. Let $\vec{\mathcal{V}}$ be the velocity field induced by a global parameterization of $\mathcal{G}_T$. Then it holds that*

$$\frac{d}{dt} E(\Gamma(t)) = - \left\langle \frac{1}{2} |\vec{\mathcal{Z}}|^2 + \nabla_s \cdot \vec{\mathcal{Z}}, \nabla_s \cdot \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} + \left\langle \nabla_s \vec{\mathcal{Z}}, 2 \underline{D}_s(\vec{\mathcal{V}}) - \nabla_s \vec{\mathcal{V}} \right\rangle_{\Gamma(t)},$$

where $\underline{D}_s(\vec{\mathcal{V}})$ is the rate of deformation tensor, recall Definition 2.25(iv).

Proof. It follows from Definition 2.11(iii) and Theorem 2.32 that

$$\frac{d}{dt} E(\Gamma(t)) = \frac{1}{2} \frac{d}{dt} \langle |\vec{\mathcal{Z}}|^2, 1 \rangle_{\Gamma(t)} = \langle \vec{\mathcal{Z}}, \partial_t^\circ \vec{\mathcal{Z}} \rangle_{\Gamma(t)} + \frac{1}{2} \left\langle |\vec{\mathcal{Z}}|^2, \nabla_s \cdot \vec{\mathcal{V}} \right\rangle_{\Gamma(t)}. \quad (9.5)$$

We now slightly modify the arguments in the proof of Dziuk (2008, Lemma 3), in order to compute the term $\langle \vec{\mathcal{Z}}, \partial_t^\circ \vec{\mathcal{Z}} \rangle_{\Gamma(t)}$.

Let $\vec{x} : \Upsilon \times [0, T] \rightarrow \mathbb{R}^d$ be a global parameterization of $\mathcal{G}_T$ as described in Definition 2.25(i). For a given $\vec{\eta}_0 \in [C^1(\Upsilon)]^d$, we define $\vec{\eta} : \mathcal{G}_T \rightarrow \mathbb{R}^d$ via

$$\vec{\eta}(\vec{x}(\vec{z}, t), t) = \vec{\eta}_0(\vec{z}) \quad \text{for all } \quad \forall (\vec{z}, t) \in \Upsilon \times [0, T], \quad (9.6)$$

i.e. the values of $\vec{\eta}$ are transported with the map $\vec{x}$. Hence it follows from Definition 2.28(i) that

$$\partial_t^\circ \vec{\eta} = \vec{0} \quad \text{on } \mathcal{G}_T. \quad (9.7)$$

On recalling Remark 2.22(iv), Definition 2.11(iii) and a density argument, we have that

$$\langle \vec{\mathcal{Z}}, \vec{\eta} \rangle_{\Gamma(t)} + \left\langle \nabla_s \vec{\text{id}}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d, \quad (9.8)$$

since we assume $\Gamma(t)$ to be closed. Differentiating (9.8) with respect to t , we obtain from Theorem 2.32, on noting (9.7), that

$$\langle \partial_t^\circ \vec{\mathcal{Z}}, \vec{\eta} \rangle_{\Gamma(t)} + \left\langle \vec{\mathcal{Z}} \cdot \vec{\eta}, \nabla_s \cdot \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} + \frac{d}{dt} \left\langle \nabla_s \vec{\text{id}}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} = 0. \quad (9.9)$$

Using Lemma 2.9(ii), Theorem 2.32, Lemma 2.38(iii) and (9.7), we now compute

$$\begin{aligned} \frac{d}{dt} \left\langle \nabla_s \vec{\text{id}}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} &= \frac{d}{dt} \langle \nabla_s \cdot \vec{\eta}, 1 \rangle_{\Gamma(t)} \\ &= \left\langle \nabla_s \cdot \vec{\eta}, \nabla_s \cdot \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} + \left\langle \nabla_s \vec{\eta}, \nabla_s \vec{\mathcal{V}} - 2 \underline{D}_s(\vec{\mathcal{V}}) \right\rangle_{\Gamma(t)}. \end{aligned} \quad (9.10)$$

On combining (9.9) and (9.10), and then choosing $\vec{\eta} = \vec{\mathcal{Z}}$, we obtain

$$\langle \partial_t^\circ \vec{\mathcal{Z}}, \vec{\mathcal{Z}} \rangle_{\Gamma(t)} = - \left\langle |\vec{\mathcal{Z}}|^2 + \nabla_s \cdot \vec{\mathcal{Z}}, \nabla_s \cdot \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} - \left\langle \nabla_s \vec{\mathcal{Z}}, \nabla_s \vec{\mathcal{V}} - 2 \underline{D}_s(\vec{\mathcal{V}}) \right\rangle_{\Gamma(t)}.$$

Together with (9.5) this yields the desired result. $\square$

A weak formulation of Willmore flow based on Lemma 9.4 is then the following. Given a closed hypersurface $\Gamma(0)$, we seek an evolving hypersurface $(\Gamma(t))_{t \in [0, T]}$, with a global parameterization and induced velocity field $\vec{\mathcal{V}}$, and $\vec{\kappa} \in [L^2(\mathcal{G}_T)]^d$ as follows. For almost all $t \in (0, T)$, find $(\vec{\mathcal{V}}(\cdot, t), \vec{\kappa}(\cdot, t)) \in [L^2(\Gamma(t))]^d \times [H^1(\Gamma(t))]^d$ such that

$$\begin{aligned} \langle \vec{\mathcal{V}}, \vec{\chi} \rangle_{\Gamma(t)} &= \langle \nabla_s \vec{\kappa}, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \rangle_{\Gamma(t)} + \langle \nabla_s \cdot \vec{\kappa}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\ &\quad + \frac{1}{2} \langle |\vec{\kappa}|^2, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \quad \forall \vec{\chi} \in [H^1(\Gamma(t))]^d, \end{aligned} \quad (9.11a)$$

$$\langle \vec{\kappa}, \vec{\eta} \rangle_{\Gamma(t)} + \langle \nabla_s \text{id}, \nabla_s \vec{\eta} \rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d, \quad (9.11b)$$

where we have noted a density argument.

Remark 9.5 (Comparison to Dziuk (2008)). *We note that our notation is such that $\nabla_s \vec{\chi} = (\nabla_\Gamma \vec{\chi})^\top$, with $\nabla_\Gamma \vec{\chi}$ defined as in Dziuk (2008, (2.4)). In addition, our $\underline{D}_s(\vec{\chi}) = \frac{1}{2} \underline{P}_\Gamma \underline{D}_\Gamma(\vec{\chi}) \underline{P}_\Gamma$, where we recall Definition 2.5(vii) and $\underline{D}_\Gamma(\vec{\chi}) = \nabla_\Gamma \vec{\chi} + (\nabla_\Gamma \vec{\chi})^\top$ as defined in Dziuk (2008, (3.14)). Hence, it is easily deduced from Remark 2.6(v) and Lemma 2.9(i) that $2 \nabla_s \vec{f} : \underline{D}_s(\vec{\chi}) = \nabla_\Gamma \vec{f} : \underline{D}_\Gamma(\vec{\chi}) \nabla_\Gamma \text{id}$ for all $\vec{f}, \vec{\chi} \in [H^1(\Gamma(t))]^d$, which implies that (9.11) agrees with Dziuk (2008, Problem 2).*

We now relate the weak formulation (9.11) to the strong formulation (9.3).

Lemma 9.6. *A sufficiently smooth solution of (9.11) is a solution of the strong formulation (9.3) of Willmore flow.*

Proof. First of all, (9.11b) and Remark 2.22(iv) imply that $\vec{\kappa} = \kappa \vec{\nu}$ and the second equation in (9.3) holds.

Next, we have, on noting Definition 2.5(vii), Remark 2.6(v), Lemma 2.7(iii) and Lemma 2.12(ii), that

$$\nabla_s \vec{\kappa} : (\nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi})) = (\vec{\nu} \otimes \nabla_s \kappa) : \nabla_s \vec{\chi} - \kappa \nabla_s \vec{\nu} : \nabla_s \vec{\chi}.$$

Hence, it follows from Remark 2.22(i),(iii) and Lemma 2.7(ii),(iii) that the first term on the right hand side of (9.11a) can be rewritten as

$$\langle \nabla_s \vec{\kappa}, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \rangle_{\Gamma(t)} = \langle \kappa \Delta_s \vec{\nu} - (\Delta_s \kappa) \vec{\nu}, \vec{\chi} \rangle_{\Gamma(t)}. \quad (9.12)$$

In addition, Definition 2.5(ii) and Lemma 2.13(i) yield that $\nabla_s \cdot \vec{\kappa} = \nabla_s \cdot (\kappa \vec{\nu}) = \kappa \nabla_s \cdot \vec{\nu} = -\kappa^2$. Hence, we obtain from the second and third terms on the right hand side of (9.11a), on noting Lemma 2.7(i) and Theorem 2.21, that

$$\begin{aligned} \langle \nabla_s \cdot \vec{\kappa} + \frac{1}{2} |\vec{\kappa}|^2, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} &= -\frac{1}{2} \langle \kappa^2, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\ &= \langle \kappa \nabla_s \kappa, \vec{\chi} \rangle_{\Gamma(t)} + \frac{1}{2} \langle \kappa^3, \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)}. \end{aligned} \quad (9.13)$$

Combining (9.11a), (9.12) and (9.13) yields that

$$\vec{\mathcal{V}} = (-\Delta_s \kappa + \frac{1}{2} \kappa^3) \vec{\nu} + \kappa (\Delta_s \vec{\nu} + \nabla_s \kappa) = (-\Delta_s \kappa - \kappa |\nabla_s \vec{\nu}|^2 + \frac{1}{2} \kappa^3) \vec{\nu}, \quad (9.14)$$

where we have recalled Lemma 2.16. Therefore, we obtain the desired first result in (9.3). $\square$

We now introduce a natural semidiscrete variant of (9.11). Given the closed polyhedral hypersurface $\Gamma^h(0)$, find an evolving polyhedral hypersurface $\mathcal{G}_T^h$ with induced velocity $\vec{\mathcal{V}}^h \in \underline{V}(\mathcal{G}_T^h)$, and $\vec{\kappa}^h \in \underline{V}(\mathcal{G}_T^h)$, i.e. $(\vec{\mathcal{V}}^h(\cdot, t), \vec{\kappa}^h(\cdot, t)) \in \underline{V}(\Gamma^h(t)) \times \underline{V}(\Gamma^h(t))$ for all $t \in [0, T]$, such that, for all $t \in (0, T]$,

$$\begin{aligned} \left\langle \vec{\mathcal{V}}^h, \vec{\chi} \right\rangle_{\Gamma^h(t)}^h &= \left\langle \nabla_s \vec{\kappa}^h, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \right\rangle_{\Gamma^h(t)} + \left\langle \nabla_s \cdot \vec{\kappa}^h, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^h(t)} \\ &\quad + \frac{1}{2} \left\langle |\vec{\kappa}^h|^2, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\chi} \in \underline{V}(\Gamma^h(t)), \end{aligned} \quad (9.15a)$$

$$\left\langle \vec{\kappa}^h, \vec{\eta} \right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h(t)), \quad (9.15b)$$

where we recall the definition of $\underline{D}_s$ on $\Gamma^h(t)$ from Lemma 3.33.

We now prove the following stability theorem.

Theorem 9.7. *Let $(\mathcal{G}_T^h, \vec{\kappa}^h)$ be a solution of (9.15), and let $\vec{\kappa}^h \in \underline{V}_T(\mathcal{G}_T^h)$. Then it holds that*

$$\frac{d}{dt} \frac{1}{2} \left(|\vec{\kappa}^h|_{\Gamma^h(t)}^h \right)^2 = - \left(|\vec{\mathcal{V}}^h|_{\Gamma^h(t)}^h \right)^2 \leq 0.$$

Proof. We argue as in the proof of Lemma 9.4. Similarly to (9.7), we extend test functions $\vec{\eta} \in \underline{V}(\Gamma^h(t))$ in (9.15b) to $\vec{\eta} \in \underline{V}_T(\mathcal{G}_T^h)$ such that $\partial_t^{\circ, h} \vec{\eta} = \vec{0}$ on $\mathcal{G}_T^h$. Then taking the time derivative of (9.15b), on noting Theorem 3.30 and Lemma 3.33(iii), yields

$$\begin{aligned} \left\langle \partial_t^{\circ, h} \vec{\kappa}^h, \vec{\eta} \right\rangle_{\Gamma^h(t)}^h &+ \left\langle \vec{\kappa}^h \cdot \vec{\eta}, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s \cdot \vec{\mathcal{V}}^h, \nabla_s \cdot \vec{\eta} \right\rangle_{\Gamma^h(t)} \\ &+ \left\langle \nabla_s \vec{\mathcal{V}}^h, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)} - 2 \left\langle \underline{D}_s(\vec{\mathcal{V}}^h), \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)} = 0. \end{aligned} \quad (9.16)$$

We now choose $\vec{\eta} = \vec{\kappa}^h$ in (9.16) and $\vec{\chi} = \vec{\mathcal{V}}^h$ in (9.15a), to obtain that

$$\left\langle \partial_t^{\circ, h} \vec{\kappa}^h, \vec{\kappa}^h \right\rangle_{\Gamma^h(t)}^h + \frac{1}{2} \left\langle |\vec{\kappa}^h|^2, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \vec{\mathcal{V}}^h, \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h = 0.$$

The desired result then follows on noting Theorem 3.30(ii) and (3.2). $\square$

Remark 9.8.

- (i) For the case $d = 2$ an error analysis of (9.15) can be found in Deckelnick and Dziuk (2009).
- (ii) We note the version of (9.15) proposed in Dziuk (2008, Problem 3) is without mass lumping. Nevertheless, either version of (9.15), in contrast to (9.4), does not have good mesh properties. This is due to the fact that the mesh movements are almost exclusively in the normal direction, which in general leads to bad meshes. This is because (9.15a) approximates (9.11a), which is a weak formulation of

$$\vec{\mathcal{V}} = \left[-\Delta_s \varkappa - \varkappa |\nabla_s \vec{v}|^2 + \frac{1}{2} \varkappa^3 \right] \vec{v} \quad \text{on } \Gamma(t),$$

where we have recalled (9.14).

We now wish to derive a weak formulation, which leads to semidiscretizations that are both stable and have good mesh properties. A main ingredient is to ensure that the equation

$$\langle \kappa \vec{\nu}, \vec{\eta} \rangle_{\Gamma(t)} + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d \quad (9.17)$$

holds. This then leads to good meshes on the discrete level, recall §4.6. We hence want to compute the time derivative of $\frac{1}{2} \langle \kappa, \kappa \rangle_{\Gamma(t)}$ by taking the constraint (9.17) into account. To this end, we use the calculus of PDE constrained optimization, see e.g. Hinze et al. (2009); Tröltzsch (2010), and define the Lagrangian

$$L(\Gamma(t), \kappa^*, \vec{y}) = \frac{1}{2} \langle \kappa^*, \kappa^* \rangle_{\Gamma(t)} - \langle \kappa^* \vec{\nu}, \vec{y} \rangle_{\Gamma(t)} - \left\langle \nabla_s \text{id}, \nabla_s \vec{y} \right\rangle_{\Gamma(t)}, \quad (9.18)$$

where $\vec{y} \in [H^1(\Gamma(t))]^d$ is the Lagrange multiplier associated with the constraint (9.17) with κ replaced by κ^* . We note at this stage that $\kappa^*(t)$ is an independent variable, and not the mean curvature, $\kappa(t)$, of $\Gamma(t)$. We now need to take variations of $L(\Gamma(t), \kappa^*, \vec{y})$ with respect to $\Gamma(t)$, κ^* and $\vec{y}$.

To this end, for any $\vec{\chi} \in [H^1(\Gamma(t))]^d$ and for any $\varepsilon \in \mathbb{R}$ let

$$\Gamma_\varepsilon(t) = \vec{\Phi}(\Gamma(t), \varepsilon), \quad \text{where} \quad \vec{\Phi}(\cdot, \varepsilon) = \text{id}_{|\Gamma(t)} + \varepsilon \vec{\chi}. \quad (9.19)$$

For $\varepsilon_0 > 0$, we now consider a smooth function f defined on $\bigcup_{\varepsilon \in [-\varepsilon_0, \varepsilon_0]} (\Gamma_\varepsilon(t) \times \{\varepsilon\})$. Then, similarly to Definition 2.28(i), we define

$$(\partial_\varepsilon^\circ f)(\vec{\Phi}(\vec{z}, \varepsilon), \varepsilon) = \frac{d}{d\varepsilon} f(\vec{\Phi}(\vec{z}, \varepsilon), \varepsilon) \quad \forall (\vec{z}, \varepsilon) \in \Gamma(t) \times [-\varepsilon_0, \varepsilon_0], \quad (9.20)$$

and note that

$$\partial_\varepsilon^\circ f = \left(\frac{d}{d\varepsilon} f(\vec{\Phi}(\cdot, \varepsilon), \varepsilon) \right)_{|\varepsilon=0} = \lim_{\varepsilon \rightarrow 0} \frac{f(\vec{\Phi}(\cdot, \varepsilon), \varepsilon) - f}{\varepsilon} \quad \text{on } \Gamma(t). \quad (9.21)$$

In what follows, and similarly to §2.4, we often identify $\Gamma_\varepsilon(t) \times \{\varepsilon\}$ with $\Gamma_\varepsilon(t)$, and hence $(\Gamma_\varepsilon(t) \times \{\varepsilon\})_{|\varepsilon=0}$ with $\Gamma(t)$. With the help of a direct analogue of Theorem 2.32, we then obtain that the first variation of $\langle f, 1 \rangle_{\Gamma(t)}$ is given by

$$\left[\frac{\delta}{\delta \Gamma} \langle f, 1 \rangle_{\Gamma(t)} \right] (\vec{\chi}) = \left(\frac{d}{d\varepsilon} \langle f, 1 \rangle_{\Gamma_\varepsilon(t)} \right)_{|\varepsilon=0} = \langle \partial_\varepsilon^\circ f + f \nabla_s \cdot \vec{\chi}, 1 \rangle_{\Gamma(t)}. \quad (9.22)$$

In addition, if $\vec{\nu}_\varepsilon$ is the unit normal on $\Gamma_\varepsilon(t)$, corresponding to $\vec{\nu}$ on $\Gamma(t)$, then a direct analogue of Lemma 2.37(i) yields that

$$\left[\frac{\delta}{\delta \Gamma} \vec{\nu} \right] (\vec{\chi}) = (\partial_\varepsilon^\circ \vec{\nu}_\varepsilon)_{|\varepsilon=0} = -(\nabla_s \vec{\chi})^\top \vec{\nu} \quad \text{on } \Gamma(t). \quad (9.23)$$

Similarly to (9.6), for any $\eta \in L^\infty(\Gamma(t))$, one can define $\eta_{(\varepsilon)}$ on $\bigcup_{\varepsilon \in [-\varepsilon_0, \varepsilon_0]} (\Gamma_\varepsilon(t) \times \{\varepsilon\})$ via

$$\eta_{(\varepsilon)}(\vec{\Phi}(\vec{z}, \varepsilon), \varepsilon) = \eta(\vec{z}) \quad \forall (\vec{z}, \varepsilon) \in \Gamma(t) \times [-\varepsilon_0, \varepsilon_0], \quad (9.24)$$

and analogously for $\vec{\eta} \in [L^\infty(\Gamma(t))]^d$. Similarly to (9.7), it follows from this extension and (9.21) that

$$\left[\frac{\delta}{\delta \Gamma} \vec{\eta} \right] (\vec{\chi}) = (\partial_\varepsilon^\circ \vec{\eta}_{(\varepsilon)})|_{\varepsilon=0} = \vec{0} \quad \text{on } \Gamma(t).$$

In particular, we have the following analogue of (9.10),

$$\begin{aligned} \left[\frac{\delta}{\delta \Gamma} \langle \nabla_s \text{id}, \nabla_s \vec{\eta} \rangle_{\Gamma(t)} \right] (\vec{\chi}) &= \left(\frac{d}{d\varepsilon} \langle \nabla_s \text{id}, \nabla_s \vec{\eta}_{(\varepsilon)} \rangle_{\Gamma_\varepsilon(t)} \right) \Big|_{\varepsilon=0} \\ &= \langle \nabla_s \cdot \vec{\eta}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} + \langle \nabla_s \vec{\eta}, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \rangle_{\Gamma(t)}. \end{aligned} \quad (9.25)$$

We now consider the variations of $L(\Gamma(t), \varkappa^*, \vec{y})$ with respect to $\Gamma(t)$, $\varkappa^*$ and $\vec{y}$. In particular, for all $\vec{\chi} \in [H^1(\Gamma(t))]^d$, $\xi \in L^2(\Gamma(t))$ and $\vec{\eta} \in [H^1(\Gamma(t))]^d$, we let

$$\left[\frac{\delta}{\delta \Gamma} L \right] (\vec{\chi}) = \left(\frac{d}{d\varepsilon} L(\Gamma_\varepsilon(t), \varkappa_{(\varepsilon)}^*, \vec{y}_{(\varepsilon)}) \right) \Big|_{\varepsilon=0}, \quad (9.26a)$$

$$\left[\frac{\delta}{\delta \varkappa^*} L \right] (\xi) = \left(\frac{d}{d\varepsilon} L(\Gamma(t), \varkappa^* + \varepsilon \xi, \vec{y}) \right) \Big|_{\varepsilon=0}, \quad (9.26b)$$

$$\left[\frac{\delta}{\delta \vec{y}} L \right] (\vec{\eta}) = \left(\frac{d}{d\varepsilon} L(\Gamma(t), \varkappa^*, \vec{y} + \varepsilon \vec{\eta}) \right) \Big|_{\varepsilon=0}, \quad (9.26c)$$

where $\varkappa_{(\varepsilon)}^* \in L^2(\Gamma_\varepsilon(t))$ and $\vec{y}_{(\varepsilon)} \in [H^1(\Gamma_\varepsilon(t))]^d$ are defined by transporting the values of $\varkappa^* \in L^2(\Gamma(t))$ and $\vec{y} \in [H^1(\Gamma(t))]^d$ as defined in (9.24), recall (9.19) for the $\vec{\chi}$ at hand. Setting the variation $\left[\frac{\delta}{\delta \vec{y}} L \right] (\vec{\eta}) = 0$, yields (9.17) with $\varkappa$ replaced by $\varkappa^*$. Hence, comparing this with the original (9.17), we obtain that $\varkappa^* = \varkappa$. Setting $\left[\frac{\delta}{\delta \varkappa^*} L \right] (\xi) = 0$, yields, on noting $\varkappa^* = \varkappa$, that

$$\varkappa = \vec{y} \cdot \vec{\nu} \quad \text{on } \Gamma(t). \quad (9.27)$$

Finally, setting the variation $\left[\frac{\delta}{\delta \Gamma} L \right] (\vec{\chi}) = -\langle \vec{\mathcal{V}} \cdot \vec{\nu}, \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)}$ and noting (9.22), (9.23), (9.25) and that $\varkappa^* = \varkappa$, we obtain

$$\begin{aligned} \langle \vec{\mathcal{V}} \cdot \vec{\nu}, \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} &= \langle \nabla_s \vec{y}, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \rangle_{\Gamma(t)} + \langle \nabla_s \cdot \vec{y}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\ &\quad - \langle \varkappa \left(\frac{1}{2} \varkappa - \vec{y} \cdot \vec{\nu} \right), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} - \langle \varkappa \vec{y}, (\nabla_s \vec{\chi})^\top \vec{\nu} \rangle_{\Gamma(t)} \\ &\quad \forall \vec{\chi} \in [H^1(\Gamma(t))]^d. \end{aligned} \quad (9.28)$$

Therefore we have the following weak formulation. Given a closed hypersurface $\Gamma(0)$, we seek an evolving hypersurface $(\Gamma(t))_{t \in [0, T]}$, with a global parameterization and induced velocity field $\vec{\mathcal{V}}$, $\varkappa \in L^2(\mathcal{G}_T)$ and $\vec{y} \in [L^2(\mathcal{G}_T)]^d$ as follows. For almost all $t \in (0, T)$, find $(\vec{\mathcal{V}}(\cdot, t), \varkappa(\cdot, t), \vec{y}(\cdot, t)) \in [L^2(\Gamma(t))]^d \times L^2(\Gamma(t)) \times [H^1(\Gamma(t))]^d$ such that (9.28), (9.27) and (9.17) hold.

Remark 9.9.

- (i) *Using the techniques in Barrett et al. (2017c, Appendix A) one can show, similarly to Lemma 9.6, that a sufficiently smooth solution of this weak formulation is a solution of the strong formulation (9.3).*
- (ii) *Clearly, using (9.27) one can eliminate $\varkappa$ from (9.28) and (9.17) in this weak formulation.*

We now consider a discrete analogue of (9.28), (9.27) and (9.17), by first introducing the discrete analogue of (9.18)

$$L^h(\Gamma^h(t), \kappa^h, \vec{Y}^h) = \frac{1}{2} \langle \kappa^h, \kappa^h \rangle_{\Gamma^h(t)}^h - \langle \kappa^h \vec{\nu}^h, \vec{Y}^h \rangle_{\Gamma^h(t)}^h - \langle \nabla_s \text{id}, \nabla_s \vec{Y}^h \rangle_{\Gamma^h(t)}^h, \quad (9.29)$$

where $\vec{Y}^h(\cdot, t) \in \underline{V}(\Gamma^h(t))$ is the Lagrange multiplier associated with the constraint $\kappa^h(\cdot, t) \in V(\Gamma^h(t))$ satisfying

$$\langle \kappa^h \vec{\nu}^h, \vec{\eta} \rangle_{\Gamma^h(t)}^h + \langle \nabla_s \text{id}, \nabla_s \vec{\eta} \rangle_{\Gamma^h(t)}^h = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h(t)). \quad (9.30)$$

Setting $\left[\frac{\delta}{\delta \vec{Y}^h} L^h \right] (\vec{\eta}) = 0$ yields (9.30). Setting $\left[\frac{\delta}{\delta \kappa^h} L^h \right] (\xi) = 0$ yields that

$$\langle \kappa^h - \vec{Y}^h \cdot \vec{\nu}^h, \xi \rangle_{\Gamma^h(t)}^h = 0 \quad \forall \xi \in V(\Gamma^h(t)). \quad (9.31)$$

Finally, we need to take the variation of $L^h(\Gamma^h(t), \kappa^h, \vec{Y}^h)$ with respect to $\Gamma^h(t)$. To this end, we have the following discrete analogue of (9.19). For any $\vec{\chi} \in \underline{V}(\Gamma^h(t))$ and for any $\varepsilon \in \mathbb{R}$, let

$$\Gamma_\varepsilon^h(t) = \vec{\Phi}^h(\Gamma^h(t), \varepsilon), \quad \text{where} \quad \vec{\Phi}^h(\cdot, \varepsilon) = \text{id}_{\Gamma^h(t)} + \varepsilon \vec{\chi}.$$

We also define $\partial_\varepsilon^{\circ, h}$ to be the discrete analogue of (9.20). Similarly to Theorem 3.30(ii), we then have that

$$\begin{aligned} \left[\frac{\delta}{\delta \Gamma^h} \langle \kappa^h, \vec{Y}^h \cdot \vec{\nu}^h \rangle_{\Gamma^h(t)}^h \right] (\vec{\chi}) &= \left(\frac{d}{d\varepsilon} \langle \kappa_{(\varepsilon)}^h, \vec{Y}_{(\varepsilon)}^h \cdot \vec{\nu}_\varepsilon^h \rangle_{\Gamma_\varepsilon^h(t)}^h \right) \Big|_{\varepsilon=0} \\ &= \left(\langle \kappa_{(\varepsilon)}^h, \vec{Y}_{(\varepsilon)}^h \cdot \partial_\varepsilon^{\circ, h} \vec{\nu}_\varepsilon^h \rangle_{\Gamma_\varepsilon^h(t)}^h \right) \Big|_{\varepsilon=0} + \langle \kappa^h \vec{Y}^h \cdot \vec{\nu}^h, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^h(t)}^h \\ &= \left\langle \kappa^h, \vec{Y}^h \cdot \left[\frac{\delta}{\delta \Gamma^h} \vec{\nu}^h \right] (\vec{\chi}) \right\rangle_{\Gamma^h(t)}^h + \langle \kappa^h \vec{Y}^h \cdot \vec{\nu}^h, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^h(t)}^h, \end{aligned} \quad (9.32)$$

where $\kappa_{(\varepsilon)}^h$ and $\vec{Y}_{(\varepsilon)}^h$ are defined similarly to (9.24), with the help of the map $\vec{\Phi}^h$, and $\vec{\nu}_\varepsilon^h$ is the unit normal on $\Gamma_\varepsilon^h(t)$. Hence, setting the variation $\left[\frac{\delta}{\delta \Gamma^h} L^h \right] (\vec{\chi}) =$

$-\left\langle \vec{\mathcal{V}}^h \cdot \vec{\omega}^h, \vec{\chi} \cdot \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h$, on noting (9.32), the discrete analogue of (9.23) for $\vec{\nu}^h$ on $\Gamma^h(t)$, compare Lemma 3.32, and (9.25) for $\Gamma^h(t)$, we obtain

$$\begin{aligned} \left\langle \vec{\mathcal{V}}^h \cdot \vec{\omega}^h, \vec{\chi} \cdot \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h &= \left\langle \nabla_s \vec{Y}^h, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \right\rangle_{\Gamma^h(t)} + \left\langle \nabla_s \cdot \vec{Y}^h, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^h(t)} \\ &\quad - \left\langle \kappa^h \left(\frac{1}{2} \kappa^h - \vec{Y}^h \cdot \vec{\nu}^h \right), \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^h(t)}^h - \left\langle \kappa^h \vec{Y}^h, (\nabla_s \vec{\chi})^\top \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h \\ &\quad \forall \vec{\chi} \in \underline{V}(\Gamma^h(t)). \end{aligned} \quad (9.33)$$

Therefore we have the following semidiscrete finite element approximation of (9.28), (9.27) and (9.17). Given the closed polyhedral hypersurface $\Gamma^h(0)$, find an evolving polyhedral hypersurface $\mathcal{G}_T^h$ with induced velocity $\vec{\mathcal{V}}^h \in \underline{V}(\mathcal{G}_T^h)$, and $\kappa^h \in V(\mathcal{G}_T^h)$, $\vec{Y}^h \in \underline{V}(\mathcal{G}_T^h)$, i.e. $(\vec{\mathcal{V}}^h(\cdot, t), \kappa^h(\cdot, t), \vec{Y}^h(\cdot, t)) \in \underline{V}(\Gamma^h(t)) \times V(\Gamma^h(t)) \times \underline{V}(\Gamma^h(t))$ for all $t \in [0, T]$, such that, for all $t \in (0, T]$, (9.33), (9.31) and (9.30) hold.

Remark 9.10.

- (i) Similarly to Remark 9.9(ii), using (9.31), one can eliminate κ^h from (9.33) and (9.30) in this semidiscrete finite element approximation.
- (ii) The scheme (9.33), (9.31) and (9.30) satisfies Theorem 5.3(iii).

We have the following stability result.

Theorem 9.11. Let $(\mathcal{G}_T^h, \kappa^h, \vec{Y}^h)$ be a solution of (9.33), (9.31) and (9.30), and let $\kappa^h \in V_T(\mathcal{G}_T^h)$. Then it holds that

$$\frac{d}{dt} \frac{1}{2} \left(|\kappa^h|_{\Gamma^h(t)}^h \right)^2 = - \left(|\vec{\mathcal{V}}^h \cdot \vec{\omega}^h|_{\Gamma^h(t)}^h \right)^2 \leq 0.$$

Proof. Similarly to (9.16), we extend test functions $\vec{\eta} \in \underline{V}(\Gamma^h(t))$ in (9.30) to $\vec{\eta} \in \underline{V}_T(\mathcal{G}_T^h)$ such that $\partial_t^{\circ, h} \vec{\eta} = \vec{0}$ on $\mathcal{G}_T^h$. Then taking the time derivative of (9.30), on noting Theorem 3.30 and Lemma 3.33(iii), yields

$$\begin{aligned} &\left\langle \partial_t^{\circ, h} \kappa^h, \vec{\nu}^h \cdot \vec{\eta} \right\rangle_{\Gamma^h(t)}^h + \left\langle \kappa^h \partial_t^{\circ, h} \vec{\nu}^h, \vec{\eta} \right\rangle_{\Gamma^h(t)}^h + \left\langle \kappa^h \vec{\nu}^h \cdot \vec{\eta}, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h \\ &\quad + \left\langle \nabla_s \cdot \vec{\mathcal{V}}^h, \nabla_s \cdot \vec{\eta} \right\rangle_{\Gamma^h(t)} + \left\langle \nabla_s \vec{\mathcal{V}}^h, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)} - 2 \left\langle \underline{D}_s(\vec{\mathcal{V}}^h), \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)} = 0. \end{aligned} \quad (9.34)$$

We now take $\vec{\eta} = \vec{Y}^h$ in (9.34) and $\vec{\chi} = \vec{\mathcal{V}}^h$ in (9.33), to obtain, on noting (9.31), (3.5) and Lemma 3.32, that

$$\left\langle \partial_t^{\circ, h} \kappa^h, \kappa^h \right\rangle_{\Gamma^h(t)}^h + \frac{1}{2} \left\langle |\kappa^h|^2, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \vec{\mathcal{V}}^h \cdot \vec{\omega}^h, \vec{\mathcal{V}}^h \cdot \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h = 0.$$

The desired result then follows on noting Theorem 3.30(ii) and (3.2). $\square$

We now state a fully discrete version of (9.33), (9.31) and (9.30), on recalling (3.5).

Let the closed polyhedral hypersurface Γ^0 be an approximation to $\Gamma(0)$, and let $\kappa_{\Gamma^0}^0 \in V(\Gamma^0)$ and $\vec{Y}_{\Gamma^0}^0 \in \underline{V}(\Gamma^0)$ be approximations to its mean curvature and mean curvature vector, respectively. We also recall the time interval partitioning (4.5). Then, for $m = 0, \dots, M-1$, find $(\vec{X}^{m+1}, \kappa^{m+1}, \vec{Y}^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m) \times \underline{V}(\Gamma^m)$ such that

$$\begin{aligned} & \left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m} \cdot \vec{\omega}^m, \vec{\chi} \cdot \vec{\omega}^m \right\rangle_{\Gamma^m}^h - \left\langle \nabla_s \vec{Y}^{m+1}, \nabla_s \vec{\chi} \right\rangle_{\Gamma^m} \\ &= - \left\langle \kappa_{\Gamma^m}^m \left(\frac{1}{2} \kappa_{\Gamma^m}^m - \vec{Y}_{\Gamma^m}^m \cdot \vec{\nu}^m \right), \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^m}^h - \left\langle \kappa_{\Gamma^m}^m \vec{Y}_{\Gamma^m}^m, (\nabla_s \vec{\chi})^\top \vec{\nu}^m \right\rangle_{\Gamma^m}^h \\ &+ \left\langle \nabla_s \cdot \vec{Y}_{\Gamma^m}^m, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^m} - 2 \left\langle \nabla_s \vec{Y}_{\Gamma^m}^m, \underline{D}_s(\vec{\chi}) \right\rangle_{\Gamma^m} \quad \forall \vec{\chi} \in \underline{V}(\Gamma^m), \end{aligned} \quad (9.35a)$$

$$\kappa^{m+1} = \pi_{\Gamma^m} \left[\vec{Y}^{m+1} \cdot \vec{\omega}^m \right], \quad (9.35b)$$

$$\left\langle \kappa^{m+1} \vec{\nu}^m, \vec{\eta} \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (9.35c)$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$, $\kappa_{\Gamma^{m+1}}^{m+1} = \kappa^{m+1} \circ (\vec{X}^{m+1})^{-1} \in V(\Gamma^{m+1})$ and $\vec{Y}_{\Gamma^{m+1}}^{m+1} = \vec{Y}^{m+1} \circ (\vec{X}^{m+1})^{-1} \in \underline{V}(\Gamma^{m+1})$. We have the following result.

Theorem 9.12. *Let Γ^m satisfy Assumption 3.24(i) and let $\kappa_{\Gamma^m}^m \in V(\Gamma^m)$ and $\vec{Y}_{\Gamma^m}^m \in \underline{V}(\Gamma^m)$. Then there exists a unique solution $(\vec{X}^{m+1}, \kappa^{m+1}, \vec{Y}^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m) \times \underline{V}(\Gamma^m)$ to (9.35).*

Proof. The proof is very similar to the proof of Theorem 5.1. We consider a solution $(\vec{X}, \kappa, \vec{Y}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m) \times \underline{V}(\Gamma^m)$ of the homogeneous system

$$\left\langle \vec{X} \cdot \vec{\omega}^m, \vec{\chi} \cdot \vec{\omega}^m \right\rangle_{\Gamma^m}^h - \Delta t_m \left\langle \nabla_s \vec{Y}, \nabla_s \vec{\chi} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\chi} \in \underline{V}(\Gamma^m), \quad (9.36a)$$

$$\kappa - \pi_{\Gamma^m} \left[\vec{Y} \cdot \vec{\omega}^m \right] = 0, \quad (9.36b)$$

$$\left\langle \kappa \vec{\nu}^m, \vec{\eta} \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m). \quad (9.36c)$$

Choosing $\vec{\chi} = \vec{Y} \in \underline{V}(\Gamma^m)$ in (9.36a) and $\vec{\eta} = \vec{X} \in \underline{V}(\Gamma^m)$ in (9.36c) yields, on noting (3.5) and (9.36b), that

$$\left| \nabla_s \vec{X} \right|_{\Gamma^m}^2 + \Delta t_m \left| \nabla_s \vec{Y} \right|_{\Gamma^m}^2 = 0.$$

We deduce from this that $\vec{X} = \vec{X}^c$ and $\vec{Y} = \vec{Y}^c$ on Γ^m , for $\vec{X}^c, \vec{Y}^c \in \mathbb{R}^d$. Hence, on substituting (9.36b) into (9.36c), it follows from (9.36) and (3.5) that

$$\left(\left| \vec{X}^c \cdot \vec{\omega}^m \right|_{\Gamma^m}^h \right)^2 + \left(\left| \vec{Y}^c \cdot \vec{\omega}^m \right|_{\Gamma^m}^h \right)^2 = 0,$$

i.e. $\vec{X}^c \cdot \vec{\omega}^m = \vec{Y}^c \cdot \vec{\omega}^m = 0$. Therefore Assumption 3.24(i) yields that $\vec{X}^c = \vec{Y}^c = \vec{0}$, and hence $\kappa = 0$. $\square$

Remark 9.13 (Stability). *Unfortunately, it does not seem possible to prove a stability bound for the fully discrete scheme (9.35) or its generalizations. A similar comment applies to a fully discrete approximation of the Dziuk scheme (9.15).*

Remark 9.14 (Discrete linear systems). *On recalling the notation from §4.3, we can formulate the linear systems of equations to be solved at each time level for (9.35) as follows. Find $(\vec{Y}^{m+1}, \kappa^{m+1}, \delta \vec{X}^{m+1}) \in (\mathbb{R}^d)^K \times \mathbb{R}^K \times (\mathbb{R}^d)^K$ such that*

$$\begin{pmatrix} \underline{A}_{\Gamma^m} & 0 & -\frac{1}{\Delta t_m} \underline{M}_{\Gamma^m} \\ -\vec{N}_{\Gamma^m}^\top & M_{\Gamma^m} & 0 \\ 0 & \vec{N}_{\Gamma^m} & \underline{A}_{\Gamma^m} \end{pmatrix} \begin{pmatrix} \vec{Y}^{m+1} \\ \kappa^{m+1} \\ \delta \vec{X}^{m+1} \end{pmatrix} = \begin{pmatrix} \vec{g}_{\Gamma^m} \\ 0 \\ -\underline{A}_{\Gamma^m} \vec{X}^m \end{pmatrix}, \quad (9.37)$$

where we use a similar abuse of notation as in (4.11). The definitions of the matrices and vectors in (9.37) are either given in (4.10), or they follow directly from (9.35). In practice, the linear system (9.37) can be efficiently solved with a sparse direct solution method like UMFPACK, see Davis (2004).

9.4 Willmore flow with spontaneous curvature and area difference elasticity effects

Curvature energies also play an important role for vesicles and biomembranes. As in many membrane elastic energies, the curvature of the membrane enters the elastic energy density. However, for biomembranes, additional effects play a role, which we would like to discuss now. In the original curvature energies for biomembranes a possible asymmetry of the membrane in the normal direction was taken into account, which can result, for example, from a different chemical environment on the two sides of the membrane. This top-down asymmetry makes it necessary to generalize the Willmore energy, and one example of such a model is the spontaneous curvature model introduced by Canham (1970) and Helfrich (1973). The simplest such energy, in a nondimensional form, is

$$E_{\overline{\kappa}}(\Gamma) = \frac{1}{2} \int_{\Gamma} (\kappa - \overline{\kappa})^2 \, d\mathcal{H}^{d-1},$$

where $\overline{\kappa} \in \mathbb{R}$ is the given so-called spontaneous curvature. Biomembranes consist of two layers of lipids, and the number of lipid molecules is conserved. In addition, there are osmotic pressure effects, arising from the chemistry around the lipid. These two effects lead to constraints on the possible membrane configurations. Early models for bilayer membranes modelled this by taking hard constraints on the total surface area and the enclosed volume of the membrane into account. The fact that it is difficult to exchange molecules between the two layers imply that the total number of lipids in each layer is conserved, and hence a surface area difference between the two layers will appear. The area difference is to first order given by the total integrated mean curvature. This follows from the first variation formula for surface area, recall (4.1). Different models incorporate this area difference either by a hard constraint or penalize deviations from an optimal

area difference. In the latter case, we obtain the energy

$$E_{\bar{\kappa},\beta}(\Gamma) = E_{\bar{\kappa}}(\Gamma) + \frac{1}{2} \beta (\langle \kappa, 1 \rangle_{\Gamma} - M_0)^2 \quad (9.38)$$

with given constants $\beta \in \mathbb{R}_{\geq 0}$, $M_0 \in \mathbb{R}$. A model based on the energy (9.38) is called an area difference elasticity (ADE) model, see Seifert (1997). We now extend Lemma 9.1 to $E_{\bar{\kappa},\beta}(\Gamma(t))$, where for notational convenience we define

$$A(t) = \langle \kappa, 1 \rangle_{\Gamma(t)} - M_0. \quad (9.39)$$

Lemma 9.15. *Let $\mathcal{G}_T$ be a closed C^4 -evolving orientable hypersurface. Then it holds that*

$$\begin{aligned} \frac{d}{dt} E_{\bar{\kappa},\beta}(\Gamma(t)) \\ = \langle \Delta_s \kappa + (\kappa - \bar{\kappa}) |\nabla_s \vec{\nu}|^2 - \frac{1}{2} (\kappa - \bar{\kappa})^2 \kappa + \beta A(t) (|\nabla_s \vec{\nu}|^2 - \kappa^2), \mathcal{V} \rangle_{\Gamma(t)}. \end{aligned}$$

Proof. Generalising (9.1) to $E_{\bar{\kappa}}(\Gamma(t))$ yields that

$$\begin{aligned} \frac{d}{dt} E_{\bar{\kappa}}(\Gamma(t)) &= \langle \kappa - \bar{\kappa}, \partial_t^\square \kappa - \frac{1}{2} (\kappa - \bar{\kappa}) \kappa \mathcal{V} \rangle_{\Gamma(t)} \\ &= \langle \kappa - \bar{\kappa}, \Delta_s \mathcal{V} + \mathcal{V} |\nabla_s \vec{\nu}|^2 - \frac{1}{2} (\kappa - \bar{\kappa}) \kappa \mathcal{V} \rangle_{\Gamma(t)} \\ &= \langle \Delta_s \kappa + (\kappa - \bar{\kappa}) |\nabla_s \vec{\nu}|^2 - \frac{1}{2} (\kappa - \bar{\kappa})^2 \kappa, \mathcal{V} \rangle_{\Gamma(t)}. \end{aligned} \quad (9.40)$$

Next, we compute, on recalling Theorem 2.32 and Lemma 2.39(ii), that

$$\begin{aligned} \frac{d}{dt} \left[\frac{1}{2} (\langle \kappa, 1 \rangle_{\Gamma(t)} - M_0)^2 \right] &= A(t) \frac{d}{dt} \langle \kappa, 1 \rangle_{\Gamma(t)} = A(t) \langle \partial_t^\square \kappa - \kappa^2 \mathcal{V}, 1 \rangle_{\Gamma(t)} \\ &= A(t) \langle |\nabla_s \vec{\nu}|^2 - \kappa^2, \mathcal{V} \rangle_{\Gamma(t)}. \end{aligned}$$

Combining the above with (9.40) yields the claim, on noting (9.38). $\square$

Hence the L^2 -gradient flow of $E_{\bar{\kappa},\beta}(\Gamma(t))$, (9.38), is given as

$$\mathcal{V} = -\Delta_s \kappa - (\kappa - \bar{\kappa}) |\nabla_s \vec{\nu}|^2 + \frac{1}{2} (\kappa - \bar{\kappa})^2 \kappa - \beta A(t) (|\nabla_s \vec{\nu}|^2 - \kappa^2) \quad \text{on } \Gamma(t). \quad (9.41)$$

Taking our discussion above into account, the volume preserving and surface area preserving flows are also of interest. In the case $\beta = 0$, the volume and surface area preserving flow is called Helfrich flow. We consider the two side constraints

$$\langle \kappa, \mathcal{V} \rangle_{\Gamma(t)} = 0 \quad \text{and} \quad \langle 1, \mathcal{V} \rangle_{\Gamma(t)} = 0 \quad (9.42)$$

for surface area and volume preservation, where we have recalled Theorem 2.32 and Theorem 2.33, respectively. In particular, we introduce Lagrange multipliers $(\lambda_A(t), \lambda_V(t))^T \in \mathbb{R}^2$ and then, on writing (9.41) as $\mathcal{V} = f$, we adapt (9.41) to

$$\mathcal{V} = f + \lambda_A \kappa + \lambda_V \quad \text{on } \Gamma(t). \quad (9.43)$$

We see that the constraints (9.42) are satisfied if $(\lambda_A(t), \lambda_V(t))^T \in \mathbb{R}^2$ solve the symmetric system

$$\begin{pmatrix} \langle \varkappa, \varkappa \rangle_{\Gamma(t)} & \langle \varkappa, 1 \rangle_{\Gamma(t)} \\ \langle \varkappa, 1 \rangle_{\Gamma(t)} & \langle 1, 1 \rangle_{\Gamma(t)} \end{pmatrix} \begin{pmatrix} \lambda_A \\ \lambda_V \end{pmatrix} = - \begin{pmatrix} \langle f, \varkappa \rangle_{\Gamma(t)} \\ \langle f, 1 \rangle_{\Gamma(t)} \end{pmatrix}. \quad (9.44)$$

We observe that the matrix in (9.44) is symmetric positive semidefinite, and it is singular if and only if $\varkappa$ is constant, i.e. $\Gamma(t)$ is sphere. In the case of just one constraint, the Lagrange multiplier corresponding to the other constraint is set to zero and the corresponding equation is removed from (9.44). Equivalently to (9.44), in the two constraint case and on assuming that $\varkappa$ is not constant, $\lambda_A = - \langle f, \varkappa - f_{\Gamma(t)} \varkappa \rangle_{\Gamma(t)} / |\varkappa - f_{\Gamma(t)} \varkappa|_{\Gamma(t)}^2$ and λ_V is obtained from the second equation in (9.44). Here, we have recalled the definition of $f_{\Gamma(t)} \varkappa$ from (5.15).

The corresponding changes to the finite element approximation (9.4) is to replace (9.4a) by

$$\begin{aligned} & \left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \chi \vec{\nu}^m \right\rangle_{\Gamma^m}^h - \langle \nabla_s \kappa^{m+1}, \nabla_s \chi \rangle_{\Gamma^m} - \frac{1}{2} \langle (\kappa_{\Gamma^m}^m - \bar{\varkappa})^2 \kappa^{m+1}, \chi \rangle_{\Gamma^m}^h \\ & \quad - [\lambda_A^m]_+ \langle \kappa^{m+1}, \chi \rangle_{\Gamma^m}^h \\ & = \langle g^m, \chi \rangle_{\Gamma^m}^h + [\lambda_A^m]_- \langle \kappa_{\Gamma^m}^m, \chi \rangle_{\Gamma^m}^h + \lambda_V^m \langle 1, \chi \rangle_{\Gamma^m}^h \quad \forall \chi \in V(\Gamma^m), \end{aligned} \quad (9.45)$$

where $g^m \in V(\Gamma^m)$ is such that

$$\begin{aligned} \langle g^m, \chi \rangle_{\Gamma^m}^h & = - \langle (\kappa_{\Gamma^m}^m - \bar{\varkappa}) |\underline{W}^{m+1}|^2, \chi \rangle_{\Gamma^m}^h - \beta A^m \langle |\underline{W}^{m+1}|^2 - (\kappa_{\Gamma^m}^m)^2, \chi \rangle_{\Gamma^m}^h \\ & \quad \forall \chi \in V(\Gamma^m), \end{aligned}$$

$$A^m = \langle \kappa_{\Gamma^m}^m, 1 \rangle_{\Gamma^m}^h - M_0.$$

In addition, $[\lambda_A^m]_{\pm} = \pm \max\{\pm \lambda_A^m, 0\}$ and the Lagrange multipliers $(\lambda_A^m, \lambda_V^m)^T \in \mathbb{R}^2$ satisfy the symmetric system

$$\begin{aligned} & \begin{pmatrix} \langle \kappa_{\Gamma^m}^m, \kappa_{\Gamma^m}^m \rangle_{\Gamma^m}^h & \langle \kappa_{\Gamma^m}^m, 1 \rangle_{\Gamma^m} \\ \langle \kappa_{\Gamma^m}^m, 1 \rangle_{\Gamma^m} & \langle 1, 1 \rangle_{\Gamma^m} \end{pmatrix} \begin{pmatrix} \lambda_A^m \\ \lambda_V^m \end{pmatrix} \\ & = - \begin{pmatrix} \langle g^m + \frac{1}{2} (\kappa_{\Gamma^m}^m - \bar{\varkappa})^2 \kappa_{\Gamma^m}^m, \kappa_{\Gamma^m}^m \rangle_{\Gamma^m}^h + |\nabla_s \kappa_{\Gamma^m}^m|_{\Gamma^m}^2 \\ \langle g^m + \frac{1}{2} (\kappa_{\Gamma^m}^m - \bar{\varkappa})^2 \kappa_{\Gamma^m}^m, 1 \rangle_{\Gamma^m}^h \end{pmatrix}. \end{aligned} \quad (9.46)$$

Once again, we observe that the matrix in (9.46) is symmetric positive semidefinite, and it is singular if and only if $\kappa_{\Gamma^m}^m$ is constant. Similarly, in the case of just one constraint, the Lagrange multiplier corresponding to the other constraint is set to zero and the corresponding equation removed from (9.46). Moreover, this modified scheme satisfies the suitably modified versions of Theorem 9.2 and Remark 9.3; see Barrett et al. (2008d) for details.

We now discuss generalizations of the stable approximations of Willmore flow in §9.3 to the case of Willmore flow with spontaneous curvature and area difference effects. In

Barrett et al. (2016b), the present authors extended the approach of Dziuk (2008), see (9.15), to the case of nonzero $\bar{\kappa}$ and β .

First of all, we consider the variation of $E_{\bar{\kappa},\beta}(\Gamma(t))$ subject to the side constraint (9.8). Similarly to (9.18), we introduce the Lagrangian

$$\begin{aligned} \widehat{L}_{\bar{\kappa},\beta}(\Gamma(t), \bar{\kappa}^*, \vec{y}) &= \frac{1}{2} \langle |\bar{\kappa}^* - \bar{\kappa} \vec{\nu}|^2, 1 \rangle_{\Gamma(t)} + \frac{1}{2} \beta \left(\langle \bar{\kappa}^*, \vec{\nu} \rangle_{\Gamma(t)} - M_0 \right)^2 \\ &\quad - \langle \bar{\kappa}^*, \vec{y} \rangle_{\Gamma(t)} - \left\langle \nabla_s \text{id}, \nabla_s \vec{y} \right\rangle_{\Gamma(t)}, \end{aligned}$$

where $\vec{y}(\cdot, t) \in [H^1(\Gamma(t))]^d$ is the Lagrange multiplier for (9.8) with $\bar{\kappa}(\cdot, t) \in [L^2(\Gamma(t))]^d$ replaced by $\bar{\kappa}^*(\cdot, t) \in [L^2(\Gamma(t))]^d$. As in (9.26), we consider the variations, for all $\vec{\chi} \in [H^1(\Gamma(t))]^d$, $\vec{\xi} \in [L^2(\Gamma(t))]^d$ and $\vec{\eta} \in [H^1(\Gamma(t))]^d$,

$$\begin{aligned} \left[\frac{\delta}{\delta \Gamma} \widehat{L}_{\bar{\kappa},\beta} \right] (\vec{\chi}) &= \left(\frac{d}{d\varepsilon} \widehat{L}_{\bar{\kappa},\beta}(\Gamma_\varepsilon(t), \bar{\kappa}_{(\varepsilon)}^*, \vec{y}_{(\varepsilon)}) \right)_{\big|_{\varepsilon=0}}, \\ \left[\frac{\delta}{\delta \bar{\kappa}^*} \widehat{L}_{\bar{\kappa},\beta} \right] (\vec{\xi}) &= \left(\frac{d}{d\varepsilon} \widehat{L}_{\bar{\kappa},\beta}(\Gamma(t), \bar{\kappa}^* + \varepsilon \vec{\xi}, \vec{y}) \right)_{\big|_{\varepsilon=0}}, \\ \left[\frac{\delta}{\delta \vec{y}} \widehat{L}_{\bar{\kappa},\beta} \right] (\vec{\eta}) &= \left(\frac{d}{d\varepsilon} \widehat{L}_{\bar{\kappa},\beta}(\Gamma(t), \bar{\kappa}^*, \vec{y} + \varepsilon \vec{\eta}) \right)_{\big|_{\varepsilon=0}}, \end{aligned}$$

where $\bar{\kappa}_{(\varepsilon)}^*(\cdot, t), \vec{y}_{(\varepsilon)}(\cdot, t) \in [H^1(\Gamma_\varepsilon(t))]^d$ are defined by transporting the values of $\bar{\kappa}^*$ and $\vec{y}$ as in (9.24). Setting $\left[\frac{\delta}{\delta \vec{y}} \widehat{L}_{\bar{\kappa},\beta} \right] (\vec{\eta}) = 0$ and comparing with (9.8) leads to $\bar{\kappa}^* = \bar{\kappa}$. Moreover, on setting $\left[\frac{\delta}{\delta \bar{\kappa}^*} \widehat{L}_{\bar{\kappa},\beta} \right] (\vec{\xi}) = 0$ and $\langle \vec{\nu}, \vec{\chi} \rangle_{\Gamma(t)} = - \left[\frac{\delta}{\delta \Gamma} \widehat{L}_{\bar{\kappa},\beta} \right] (\vec{\chi})$, we obtain, on noting (9.22), (9.23) and (9.25), the following weak formulation of $\vec{\nu} = f \vec{\nu}$ and Lemma 2.13(ii), where f is the right hand side of (9.41); recall Remark 9.8(ii) in the absence of spontaneous curvature and ADE effects. Given a closed hypersurface $\Gamma(0)$, we seek an evolving hypersurface $(\Gamma(t))_{t \in [0, T]}$, with a global parameterization and induced velocity field $\vec{\nu}$, $\bar{\kappa} \in [L^2(\mathcal{G}_T)]^d$ and $\vec{y} \in [L^2(\mathcal{G}_T)]^d$ as follows. For almost all $t \in (0, T)$, find $(\vec{\nu}(\cdot, t), \bar{\kappa}(\cdot, t), \vec{y}(\cdot, t)) \in [L^2(\Gamma(t))]^d \times [L^2(\Gamma(t))]^d \times [H^1(\Gamma(t))]^d$ such that

$$\begin{aligned} \langle \vec{\nu}, \vec{\chi} \rangle_{\Gamma(t)} &= \langle \nabla_s \vec{y}, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \rangle_{\Gamma(t)} + \langle \nabla_s \cdot \vec{y}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\ &\quad - \left\langle \frac{1}{2} |\bar{\kappa} - \bar{\kappa} \vec{\nu}|^2 - \bar{\kappa} \cdot (\vec{y} - \beta A(t) \vec{\nu}), \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma(t)} \\ &\quad + (\beta A(t) - \bar{\kappa}) \langle \bar{\kappa}, (\nabla_s \vec{\chi})^\top \vec{\nu} \rangle_{\Gamma(t)} \quad \forall \vec{\chi} \in [H^1(\Gamma(t))]^d, \end{aligned} \quad (9.47a)$$

$$\langle \bar{\kappa} + (\beta A(t) - \bar{\kappa}) \vec{\nu} - \vec{y}, \vec{\xi} \rangle_{\Gamma(t)} = 0 \quad \forall \vec{\xi} \in [L^2(\Gamma(t))]^d, \quad (9.47b)$$

$$\langle \bar{\kappa}, \vec{\eta} \rangle_{\Gamma(t)} + \langle \nabla_s \text{id}, \nabla_s \vec{\eta} \rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d \quad (9.47c)$$

with

$$A(t) = \langle \bar{\kappa}, \vec{\nu} \rangle_{\Gamma(t)} - M_0. \quad (9.47d)$$

We note that if $\bar{\kappa} = \beta = 0$ then $\vec{y} = \vec{\kappa}$, and so the system (9.47) reduces to (9.11).

We now introduce a semidiscrete variant of (9.47) with the help of the first variation of the discrete energy

$$E_{\bar{\kappa},\beta}^h(\Gamma^h(t)) = \frac{1}{2} \left\langle |\vec{\kappa}^h - \bar{\kappa} \vec{\nu}^h|^2, 1 \right\rangle_{\Gamma^h(t)}^h + \frac{1}{2} \beta \left(\left\langle \vec{\kappa}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)} - M_0 \right)^2 \quad (9.48)$$

subject to the side constraint (9.15b). Hence, we define the Lagrangian

$$\widehat{L}_{\bar{\kappa},\beta}^h(\Gamma^h(t), \vec{\kappa}^h, \vec{Y}^h) = E_{\bar{\kappa},\beta}^h(\Gamma^h(t)) - \left\langle \vec{\kappa}^h, \vec{Y}^h \right\rangle_{\Gamma^h(t)}^h - \left\langle \nabla_s \text{id}, \nabla_s \vec{Y}^h \right\rangle_{\Gamma^h(t)},$$

where $\vec{Y}^h(\cdot, t) \in \underline{V}(\Gamma^h(t))$ is the Lagrange multiplier for (9.15b). Similarly to (9.29), we set $\left[\frac{\delta}{\delta \Gamma^h} \widehat{L}_{\bar{\kappa},\beta}^h \right](\vec{\chi}) = -\langle \vec{\nu}^h, \vec{\chi} \rangle_{\Gamma^h(t)}$ for $\vec{\chi} \in \underline{V}(\Gamma^h(t))$, $\left[\frac{\delta}{\delta \vec{\kappa}^h} \widehat{L}_{\bar{\kappa},\beta}^h \right](\vec{\xi}) = 0$ for $\vec{\xi} \in \underline{V}(\Gamma^h(t))$ and $\left[\frac{\delta}{\delta \vec{Y}^h} \widehat{L}_{\bar{\kappa},\beta}^h \right](\vec{\eta}) = 0$ for $\vec{\eta} \in \underline{V}(\Gamma^h(t))$. Therefore, on noting the analogue of (9.32), the discrete analogue of (9.23) for $\vec{\nu}^h$ on $\Gamma^h(t)$ and (9.25) for $\Gamma^h(t)$, we have the following semidiscrete finite element approximation of (9.47). Given the closed polyhedral hypersurface $\Gamma^h(0)$, find an evolving polyhedral hypersurface $\mathcal{G}_T^h$ with induced velocity $\vec{\nu}^h \in \underline{V}(\mathcal{G}_T^h)$, $\vec{\kappa}^h \in \underline{V}(\mathcal{G}_T^h)$ and $\vec{Y}^h \in \underline{V}(\mathcal{G}_T^h)$ as follows. For all $t \in (0, T]$, find $(\vec{\nu}^h(\cdot, t), \vec{\kappa}^h(\cdot, t), \vec{Y}^h(\cdot, t)) \in \underline{V}(\Gamma^h(t)) \times \underline{V}(\Gamma^h(t)) \times \underline{V}(\Gamma^h(t))$ such that

$$\begin{aligned} \left\langle \vec{\nu}^h, \vec{\chi} \right\rangle_{\Gamma^h(t)}^h &= \left\langle \nabla_s \vec{Y}^h, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \right\rangle_{\Gamma^h(t)} + \left\langle \nabla_s \cdot \vec{Y}^h, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^h(t)} \\ &\quad - \left\langle \frac{1}{2} |\vec{\kappa}^h - \bar{\kappa} \vec{\nu}^h|^2 - \vec{\kappa}^h \cdot (\vec{Y}^h - \beta A^h(t) \vec{\nu}^h), \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^h(t)}^h \\ &\quad + (\beta A^h(t) - \bar{\kappa}) \left\langle \vec{\kappa}^h, (\nabla_s \vec{\chi})^\top \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\chi} \in \underline{V}(\Gamma^h(t)), \end{aligned} \quad (9.49a)$$

$$\left\langle \vec{\kappa}^h + (\beta A^h(t) - \bar{\kappa}) \vec{\nu}^h - \vec{Y}^h, \vec{\xi} \right\rangle_{\Gamma^h(t)}^h = 0 \quad \forall \vec{\xi} \in \underline{V}(\Gamma^h(t)), \quad (9.49b)$$

$$\left\langle \vec{\kappa}^h, \vec{\eta} \right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)}^h = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h(t)), \quad (9.49c)$$

where

$$A^h(t) = \left\langle \vec{\kappa}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h - M_0. \quad (9.49d)$$

We note that (9.49b) and (3.5) imply that $\vec{\kappa}^h + (\beta A^h(t) - \bar{\kappa}) \vec{\nu}^h = \vec{Y}^h$ on $\Gamma^h(t)$. Of course, $\vec{\kappa}^h$ can be eliminated from (9.49).

We now prove the analogue of Theorem 9.7 for the semidiscrete scheme (9.49).

Theorem 9.16. *Let $(\mathcal{G}_T^h, \vec{\kappa}^h, \vec{Y}^h)$ be a solution of (9.49), and let $\vec{\kappa}^h \in \underline{V}_T(\mathcal{G}_T^h)$. Then it follows that*

$$\frac{d}{dt} E_{\bar{\kappa},\beta}^h(\Gamma^h(t)) = - \left(\left| \vec{\nu}^h \right|_{\Gamma^h(t)}^h \right)^2 \leq 0. \quad (9.50)$$

Proof. As in the proof of Theorem 9.7, on taking the derivative with respect to t of (9.49c) we obtain (9.16). Choosing $\vec{\eta} = \vec{Y}^h$ in (9.16) leads to

$$\begin{aligned} & \left\langle \partial_t^{\circ, h} \vec{\kappa}^h, \vec{Y}^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \vec{\kappa}^h \cdot \vec{Y}^h, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s \cdot \vec{\mathcal{V}}^h, \nabla_s \cdot \vec{Y}^h \right\rangle_{\Gamma^h(t)} \\ & + \left\langle \nabla_s \vec{\mathcal{V}}^h, \nabla_s \vec{Y}^h \right\rangle_{\Gamma^h(t)} - 2 \left\langle \underline{D}_s(\vec{\mathcal{V}}^h), \nabla_s \vec{Y}^h \right\rangle_{\Gamma^h(t)} = 0. \end{aligned} \quad (9.51)$$

Combining (9.49a) with $\vec{\chi} = \vec{\mathcal{V}}^h$ and (9.51), we obtain, on noting Lemma 3.32 and (9.49b), that

$$\begin{aligned} & \left\langle \vec{\mathcal{V}}^h, \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \frac{1}{2} |\vec{\kappa}^h - \bar{\kappa} \vec{\nu}^h|^2 + \beta A^h(t) \vec{\kappa}^h \cdot \vec{\nu}^h, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h \\ & + (\beta A^h(t) - \bar{\kappa}) \left\langle \vec{\kappa}^h, \partial_t^{\circ, h} \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h \\ & = - \left\langle \partial_t^{\circ, h} \vec{\kappa}^h, \vec{Y}^h \right\rangle_{\Gamma^h(t)}^h = - \left\langle \partial_t^{\circ, h} \vec{\kappa}^h, \vec{\kappa}^h + (\beta A^h(t) - \bar{\kappa}) \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h. \end{aligned} \quad (9.52)$$

The desired result (9.50) then follows from (9.52), (9.48), (3.2), Theorem 3.30 and (9.49d), where we have observed that

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \left(\left\langle \vec{\kappa}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h - M_0 \right)^2 \\ & = A^h(t) \left[\left\langle \partial_t^{\circ, h} \vec{\kappa}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \vec{\kappa}^h, \partial_t^{\circ, h} \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \vec{\kappa}^h \cdot \vec{\nu}^h, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h \right]. \end{aligned}$$

□

We now state a fully discrete variant of the semidiscrete scheme (9.49). Let the closed polyhedral hypersurface Γ^0 be an approximation to $\Gamma(0)$, and let $\vec{\kappa}_{\Gamma^0}^0, \vec{Y}_{\Gamma^0}^0 \in \underline{V}(\Gamma^0)$ and $A^0 \in \mathbb{R}$ be given. Then, for $m = 0, \dots, M-1$, find $(\vec{X}^{m+1}, \vec{\kappa}^{m+1}, \vec{Y}^{m+1}) \in \underline{V}(\Gamma^m) \times \underline{V}(\Gamma^m) \times \underline{V}(\Gamma^m)$ such that

$$\begin{aligned} \left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \vec{\eta} \right\rangle_{\Gamma^m} &= \left\langle \nabla_s \vec{Y}^{m+1}, \nabla_s \vec{\chi} \right\rangle_{\Gamma^m} + \left\langle \nabla_s \cdot \vec{Y}_{\Gamma^m}^m, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^m} \\ &- 2 \left\langle \nabla_s \vec{Y}_{\Gamma^m}^m, \underline{D}_s(\vec{\chi}) \right\rangle_{\Gamma^m} + (\beta A^m - \bar{\kappa}) \left\langle \vec{\kappa}_{\Gamma^m}^m, (\nabla_s \vec{\chi})^\top \vec{\nu}^m \right\rangle_{\Gamma^m}^h \\ &- \left\langle \frac{1}{2} |\vec{\kappa}_{\Gamma^m}^m - \bar{\kappa} \vec{\nu}^m|^2 - \vec{\kappa}_{\Gamma^m}^m \cdot (\vec{Y}_{\Gamma^m}^m - \beta A^m \vec{\nu}^m), \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^m}^h \\ &\quad \forall \vec{\chi} \in \underline{V}(\Gamma^m), \end{aligned} \quad (9.53a)$$

$$\vec{\kappa}^{m+1} = \vec{Y}^{m+1} - (\beta A^m - \bar{\kappa}) \vec{\omega}^m, \quad (9.53b)$$

$$\left\langle \vec{\kappa}^{m+1}, \vec{\eta} \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m) \quad (9.53c)$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$, $A^{m+1} = \langle \vec{\kappa}^{m+1}, \vec{\nu}^m \rangle_{\Gamma^m} - M_0$, $\vec{\kappa}_{\Gamma^{m+1}}^{m+1} = \vec{\kappa}^{m+1} \circ (\vec{X}^{m+1})^{-1} \in \underline{V}(\Gamma^{m+1})$ and $\vec{Y}_{\Gamma^{m+1}}^{m+1} = \vec{Y}^{m+1} \circ (\vec{X}^{m+1})^{-1} \in \underline{V}(\Gamma^{m+1})$. Of course, $\vec{\kappa}^{m+1}$ can be eliminated from (9.53).

Theorem 9.17. *Let $\vec{\kappa}_{\Gamma^m}^m, \vec{Y}_{\Gamma^m}^m \in \underline{V}(\Gamma^m)$ and $A^m \in \mathbb{R}$. Then there exists a unique solution $(\vec{X}^{m+1}, \vec{\kappa}^{m+1}, \vec{Y}^{m+1}) \in \underline{V}(\Gamma^m) \times \underline{V}(\Gamma^m) \times \underline{V}(\Gamma^m)$ to (9.53).*

Proof. It is a simple matter to adapt the proof of Theorem 9.12. $\square$

Remark 9.18 (Discrete linear systems). *Similarly to Remark 9.14, the linear systems of equations to be solved at each time level for (9.53) can be formulated as follows. Find $(\vec{Y}^{m+1}, \vec{\kappa}^{m+1}, \delta \vec{X}^{m+1}) \in (\mathbb{R}^d)^K \times (\mathbb{R}^d)^K \times (\mathbb{R}^d)^K$ such that*

$$\begin{pmatrix} \underline{A}_{\Gamma^m} & 0 & -\frac{1}{\Delta t_m} \underline{M}_{\Gamma^m} \\ -\underline{M}_{\Gamma^m} & \underline{M}_{\Gamma^m} & 0 \\ 0 & \underline{M}_{\Gamma^m} & \underline{A}_{\Gamma^m} \end{pmatrix} \begin{pmatrix} \vec{Y}^{m+1} \\ \vec{\kappa}^{m+1} \\ \delta \vec{X}^{m+1} \end{pmatrix} = \begin{pmatrix} \vec{g}_{\Gamma^m} \\ -(\beta A^m - \bar{\kappa}) \underline{M}_{\Gamma^m} \vec{\omega}^m \\ -\underline{A}_{\Gamma^m} \vec{X}^m \end{pmatrix},$$

and this system can be efficiently solved with a sparse direct solution method like UMF-PACK, see Davis (2004).

Similarly to Remark 9.8(ii), the semidiscrete scheme (9.49) and its fully discrete version (9.53) do not have good mesh properties. In order to obtain a scheme with good mesh properties, we extend the semidiscrete approximation (9.33), (9.31) and (9.30) to take into account spontaneous curvature and ADE effects. First, we extend the weak formulation (9.28), (9.27) and (9.17) to include spontaneous curvature and ADE effects. In order to do so, we extend the Lagrangian (9.18) to

$$\begin{aligned} L_{\bar{\kappa}, \beta}(\Gamma(t), \kappa^*, \vec{y}) &= \frac{1}{2} \langle \kappa^* - \bar{\kappa}, \kappa^* - \bar{\kappa} \rangle_{\Gamma(t)} + \frac{1}{2} \beta \left(\langle \kappa^*, 1 \rangle_{\Gamma(t)} - M_0 \right)^2 \\ &\quad - \langle \kappa^* \vec{\nu}, \vec{y} \rangle_{\Gamma(t)} - \left\langle \nabla_s \text{id}, \nabla_s \vec{y} \right\rangle_{\Gamma(t)}. \end{aligned} \quad (9.54)$$

Once again, setting the variation $\left[\frac{\delta}{\delta \vec{y}} L_{\bar{\kappa}, \beta} \right](\vec{\eta}) = 0$, yields (9.17) with κ replaced by κ^* , and so $\kappa^* = \kappa$. Setting $\left[\frac{\delta}{\delta \kappa^*} L_{\bar{\kappa}, \beta} \right](\xi) = 0$, yields, on noting $\kappa^* = \kappa$ and (9.39), that

$$\kappa - \bar{\kappa} = \vec{y} \cdot \vec{\nu} - \beta A(t) \quad \text{on } \Gamma(t). \quad (9.55)$$

Finally, on setting the variation $\left[\frac{\delta}{\delta \vec{\chi}} L_{\bar{\kappa}, \beta} \right](\vec{\chi}) = -\left\langle \vec{\nu} \cdot \vec{\nu}, \vec{\chi} \cdot \vec{\nu} \right\rangle_{\Gamma(t)}$ and noting (9.22), (9.23), (9.25) and that $\kappa^* = \kappa$, we obtain

$$\begin{aligned} \left\langle \vec{\nu} \cdot \vec{\nu}, \vec{\chi} \cdot \vec{\nu} \right\rangle_{\Gamma(t)} &= \langle \nabla_s \vec{y}, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \rangle_{\Gamma(t)} + \langle \nabla_s \cdot \vec{y}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\ &\quad - \left\langle \frac{1}{2} (\kappa - \bar{\kappa})^2 - \kappa (\vec{y} \cdot \vec{\nu} - \beta A(t)), \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma(t)} \\ &\quad - \langle \kappa \vec{y}, (\nabla_s \vec{\chi})^\top \vec{\nu} \rangle_{\Gamma(t)} \quad \forall \vec{\chi} \in [H^1(\Gamma(t))]^d. \end{aligned} \quad (9.56)$$

Therefore we have the following weak formulation. Given a closed hypersurface $\Gamma(0)$, we seek an evolving hypersurface $(\Gamma(t))_{t \in [0, T]}$, with a global parameterization and induced velocity field $\vec{\mathcal{V}}$, $\kappa \in L^2(\mathcal{G}_T)$ and $\vec{y} \in [L^2(\mathcal{G}_T)]^d$ as follows. For almost all $t \in (0, T)$, find

$(\vec{\mathcal{V}}(\cdot, t), \varkappa(\cdot, t), \vec{y}(\cdot, t)) \in [L^2(\Gamma(t))]^d \times L^2(\Gamma(t)) \times [H^1(\Gamma(t))]^d$ such that (9.56), (9.55) and (9.17) hold.

Once again, a remark equivalent to Remark 9.9 for this weak formulation holds. In addition, one can extend the semidiscrete finite element approximation (9.33), (9.31) and (9.30) to approximate the weak formulation (9.56), (9.55) and (9.17). Moreover, one can extend Remark 9.10 and Theorem 9.11 to this approximation. Furthermore, one can also incorporate volume and surface area constraints and still prove stability of the approximation.

In Barrett et al. (2016b), we considered an extension of the semidiscrete approximation (9.33), (9.31) and (9.30), and its extension to incorporate spontaneous curvature and ADE effects, which possibly reduces the tangential motion. This is based on the Lagrangian

$$\widehat{L}_{\vec{\kappa}, \beta, \theta}^h(\Gamma^h(t), \vec{\kappa}^h, \vec{Y}^h) = E_{\vec{\kappa}, \beta}^h(\Gamma^h(t)) - \left\langle \underline{Q}_{\theta}^h \vec{\kappa}^h, \vec{Y}^h \right\rangle_{\Gamma^h(t)}^h - \left\langle \nabla_s \text{id}, \nabla_s \vec{Y}^h \right\rangle_{\Gamma^h(t)}, \quad (9.57)$$

where $\vec{Y}^h(\cdot, t) \in \underline{V}(\Gamma^h(t))$ is the Lagrange multiplier associated with the constraint $\vec{\kappa}^h(\cdot, t) \in \underline{V}(\Gamma^h(t))$ satisfying

$$\left\langle \underline{Q}_{\theta}^h \vec{\kappa}^h, \vec{\eta} \right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h(t)). \quad (9.58)$$

Here, $\underline{Q}_{\theta}^h$, for a given $\theta \in [0, 1]$, is the semidiscrete version of (5.24), where $\vec{\omega}^m$ is replaced by $\vec{\omega}^h$, and where we assume that Assumption 3.24(ii) holds.

Setting $\left[\frac{\delta}{\delta \vec{Y}^h} \widehat{L}_{\vec{\kappa}, \beta, \theta}^h \right] (\vec{\eta}) = 0$, for all $\vec{\eta} \in \underline{V}(\Gamma^h(t))$, yields (9.58). Setting $\left[\frac{\delta}{\delta \vec{\kappa}^h} \widehat{L}_{\vec{\kappa}, \beta, \theta}^h \right] (\vec{\xi}) = 0$, for all $\vec{\xi} \in \underline{V}(\Gamma^h(t))$, yields that $\vec{\kappa}^h + (\beta A^h(t) - \vec{\kappa}) \vec{\omega}^h = \vec{\pi}_{\Gamma^h} \left[\underline{Q}_{\theta}^h \vec{Y}^h \right]$, where $A^h(t)$ is given by (9.49d). Finally, we set $\left[\frac{\delta}{\delta \Gamma^h} \widehat{L}_{\vec{\kappa}, \beta, \theta}^h \right] (\vec{\chi}) = -\left\langle \underline{Q}_{\theta}^h \vec{\mathcal{V}}^h, \vec{\chi} \right\rangle_{\Gamma(t)}^h$, for all $\vec{\chi} \in \underline{V}(\Gamma^h(t))$. If $\theta = 1$, the resulting scheme collapses to the semidiscrete Dziuk scheme (9.49). If $\theta = 0$, this scheme collapses to a variant of (9.33), (9.31) and (9.30), which takes spontaneous curvature and ADE effects into account, and this scheme still satisfies Theorem 5.3(iii). For any $\theta \in (0, 1)$, the scheme interpolates between these two extremes. Moreover, this scheme, for any given $\theta \in [0, 1]$, satisfies a stability bound, a generalization of Theorem 9.16; see Barrett et al. (2016b, Theorem 3.3) for details. In addition, this stability bound holds for a variant involving volume and surface area constraints.

Remark 9.19 (Surfaces with boundary). *For an evolving surface with a boundary, the result of Lemma 9.15 can be generalized as follows, where we recall the shorthand notation $\mathcal{V} = f$ for (9.41). On noting Theorem 2.32, Remark 2.39(ii) and Theorem 2.21, it holds that*

$$\begin{aligned} \frac{d}{dt} E_{\vec{\kappa}, \beta}(\Gamma(t)) &= -\langle f, \mathcal{V} \rangle_{\Gamma(t)} + \int_{\partial \Gamma(t)} \left(\frac{1}{2} (\varkappa - \bar{\varkappa})^2 + \beta A(t) \varkappa \right) \vec{\mathcal{V}} \cdot \vec{\mu} \, d\mathcal{H}^{d-2} \\ &\quad - \int_{\partial \Gamma(t)} \mathcal{V} \vec{\mu} \cdot \nabla_s \varkappa \, d\mathcal{H}^{d-2} + \int_{\partial \Gamma(t)} (\varkappa - \bar{\varkappa} + \beta A(t)) \vec{\mu} \cdot \nabla_s \mathcal{V} \, d\mathcal{H}^{d-2}, \end{aligned} \quad (9.59)$$

where $\vec{\mathcal{V}}$ is the velocity field induced by a global parameterization of the evolving hypersurface, and $\vec{\mu}(t)$ denotes the outer unit conormal on $\partial\Gamma(t)$. Hence, in order to ensure that (9.41) is still the L^2 -gradient flow of $E_{\bar{\kappa},\beta}(\Gamma(t))$, conditions need to be prescribed at the boundary so that the boundary terms in (9.59) vanish. In particular, the following boundary conditions may be considered. In the simplest situation the boundary is kept fixed, i.e. $\partial\Gamma(t) = \partial\Gamma(0)$ for all $t \in (0, T]$, which is the same as (4.8). This leads to the first two boundary terms vanishing in (9.59). The third boundary term vanishes if either $\kappa - \bar{\kappa} + \beta A(t) = 0$ or $\vec{\mu} \cdot \nabla_s \mathcal{V} = 0$ on $\partial\Gamma(t)$. Setting $\partial\Gamma(t) = \partial\Gamma(0)$ and $\kappa - \bar{\kappa} + \beta A(t) = 0$ on $\partial\Gamma(t)$ for all $t \in (0, T]$ are called Navier boundary conditions. Whereas, for a given $\vec{\zeta} \in C(\partial\Gamma(0), \mathbb{S}^{d-1})$, setting $\partial\Gamma(t) = \partial\Gamma(0)$ and $\vec{\mu}(t) = \vec{\zeta}$ on $\partial\Gamma(t)$ for all $t \in (0, T]$ are called clamped boundary conditions. It is a simple matter to show that clamped boundary conditions lead to $\vec{\mu} \cdot \nabla_s \mathcal{V} = 0$ on $\partial\Gamma(t)$, and hence to all three boundary terms vanishing in (9.59).

A third type of possible boundary conditions are called free boundary conditions. Here the boundary can move freely and the three boundary terms in (9.59) vanish on imposing

$$\frac{1}{2}(\kappa - \bar{\kappa})^2 + \beta A(t) \kappa = 0, \quad \vec{\mu} \cdot \nabla_s \kappa = 0, \quad \kappa - \bar{\kappa} + \beta A(t) = 0 \quad \text{on } \partial\Gamma(t).$$

We refer to Barrett et al. (2012b) for more details in the case $d = 2$, and to Barrett et al. (2017c) for more details in the case $d = 3$. The discussion in the latter article easily generalizes to $d > 3$. Moreover, in Barrett et al. (2017c) the present authors also included a boundary energy, $\varsigma \mathcal{H}^{d-2}(\partial\Gamma(t))$ for $\varsigma \in \mathbb{R}_{\geq 0}$, which is called line energy in the case $d = 3$, and Gaussian curvature effects. Here the inclusion of the Gaussian curvature effects is achieved via the Gauss–Bonnet theorem, recall Theorem 2.40.

In the case of Navier boundary conditions, one can easily adapt the finite element approximation (9.45), (9.4b) by replacing $\underline{V}(\Gamma^m)$ in (9.4b) by $\underline{V}_D(\Gamma^m)$, recall (4.9), by replacing $V(\Gamma^m)$ in (9.45) by $V_D(\Gamma^m)$, where $\underline{V}_D(\Gamma^m) = [V_D(\Gamma^m)]^d$, and by seeking $(\vec{X}^{m+1}, \kappa^{m+1}) \in \underline{V}(\Gamma^m) \times V(\Gamma^m)$ such that $\vec{X}^{m+1} - \text{id}|_{\Gamma^m} \in \underline{V}_D(\Gamma^m)$ and $\kappa^{m+1} - (\bar{\kappa} - \beta A^m) \in V_D(\Gamma^m)$. For clamped and free boundary conditions this finite element approximation cannot be adapted. However, the approaches based on (9.54) and (9.57) can be adapted to all three types of boundary conditions. For the latter approach, we once again refer to Barrett et al. (2012b, 2017c) for more details, including stability results for semidiscrete discretizations. Furthermore, in Barrett et al. (2018) we extended this approach to approximate gradient flows for two-phase biomembranes, where instead of boundary conditions certain matching conditions need to hold across interfaces between different phases on the hypersurface. Finally, a related problem is the evolution of curve networks under elastic flow, where two or more curves meet at junction points. This problem has been considered by the authors in Barrett et al. (2012c).

9.5 Alternative numerical approaches

We note that Rusu (2005) first introduced a mixed variational form for Willmore flow, based on position and mean curvature vectors, which allowed for the approximation by continuous piecewise linear finite elements. This approach was extended to surfaces with

boundaries and applied to surface restoration problems in Clarenz et al. (2004). We refer also to Deckelnick and Dziuk (2006); Deckelnick and Schieweck (2010); Deckelnick et al. (2015), where, on assuming a sufficiently smooth solution, an error analysis is presented for semidiscrete finite element approximations for a graph formulation of Willmore flow.

Other parametric numerical methods are discussed in Dziuk et al. (2002); Mayer and Simonett (2002); Bobenko and Schröder (2005); Bonito et al. (2010); Elliott and Stinner (2010, 2013); Bartels et al. (2012); Bartezzaghi et al. (2019). In addition, a numerical method based on a level set approach has been studied in Droske and Rumpf (2004), while phase field type approaches are discussed in Du et al. (2005); Esedoğlu et al. (2014); Bretin et al. (2015).

10 Biomembranes

In this section we will discuss how the first variation of curvature energies discussed in the previous sections appear in evolution laws involving also bulk quantities. This is relevant for the evolution of vesicles and biomembranes, where the curvature energy interacts with a fluid surrounding the membrane. Biomembranes are lipid bilayers and they form bag-like structures containing fluid and they are surrounded by a possibly different fluid. Membranes appear in a multitude of biological systems and a proper understanding of the form and the evolution of biomembranes is of major interest in the life sciences. As an example, we mention that the biconcave shapes of red blood cells appear as stationary states of the curvature energies discussed in the previous sections.

10.1 A model for the dynamics of fluidic biomembranes

We will introduce a model, which is a variant of a model introduced by Arroyo and DeSimone (2009), that couples the first variation of curvature energy to the (Navier–)Stokes equations in the bulk and on the surface. To be more precise a bulk (Navier–)Stokes system is coupled to a tangential (Navier–)Stokes system on the membrane. The tangential (Navier–)Stokes system also includes a surface incompressibility condition, which will lead to good mesh properties on the discrete level even in situations where the fluid velocity leads to a high deformation of the surface.

A generalized elastic energy for a biomembrane is given by

$$\int_{\Gamma} \frac{1}{2} \alpha (\kappa - \bar{\kappa})^2 + \alpha^G \mathcal{K} \, d\mathcal{H}^{d-1} + \frac{1}{2} \alpha \beta (\langle \kappa, 1 \rangle_{\Gamma} - M_0)^2 \quad (10.1)$$

for a compact hypersurface $\Gamma \subset \mathbb{R}^d$ without boundary, $d \geq 2$. Here $\alpha \in \mathbb{R}_{>0}$ and $\alpha^G \in \mathbb{R}$ are the bending and Gaussian bending rigidities. As before, $\bar{\kappa}$ is the spontaneous curvature, which arises for example from local inhomogeneities within the membrane and the parameters $\beta \in \mathbb{R}_{\geq 0}$, $M_0 \in \mathbb{R}$ relate the area difference elasticity (ADE) model, recall §9.4. Moreover, $\mathcal{K}$ is the Gaussian curvature. It is discussed in Nitsche (1993) that the most general form of a curvature energy of the form $\int_{\Gamma} q(\kappa_1, \dots, \kappa_{d-1}) \, d\mathcal{H}^{d-1}$, with q

being at most quadratic in the principal curvatures and invariant under permutations of its arguments, has the form $q(\kappa_1, \dots, \kappa_{d-1}) = \frac{1}{2} \alpha \kappa^2 + \alpha^G \mathcal{K} + \alpha_1 \kappa + \alpha_2$, which leads to the first term in (10.1) by choosing $\alpha_1 = -\alpha \bar{\kappa}$ and $\alpha_2 = \frac{1}{2} \alpha \bar{\kappa}^2$. If α^G is constant we obtain from the Gauss–Bonnet theorem, recall Theorem 2.40, that, as the surface has no boundary, the contribution $\int_{\Gamma} \alpha^G \mathcal{K} \, d\mathcal{H}^{d-1}$ is constant in a fixed topological class, and hence will always disappear in a first variation. For now, we will hence set $\alpha^G = 0$ and only if one considers inhomogeneous membranes, or open membranes with boundary, one has to consider this term, see Elliott and Stinner (2010); Barrett et al. (2017c,d, 2018). Hence, overall, we consider from now on $\alpha E_{\bar{\kappa}, \beta}(\Gamma(t))$ as the elastic energy for an evolving biomembrane, where $E_{\bar{\kappa}, \beta}(\Gamma(t))$ is as defined in (9.38).

We adopt the notation in §2.4, and assume that two fluids occupy regions $\Omega_-(t)$ and $\Omega_+(t) = \Omega \setminus \overline{\Omega_-(t)}$ with $\Gamma(t) = \partial\Omega_-(t)$, and with $\vec{\nu}$ denoting the outer unit normal to $\Omega_-(t)$ on $\Gamma(t)$, recall Figure 1 in §2.4. Here $\Omega \subset \mathbb{R}^d$ is a fixed domain, with $d \geq 2$. In these two fluid regions we require, as in Section 8, the incompressible Stokes equations with a no-slip boundary condition on $\partial\Omega$, i.e.

$$-\nabla \cdot \underline{\underline{\sigma}} = \vec{0}, \quad \nabla \cdot \vec{u} = 0 \quad \text{in } \Omega_{\pm}(t), \quad \vec{u} = \vec{0} \quad \text{on } \partial\Omega \quad (10.2)$$

with the stress tensor $\underline{\underline{\sigma}}$ as defined in (8.2). Once again, we refer to Remark 8.11(iv) for more general boundary conditions.

We remark that for biomembranes scales are typically such that the Stokes approximation of the Navier–Stokes equations is a very good approximation, see Barrett et al. (2015e). Therefore, we will consider the Stokes system in the bulk in what follows and refer to Barrett et al. (2016a, 2017b) and Section 8 for a discussion on how to generalize the following considerations to Navier–Stokes flow.

We now follow and generalize an approach of Arroyo and DeSimone (2009), who used the theory of interfacial fluid dynamics, which goes back to Scriven (1960), to formulate evolution laws that take the fluidic behaviour of vesicles and biomembranes into account. In fact, these lipid bilayer membranes can be described as a two-dimensional surface, where the lipid molecules have a fluid-like behaviour in the tangential direction. However, elastic forces stemming from the elastic bending energy act in normal direction. For more details on the modelling and the analysis of fluidic interfaces we refer to Slattery et al. (2007); Bothe and Prüss (2010). For our purposes it suffices to mention that in the absence of mass transfer to/from the interface from/to the bulk, and on assuming a no-slip condition between the outer and inner fluid at the interface, it is natural to assume that the bulk velocity is continuous across the interface and that the interface is moved with the bulk velocity. We refer to Barrett et al. (2015d, p. 1830) for more details.

Overall the following conditions need to hold on the free surface $\Gamma(t)$:

$$[\vec{u}]_{-}^{+} = \vec{0} \quad \text{on } \Gamma(t), \quad (10.3a)$$

$$\rho_{\Gamma} \partial_t^{\bullet} \vec{u} - \nabla_s \cdot \underline{\underline{\sigma}}_{\Gamma} = [\underline{\underline{\sigma}} \vec{\nu}]_{-}^{+} + \alpha \vec{f}_{\Gamma} \quad \text{on } \Gamma(t), \quad (10.3b)$$

$$\nabla_s \cdot \vec{u} = 0 \quad \text{on } \Gamma(t), \quad (10.3c)$$

$$\mathcal{V} = \vec{u} \cdot \vec{\nu} \quad \text{on } \Gamma(t), \quad (10.3d)$$

where $\rho_\Gamma \in \mathbb{R}_{\geq 0}$ denotes the surface material density, $\alpha \in \mathbb{R}_{>0}$ is the bending rigidity and $\vec{f}_\Gamma = f_\Gamma \vec{\nu}$, with f_Γ denoting minus the first variation of the bending energy $E_{\bar{\kappa},\beta}$, see (9.38), i.e.

$$f_\Gamma = -\Delta_s \kappa - (\kappa - \bar{\kappa})|\nabla_s \vec{\nu}|^2 + \frac{1}{2}(\kappa - \bar{\kappa})^2 \kappa - \beta A(t) (|\nabla_s \vec{\nu}|^2 - \kappa^2), \quad (10.4)$$

where κ satisfies Lemma 2.13(ii) and $A(t) = \langle \kappa, 1 \rangle_{\Gamma(t)} - M_0$, recall Lemma 9.15. Moreover,

$$\partial_t^\bullet f = \partial_t f + \vec{u} \cdot \nabla f \quad (10.5)$$

is the material time derivative with respect to the fluid velocity $\vec{u}$. This definition is related to Remark 2.29(ii), where the parameterizations $\vec{x}(\cdot, t)$ here are defined such that

$$\vec{u}(\vec{x}(\vec{q}, t), t) = (\partial_t \vec{x})(\vec{q}, t) \quad \forall (\vec{q}, t) \in \Upsilon \times [0, T], \quad (10.6)$$

as opposed to Definition 2.25(ii), so that $\vec{x}(\vec{q}, t)$ really is the trajectory of a material point. Equation (10.3c) is conservation of mass of the interface, similarly to standard incompressible (Navier–)Stokes in the bulk, recall (10.2). In particular, it implies that the membrane is locally incompressible. This can be seen by considering a surface patch $\sigma(t) \subset \Gamma(t)$ that is transported with the fluid velocity $\vec{u}$, i.e. $\sigma(t) = \vec{x}(\sigma_\Upsilon, t)$ with $\sigma_\Upsilon \subset \Upsilon$ and $\vec{x}$ satisfying (10.6). Then it follows with the help of the transport theorem, Theorem 2.32, that

$$\frac{d}{dt} \mathcal{H}^{d-1}(\sigma(t)) = \int_{\sigma(t)} \nabla_s \cdot \vec{\nu} \, d\mathcal{H}^{d-1} = \int_{\sigma(t)} \nabla_s \cdot \vec{u} \, d\mathcal{H}^{d-1} = 0,$$

see also Arroyo and DeSimone (2009). The balance of momentum on the surface implies (10.3b), see Arroyo and DeSimone (2009); Köhne and Lengeler (2018); Lengeler (2018). Here the surface stress tensor is defined by

$$\underline{\sigma}_\Gamma = 2\mu_\Gamma \underline{D}_s(\vec{u}) - p_\Gamma \underline{P}_\Gamma \quad \text{on } \Gamma(t), \quad (10.7)$$

where p_Γ is the surface pressure, $\mu_\Gamma \in \mathbb{R}_{>0}$ is the surface shear viscosity, $\underline{P}_\Gamma$ is the projection onto the tangent space and $\underline{D}_s(\vec{u})$ is the surface rate of deformation tensor, recall Definition 2.5(vii). The tensor $\underline{D}_s(\vec{u})$ is the relevant tensor for measuring the rate of change of lengths and angles through the metric tensor, cf. Lemma 2.30.

Finally, the term $[\underline{\sigma} \vec{\nu}]_\perp^+$, recall (2.12) and its generalization to vector-valued quantities in Remark 2.36, is the force exerted by the bulk on the surface. The total bending energy considered for now is given by $\alpha E_{\bar{\kappa},\beta}(\Gamma)$ with $E_{\bar{\kappa},\beta}$, the dimensionless energy defined in (9.38), and α , having the dimension of energy, is the bending rigidity. As in §8.1, (10.3d) states that the interface evolves with the normal component of the fluid velocity.

The system (10.2), (10.3) is closed with an initial condition for $\Gamma(0)$ and

$$\rho_\Gamma \vec{u}(\cdot, 0) = \rho_\Gamma \vec{u}_0 \quad \text{on } \Gamma(0),$$

where for simplicity we assume that $\vec{u}_0 : \Omega \rightarrow \mathbb{R}^d$ is a given initial velocity.

Lemma 10.1. *Let $(\mathcal{G}_T, \vec{u}, p)$ be a sufficiently smooth solution of (10.2), (10.3) and (10.4).*

(i) It holds that

$$\frac{d}{dt} |\Gamma(t)| = 0.$$

(ii) It holds that

$$\frac{d}{dt} \mathcal{L}^d(\Omega_-(t)) = 0.$$

(iii) It holds that

$$\begin{aligned} \frac{d}{dt} \left[\alpha E_{\overline{\kappa}, \beta}(\Gamma(t)) + \frac{1}{2} \rho_\Gamma |\vec{u}|_{\Gamma(t)}^2 \right] \\ = -2 \mu_\Gamma \langle \underline{D}_s(\vec{u}), \underline{D}_s(\vec{u}) \rangle_{\Gamma(t)} - 2 \langle \mu \underline{D}(\vec{u}), \underline{D}(\vec{u}) \rangle \leq 0. \end{aligned}$$

Proof. Let $\vec{x}$ be an arbitrary global parameterization of $\mathcal{G}_T$, with induced velocity field $\vec{\mathcal{V}}$.

(i) Combining the transport theorem, Theorem 2.32, and the divergence theorem, Theorem 2.21, with the tangential fields $\vec{f} = \vec{\mathcal{V}}_T$ and $\vec{f} = \underline{P}_\Gamma \vec{u}$, gives

$$\begin{aligned} \frac{d}{dt} \langle 1, 1 \rangle_{\Gamma(t)} &= \left\langle 1, \nabla_s \cdot \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} = \left\langle 1, \nabla_s \cdot (\vec{\mathcal{V}} - \vec{\mathcal{V}}_T) \right\rangle_{\Gamma(t)} = \langle 1, \nabla_s \cdot (\mathcal{V} \vec{v}) \rangle_{\Gamma(t)} \\ &= \langle 1, \nabla_s \cdot ((\vec{u} \cdot \vec{v}) \vec{v}) \rangle_{\Gamma(t)} = \langle 1, \nabla_s \cdot (\vec{u} - \underline{P}_\Gamma \vec{u}) \rangle_{\Gamma(t)} \\ &= \langle 1, \nabla_s \cdot \vec{u} \rangle_{\Gamma(t)} = 0, \end{aligned} \tag{10.8}$$

which is the claim.

(ii) As in Remark 8.1(ii), the result follows from the transport theorem, Theorem 2.33, and the facts that $\vec{\mathcal{V}} \cdot \vec{v} = \vec{u} \cdot \vec{v}$ on $\Gamma(t)$ and $\nabla \cdot \vec{u} = 0$ in $\Omega_-(t)$.

(iii) From Lemma 9.15, (10.4) and (10.3d) we obtain

$$\begin{aligned} \frac{d}{dt} E_{\overline{\kappa}, \beta}(\Gamma(t)) \\ = \left\langle \Delta_s \kappa + (\kappa - \overline{\kappa}) |\nabla_s \vec{v}|^2 - \frac{1}{2} (\kappa - \overline{\kappa})^2 \kappa + \beta A(t) (|\nabla_s \vec{v}|^2 - \kappa^2), \mathcal{V} \right\rangle_{\Gamma(t)} \\ = - \langle f_\Gamma, \mathcal{V} \rangle_{\Gamma(t)} = - \langle f_\Gamma \vec{v}, \vec{u} \rangle_{\Gamma(t)} = - \left\langle \vec{f}_\Gamma, \vec{u} \right\rangle_{\Gamma(t)}. \end{aligned} \tag{10.9}$$

It remains to analyse the right hand side in (10.9). To this end, we first of all note that it follows from Lemma 2.9(i),(ii), Definition 2.5(viii), Lemma 2.7(iii), the divergence theorem on hypersurfaces, i.e. Theorem 2.21 together with a density argument, and Remark 2.6(vi) that

$$\begin{aligned} \left\langle p_\Gamma, \nabla_s \cdot \vec{\xi} \right\rangle_{\Gamma(t)} &= \left\langle p_\Gamma \underline{P}_\Gamma, \nabla_s \vec{\xi} \right\rangle_{\Gamma(t)} \\ &= \left\langle \nabla_s \cdot (p_\Gamma \underline{P}_\Gamma \vec{\xi}), 1 \right\rangle_{\Gamma(t)} - \left\langle \nabla_s \cdot (p_\Gamma \underline{P}_\Gamma), \vec{\xi} \right\rangle_{\Gamma(t)} \\ &= - \left\langle \nabla_s \cdot (p_\Gamma \underline{P}_\Gamma), \vec{\xi} \right\rangle_{\Gamma(t)} \quad \forall \vec{\xi} \in [H^1(\Gamma(t))]^d. \end{aligned} \tag{10.10}$$

Hence it follows from (10.10), Remark 2.22(iii), together with a density argument, (10.7), (10.3b), (8.5) and (10.2) that

$$\begin{aligned} & \rho_\Gamma \left\langle \partial_t^\bullet \vec{u}, \vec{\xi} \right\rangle_{\Gamma(t)} + 2 \mu_\Gamma \left\langle \underline{D}_s(\vec{u}), \underline{D}_s(\vec{\xi}) \right\rangle_{\Gamma(t)} - \left\langle p_\Gamma, \nabla_s \cdot \vec{\xi} \right\rangle_{\Gamma(t)} \\ &= \left\langle \rho_\Gamma \partial_t^\bullet \vec{u} - \nabla_s \cdot \underline{\sigma}_\Gamma, \vec{\xi} \right\rangle_{\Gamma(t)} = \left\langle [\underline{\sigma} \vec{\nu}]^+, \vec{\xi} \right\rangle_{\Gamma(t)} + \alpha \left\langle \vec{f}_\Gamma, \vec{\xi} \right\rangle_{\Gamma(t)} \\ &= -2 \left(\mu \underline{D}(\vec{u}), \underline{D}(\vec{\xi}) \right) + \left(p, \nabla \cdot \vec{\xi} \right) + \alpha \left\langle \vec{f}_\Gamma, \vec{\xi} \right\rangle_{\Gamma(t)} \quad \forall \vec{\xi} \in \mathbb{V}_{\Gamma(t)}, \end{aligned} \quad (10.11)$$

where

$$\mathbb{V}_{\Gamma(t)} = \left\{ \vec{\xi} \in [H_0^1(\Omega)]^d : \underline{P}_\Gamma \vec{\xi}|_{\Gamma(t)} \in [H^1(\Gamma(t))]^d \right\}. \quad (10.12)$$

Here we recall from Lemma 2.14(i),(iii), together with a density argument, and a trace theorem for $\Omega_-(t)$ that all the terms in (10.11) are well-defined for $\vec{\xi} \in \mathbb{V}_{\Gamma(t)}$. Combining (10.9) and (10.11) with $\vec{\xi} = \vec{u}$, on noting (10.2) and (10.3c), yields that

$$\begin{aligned} & \alpha \frac{d}{dt} E_{\vec{\nu}, \beta}(\Gamma(t)) + \rho_\Gamma \left\langle \partial_t^\bullet \vec{u}, \vec{u} \right\rangle_{\Gamma(t)} \\ &= -2 \mu_\Gamma \left\langle \underline{D}_s(\vec{u}), \underline{D}_s(\vec{u}) \right\rangle_{\Gamma(t)} - 2 \left(\mu \underline{D}(\vec{u}), \underline{D}(\vec{u}) \right). \end{aligned} \quad (10.13)$$

Next, similarly to (10.8), it follows from (10.5), Remark 2.29(ii), (10.3d), Remark 2.8(iii), Theorem 2.21, Lemma 2.7(i), (10.3c) and Theorem 2.32 that

$$\begin{aligned} \left\langle \partial_t^\bullet \vec{u}, \vec{u} \right\rangle_{\Gamma(t)} &= \left\langle \partial_t^\circ \vec{u}, \vec{u} \right\rangle_{\Gamma(t)} + \left\langle \left[(\vec{u} - \vec{\nu}) \cdot \nabla \right] \vec{u}, \vec{u} \right\rangle_{\Gamma(t)} \\ &= \frac{1}{2} \left\langle \partial_t^\circ |\vec{u}|^2, 1 \right\rangle_{\Gamma(t)} + \left\langle \left[\underline{P}_\Gamma (\vec{u} - \vec{\nu}) \cdot \nabla_s \right] \vec{u}, \vec{u} \right\rangle_{\Gamma(t)} \\ &= \frac{1}{2} \left\langle \partial_t^\circ |\vec{u}|^2, 1 \right\rangle_{\Gamma(t)} - \frac{1}{2} \left\langle \nabla_s \cdot \left[\underline{P}_\Gamma (\vec{u} - \vec{\nu}) \right], |\vec{u}|^2 \right\rangle_{\Gamma(t)} \\ &= \frac{1}{2} \left\langle \partial_t^\circ |\vec{u}|^2, 1 \right\rangle_{\Gamma(t)} - \frac{1}{2} \left\langle \nabla_s \cdot (\vec{u} - \vec{\nu}), |\vec{u}|^2 \right\rangle_{\Gamma(t)} = \frac{1}{2} \frac{d}{dt} \left\langle |\vec{u}|^2, 1 \right\rangle_{\Gamma(t)}. \end{aligned}$$

Combining this with (10.13) yields the desired result. $\square$

We note, in particular, that the conservation properties Lemma 10.1(i), (ii) follow from the continuity equations $\nabla_s \cdot \vec{u} = 0$ on $\Gamma(t)$ and $\nabla \cdot \vec{u} = 0$ in $\Omega_\pm(t)$, respectively. Hence, in contrast to the situation in e.g. §9.4, no additional side constraints for surface area and enclosed volume are required.

10.2 A weak formulation for the dynamics of biomembranes

The most natural weak formulation for the model introduced in §10.1 uses the tangential velocity of the fluid for the evolution of $\Gamma(t)$, and hence (10.3d) is replaced by $\vec{\nu} = \vec{u}$ on $\Gamma(t)$. This mimics the procedure in §8.1.4 for two-phase Stokes flow. However, contrary to the situation there, the presence of the continuity equation $\nabla_s \cdot \vec{u} = 0$ on $\Gamma(t)$ will lead to good mesh properties for discretizations based on this natural weak formulation.

Now (10.11) leads to the following weak formulation of the system (10.2), (10.3) and (10.4). Given a closed hypersurface $\Gamma(0)$ and, if $\rho_\Gamma > 0$, $\vec{u}_0 \in [H_0^1(\Omega)]^d$, we seek an evolving hypersurface $(\Gamma(t))_{t \in [0, T]}$, with a global parameterization and induced velocity field $\vec{\mathcal{V}}, \vec{\mathcal{Z}} \in [L^2(\mathcal{G}_T)]^d$, $p_\Gamma \in L^2(\mathcal{G}_T)$, $\vec{f}_\Gamma \in [L^2(\mathcal{G}_T)]^d$, as well as $\vec{u} : \Omega \times [0, T] \rightarrow \mathbb{R}^d$, with $\vec{u}|_{\mathcal{G}_T} \in [H^1(\mathcal{G}_T)]^d$ and $\rho_\Gamma \vec{u}(\cdot, 0)|_{\Gamma(0)} = \rho_\Gamma (\vec{u}_0)|_{\Gamma(0)}$, and $p : \Omega \times [0, T] \rightarrow \mathbb{R}$ as follows. For almost all $t \in (0, T)$, find $(\vec{\mathcal{V}}(\cdot, t), \vec{\mathcal{Z}}(\cdot, t), p_\Gamma(\cdot, t), \vec{f}_\Gamma(\cdot, t), \vec{u}(\cdot, t), p(\cdot, t)) \in [L^2(\Gamma(t))]^d \times [H^1(\Gamma(t))]^d \times L^2(\Gamma(t)) \times [L^2(\Gamma(t))]^d \times \mathbb{V}_{\Gamma(t)} \times L^2(\Omega)$ such that

$$2 \left(\mu \underline{D}(\vec{u}), \underline{D}(\vec{\xi}) \right) - \left(p, \nabla \cdot \vec{\xi} \right) + \rho_\Gamma \left\langle \partial_t^\bullet \vec{u}, \vec{\xi} \right\rangle_{\Gamma(t)} + 2 \mu_\Gamma \left\langle \underline{D}_s(\vec{u}), \underline{D}_s(\vec{\xi}) \right\rangle_{\Gamma(t)} - \left\langle p_\Gamma, \nabla_s \cdot \vec{\xi} \right\rangle_{\Gamma(t)} = \alpha \left\langle \vec{f}_\Gamma, \vec{\xi} \right\rangle_{\Gamma(t)} \quad \forall \vec{\xi} \in \mathbb{V}_{\Gamma(t)}, \quad (10.14a)$$

$$(\nabla \cdot \vec{u}, \varphi) = 0 \quad \forall \varphi \in L^2(\Omega), \quad (10.14b)$$

$$\langle \nabla_s \cdot \vec{u}, \eta \rangle_{\Gamma(t)} = 0 \quad \forall \eta \in L^2(\Gamma(t)), \quad (10.14c)$$

$$\left\langle \vec{\mathcal{V}}, \vec{\chi} \right\rangle_{\Gamma(t)} = \langle \vec{u}, \vec{\chi} \rangle_{\Gamma(t)} \quad \forall \vec{\chi} \in [L^2(\Gamma(t))]^d, \quad (10.14d)$$

$$\langle \vec{\mathcal{Z}}, \vec{\eta} \rangle_{\Gamma(t)} + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d, \quad (10.14e)$$

together with an equation for $\vec{f}_\Gamma$. In the simplest case, when $\overline{\alpha} = \beta = 0$, we recall Lemma 9.4 and (9.11a), and set

$$\begin{aligned} \left\langle \vec{f}_\Gamma, \vec{\chi} \right\rangle_{\Gamma(t)} &= \langle \nabla_s \vec{\mathcal{Z}}, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \rangle_{\Gamma(t)} + \langle \nabla_s \cdot \vec{\mathcal{Z}}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\ &\quad + \frac{1}{2} \langle |\vec{\mathcal{Z}}|^2, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \quad \forall \vec{\chi} \in [H^1(\Gamma(t))]^d. \end{aligned} \quad (10.14f)$$

In the general case, for nonzero $\overline{\alpha}$ or β , we recall (9.47). Hence we require, instead of (10.14f), that in addition a $\vec{y} \in [L^2(\mathcal{G}_T)]^d$ exists such that for almost all $t \in (0, T)$ it holds that $\vec{y}(\cdot, t) \in [H^1(\Gamma(t))]^d$ and

$$\begin{aligned} \left\langle \vec{f}_\Gamma, \vec{\chi} \right\rangle_{\Gamma(t)} &= \langle \nabla_s \vec{y}, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \rangle_{\Gamma(t)} + \langle \nabla_s \cdot \vec{y}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\ &\quad - \left\langle \frac{1}{2} |\vec{\mathcal{Z}} - \overline{\alpha} \vec{\nu}|^2 - \vec{\mathcal{Z}} \cdot (\vec{y} - \beta A(t) \vec{\nu}), \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma(t)} \\ &\quad + (\beta A(t) - \overline{\alpha}) \langle \vec{\mathcal{Z}}, (\nabla_s \vec{\chi})^\top \vec{\nu} \rangle_{\Gamma(t)} \quad \forall \vec{\chi} \in [H^1(\Gamma(t))]^d, \end{aligned} \quad (10.15a)$$

$$\left\langle \vec{\mathcal{Z}} + (\beta A(t) - \overline{\alpha}) \vec{\nu} - \vec{y}, \vec{\xi} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\xi} \in [H^1(\Gamma(t))]^d, \quad (10.15b)$$

with $A(t)$ defined by (9.47d).

We now argue that if no connected component of $\Gamma(t)$ is spherical, then the surface pressure is unique and the bulk pressure is unique up to an additive constant. Recall that Figure 1 shows the special case of $\Gamma(t)$ having just a single connected component. We assume that two solutions to (10.14) are found that only differ in the pressure. Say one solution features the pressure pair $(p_1, p_{\Gamma,1})$ and the other $(p_2, p_{\Gamma,2})$. Let $\bar{p} = p_1 - p_2$ and $\bar{p}_\Gamma = p_{\Gamma,1} - p_{\Gamma,2}$. Then we obtain

$$\left(\bar{p}, \nabla \cdot \vec{\xi} \right) + \left\langle \bar{p}_\Gamma, \nabla_s \cdot \vec{\xi} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\xi} \in [H_0^1(\Omega)]^d,$$

which first of all implies that $\bar{p}$ is equal to some constants $\bar{p}_\pm$ in each connected component of $\Omega_\pm(t)$. Applying the divergence theorem in the bulk regions $\Omega_\pm(t)$, Lemma 2.7(i), and the divergence theorem on $\Gamma(t)$, Theorem 2.21, yields that

$$\nabla_s \bar{p}_\Gamma + \varkappa \bar{p}_\Gamma \vec{\nu} = -[\bar{p} \vec{\nu}]_-^+ \quad \text{on } \Gamma(t).$$

Since $\nabla_s \bar{p}_\Gamma$ is tangential, we obtain that $\nabla_s \bar{p}_\Gamma = \vec{0}$, and hence $\bar{p}_\Gamma$ is constant on connected components of $\Gamma(t)$. In addition, we obtain that $\varkappa \bar{p}_\Gamma = -[\bar{p}]_-^+$ on $\Gamma(t)$. If $\varkappa$ is not constant on a connected component of $\Gamma(t)$, which is the case if it is not a sphere, then we have $\bar{p}_\Gamma = [\bar{p}]_-^+ = 0$ on this component, and so $\bar{p}_+ = \bar{p}_-$ for the associated connected components of $\Omega_\pm(t)$. Repeating this argument for all the connected components of $\Gamma(t)$ yields, if no connected component of $\Gamma(t)$ is a sphere, that p_Γ is unique on $\Gamma(t)$ and that p is unique in Ω up to an additive constant. If $\varkappa$ is constant on a connected component of $\Gamma(t)$, however, i.e. if this component of $\Gamma(t)$ is a sphere, then on this component p_Γ is only unique up to an additive constant.

Taking the above into account we formulate the following LBB-type condition. If $\Gamma(t)$ and $\partial\Omega$ are sufficiently smooth, and provided that $\Gamma(t)$ does not contain a sphere, then there exists a constant $C \in \mathbb{R}_{>0}$ such that

$$\inf_{(\varphi, \eta) \in \widehat{\mathbb{P}} \times L^2(\Gamma(t))} \sup_{\vec{\xi} \in \mathbb{V}_{\Gamma(t)}} \frac{(\varphi, \nabla \cdot \vec{\xi}) + \langle \eta, \nabla_s \cdot \vec{\xi} \rangle_{\Gamma(t)}}{(|\varphi|_\Omega + |\eta|_{\Gamma(t)}) \left(\|\vec{\xi}\|_{1, \Omega} + \|\underline{E}_\Gamma \vec{\xi}|_{\Gamma(t)}\|_{1, \Gamma(t)} \right)} \geq C > 0. \quad (10.16)$$

Here we have recalled (10.12) as well as the definitions of the space $\widehat{\mathbb{P}}$ and the H^1 -norm $\|\cdot\|_{1, \Omega}$ from (8.10). In addition, we let $\|\cdot\|_{1, \Gamma(t)}^2 = |\cdot|_{\Gamma(t)}^2 + |\nabla_s \cdot|_{\Gamma(t)}^2$ define the H^1 -norm on $\Gamma(t)$. The LBB-type condition (10.16) can be deduced from the pressure reconstruction result in Lengeler (2015).

10.3 Semidiscrete finite element approximation

We now introduce a finite element version of the weak formulation of (10.14). We have discussed in previous sections the importance of the choice of the discrete tangential velocity of $\Gamma^h(t)$. In general, the mesh quality will deteriorate when using a velocity in the direction of the discrete normal. Similarly, for many two-phase fluid flow problems, using the tangential velocity induced by the surrounding fluid flow also leads to bad meshes. However, here it turns out that due to the approximation of the local area conservation property, $\nabla_s \cdot \vec{u} = 0$ on $\Gamma(t)$, the mesh quality typically will remain very good during the evolution even if we choose $\vec{\mathcal{V}} = \vec{u}$.

We recall the definitions of the semidiscrete finite element spaces in §8.1.2, and in particular the space (8.22). In addition, we define the space

$$\begin{aligned} \mathbb{U}_{\Gamma^h}^h = \Big\{ & \vec{\phi} \in H^1(0, T; \mathbb{U}^h) : \\ & \exists \vec{\chi} \in \underline{V}_T(\mathcal{G}_T^h) \text{ with } \vec{\chi}(\cdot, t) = \vec{\pi}_{\Gamma^h} \left[\vec{\phi}|_{\Gamma^h(t)} \right] \quad \forall t \in [0, T] \Big\}. \end{aligned}$$

Overall, we then obtain the following semidiscrete continuous-in-time finite element approximation of (10.14). First, we will state it for the simpler situation when $\overline{\alpha} = \beta = 0$. To this end, we recall the scheme (9.15).

Given the closed polyhedral hypersurface $\Gamma^h(0)$, find an evolving polyhedral hypersurface $\mathcal{G}_T^h$ with induced velocity $\vec{\mathcal{V}}^h \in \underline{V}(\mathcal{G}_T^h)$, $\vec{\kappa}^h \in \underline{V}(\mathcal{G}_T^h)$, $\vec{U}^h \in \mathbb{U}_{\Gamma^h}^h$, $P^h \in \widehat{\mathbb{P}}_T^h$, $P_\Gamma^h \in V(\mathcal{G}_T^h)$ and $\vec{F}_\Gamma^h \in \underline{V}(\mathcal{G}_T^h)$ as follows. For all $t \in (0, T]$, find $(\vec{U}^h(\cdot, t), P^h(\cdot, t), P_\Gamma^h(\cdot, t), \vec{\mathcal{V}}^h(\cdot, t), \vec{\kappa}^h(\cdot, t), \vec{F}_\Gamma^h(\cdot, t)) \in \mathbb{U}^h \times \widehat{\mathbb{P}}^h(t) \times V(\Gamma^h(t)) \times \underline{V}(\Gamma^h(t)) \times \underline{V}(\Gamma^h(t)) \times \underline{V}(\Gamma^h(t))$ such that

$$\begin{aligned} & 2 \left(\mu^h \underline{D}(\vec{U}^h), \underline{D}(\vec{\xi}) \right) - \left(P^h, \nabla \cdot \vec{\xi} \right) + \rho_\Gamma \left\langle \partial_t^{\circ, h} \vec{\pi}_{\Gamma^h} \vec{U}^h, \vec{\xi} \right\rangle_{\Gamma^h(t)}^h \\ & \quad + 2 \mu_\Gamma \left\langle \underline{D}_s(\vec{\pi}_{\Gamma^h} \vec{U}^h), \underline{D}_s(\vec{\pi}_{\Gamma^h} \vec{\xi}) \right\rangle_{\Gamma^h(t)} - \left\langle P_\Gamma^h, \nabla_s \cdot (\vec{\pi}_{\Gamma^h} \vec{\xi}) \right\rangle_{\Gamma^h(t)} \\ & = \alpha \left\langle \vec{F}_\Gamma^h, \vec{\xi} \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\xi} \in \mathbb{U}^h, \end{aligned} \quad (10.17a)$$

$$\left(\nabla \cdot \vec{U}^h, \varphi \right) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}}^h(t), \quad (10.17b)$$

$$\left\langle \nabla_s \cdot (\vec{\pi}_{\Gamma^h} \vec{U}^h), \eta \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \eta \in V(\Gamma^h(t)), \quad (10.17c)$$

$$\left\langle \vec{\mathcal{V}}^h, \vec{\chi} \right\rangle_{\Gamma^h(t)}^h = \left\langle \vec{U}^h, \vec{\chi} \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\chi} \in \underline{V}(\Gamma^h(t)), \quad (10.17d)$$

$$\left\langle \vec{\kappa}^h, \vec{\eta} \right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h(t)), \quad (10.17e)$$

$$\begin{aligned} \left\langle \vec{F}_\Gamma^h, \vec{\chi} \right\rangle_{\Gamma^h(t)}^h &= \left\langle \nabla_s \vec{\kappa}^h, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \right\rangle_{\Gamma^h(t)} + \left\langle \nabla_s \cdot \vec{\kappa}^h, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^h(t)} \\ & \quad + \frac{1}{2} \left\langle |\vec{\kappa}^h|^2, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\chi} \in \underline{V}(\Gamma^h(t)). \end{aligned} \quad (10.17f)$$

For this semidiscrete approximation we have the following stability and conservation results.

Theorem 10.2. *Let $(\mathcal{G}_T^h, \vec{U}^h, P^h, P_\Gamma^h, \vec{\kappa}^h, \vec{F}_\Gamma^h)$ be a solution to (10.17), and let $\vec{\kappa}^h \in \underline{V}_T(\mathcal{G}_T^h)$. Then it holds that*

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \left(\rho_\Gamma \left(\left| \vec{U}^h \right|_{\Gamma^h(t)}^h \right)^2 + \alpha \left(\left| \vec{\kappa}^h \right|_{\Gamma^h(t)}^h \right)^2 \right) + 2 \left(\mu^h \underline{D}(\vec{U}^h), \underline{D}(\vec{U}^h) \right) \\ & \quad + 2 \mu_\Gamma \left\langle \underline{D}_s(\vec{\pi}_{\Gamma^h} \vec{U}^h), \underline{D}_s(\vec{\pi}_{\Gamma^h} \vec{U}^h) \right\rangle_{\Gamma^h(t)} = 0. \end{aligned} \quad (10.18)$$

Moreover, it holds that

$$\frac{d}{dt} \left\langle \phi_k^{\Gamma^h(t)}, 1 \right\rangle_{\Gamma^h(t)} = 0, \quad k = 1, \dots, K, \quad (10.19)$$

and hence that

$$\frac{d}{dt} |\Gamma^h(t)| = 0. \quad (10.20)$$

Proof. Choosing $\vec{\xi} = \vec{U}^h(\cdot, t)$ in (10.17a), $\varphi = P^h(\cdot, t)$ in (10.17b) and $\eta = P_\Gamma^h(\cdot, t)$ in (10.17c), we obtain

$$\begin{aligned} & 2 \left(\mu^h \underline{D}(\vec{U}^h), \underline{D}(\vec{U}^h) \right) + \rho_\Gamma \left\langle \partial_t^{\circ, h} \vec{\pi}_{\Gamma^h} \vec{U}^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h \\ & + 2 \mu_\Gamma \left\langle \underline{D}_s(\vec{\pi}_{\Gamma^h} \vec{U}^h), \underline{D}_s(\vec{\pi}_{\Gamma^h} \vec{U}^h) \right\rangle_{\Gamma^h(t)} = \alpha \left\langle \vec{F}_\Gamma^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h. \end{aligned} \quad (10.21)$$

In addition, arguing as in the proof of Theorem 9.7 on (10.17e) and (10.17f), recall (9.15), yields

$$\frac{1}{2} \frac{d}{dt} \left(|\vec{\kappa}^h|_{\Gamma^h(t)}^h \right)^2 = - \left\langle \vec{F}_\Gamma^h, \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h = - \left\langle \vec{F}_\Gamma^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h, \quad (10.22)$$

where the last equality follows from choosing $\vec{\chi} = \vec{F}_\Gamma^h(\cdot, t)$ in (10.17d). Moreover, it follows from (10.17d) that

$$\vec{\mathcal{V}}^h(\cdot, t) = \vec{\pi}_{\Gamma^h} \left[\vec{U}_{|\Gamma^h(t)}^h \right]. \quad (10.23)$$

Noting this, Theorem 3.30(ii) and (10.17c) with $\eta = \pi_{\Gamma^h} \left[\left| \vec{U}_{|\Gamma^h(t)}^h \right|^2 \right]$ yields

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \left\langle \vec{U}^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h &= \frac{1}{2} \left\langle \partial_t^{\circ, h} \vec{\pi}_{\Gamma^h} \left[\left| \vec{U}^h \right|^2 \right], 1 \right\rangle_{\Gamma^h(t)}^h + \frac{1}{2} \left\langle \nabla_s \cdot \vec{\mathcal{V}}^h, \left| \vec{U}^h \right|^2 \right\rangle_{\Gamma^h(t)}^h \\ &= \left\langle \partial_t^{\circ, h} \vec{\pi}_{\Gamma^h} \vec{U}^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h + \frac{1}{2} \left\langle \nabla_s \cdot (\vec{\pi}_{\Gamma^h} \vec{U}^h), \left| \vec{U}^h \right|^2 \right\rangle_{\Gamma^h(t)}^h \\ &= \left\langle \partial_t^{\circ, h} \vec{\pi}_{\Gamma^h} \vec{U}^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h. \end{aligned} \quad (10.24)$$

Combining (10.21), (10.22) and (10.24) yields (10.18).

Similarly to (10.18), the identity (10.19) follows directly from Theorem 3.30(ii), Remark 3.29(i), (10.23) and choosing $\eta = \phi_k^{\Gamma^h(t)}$ in (10.17c). Finally, (10.20) follows by adding (10.19) for $k = 1, \dots, K$. $\square$

Remark 10.3 (Spontaneous curvature and ADE effects). *In the case that $\overline{\alpha}$ or β are nonzero, we replace (10.17f) in the semidiscrete approximation (10.17) with*

$$\left\langle \vec{\kappa}^h + (\beta A^h(t) - \overline{\alpha}) \vec{\nu}^h - \vec{Y}^h, \vec{\xi} \right\rangle_{\Gamma^h(t)}^h = 0 \quad \forall \vec{\xi} \in \underline{V}(\Gamma^h(t)), \quad (10.25a)$$

$$\begin{aligned} \left\langle \vec{F}_\Gamma^h, \vec{\chi} \right\rangle_{\Gamma^h(t)}^h &= \left\langle \nabla_s \vec{Y}^h, \nabla_s \vec{\chi} - 2 \underline{D}_s(\vec{\chi}) \right\rangle_{\Gamma^h(t)} + \left\langle \nabla_s \cdot \vec{Y}^h, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^h(t)} \\ &\quad - \left\langle \frac{1}{2} |\vec{\kappa}^h - \overline{\alpha} \vec{\nu}^h|^2 - \vec{\kappa}^h \cdot (\vec{Y}^h - \beta A^h(t) \vec{\nu}^h), \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^h(t)}^h \\ &\quad + (\beta A^h(t) - \overline{\alpha}) \left\langle \vec{\kappa}^h, (\nabla_s \vec{\chi})^\top \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\chi} \in \underline{V}(\Gamma^h(t)), \end{aligned} \quad (10.25b)$$

$$A^h(t) = \left\langle \vec{\kappa}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h - M_0, \quad (10.25c)$$

and seek in addition a $\vec{Y}^h \in \underline{V}(\mathcal{G}_T^h)$. Here we recall (9.49). Then a stability result as in Theorem 10.2, with $\frac{1}{2} \left(|\vec{\kappa}^h|_{\Gamma^h(t)}^h \right)^2$ replaced by $E_{\vec{\kappa}, \beta}^h(\Gamma^h(t))$ can be shown for the system (10.17a–e), (10.25), on combining the proofs of Theorem 10.2 and Theorem 9.16; see also Barrett et al. (2017b, Theorem 4.2).

Remark 10.4.

- (i) The virtual element approach introduced in §8.1.4 can be used for the semidiscrete approximation (10.17) and its generalization (10.17a–e), (10.25). In this case we obtain, in addition to $\frac{d}{dt} |\Gamma^h(t)| = 0$, also

$$\frac{d}{dt} \mathcal{L}^d(\Omega_-^h(t)) = 0,$$

which means that we obtain an approximation which conserves both the surface area and the enclosed volume, and also fulfills an energy identity.

- (ii) The identity (10.19) ensures that the measure of the support of each basis function on $\Gamma^h(t)$ is conserved. In the case of two space dimensions, and for the number of elements/vertices $J = K$ being odd, this is equivalent to each element maintaining its length. In particular, if $\Gamma^h(0)$ is equidistributed, then $\Gamma^h(t)$ will remain equidistributed throughout. For a slight modification of (10.17) one can prove that the measure of each element on $\Gamma^h(t)$ is conserved, i.e. that $\frac{d}{dt} \mathcal{H}^{d-1}(\sigma_j(t)) = 0$, $j = 1, \dots, J$, and hence (10.20), for arbitrary $J \geq 2$ and $d \geq 2$. To achieve this, one needs to replace $V(\Gamma^h(t))$ in (10.17) by $V_c(\Gamma^h(t))$, recall Definition 3.3(ii), i.e. piecewise constants are used for the trial space for $P_\Gamma^h(\cdot, t)$ and for the test space in (10.17c). However, this constraint for $d \geq 3$ can be too severe, see Barrett et al. (2016a, Remark 4.1) for more details in the case $d = 3$.
- (iii) The approximation (10.17) and its generalization (10.17a–e), (10.25) are based on continuous piecewise linear approximations of the surface velocity and surface pressure, and so are unlikely to satisfy a discrete version of the LBB condition (10.16) with a constant C independent of the mesh parameters. In fact, in practice it can lead to oscillatory surface pressure approximations, see Barrett et al. (2016a, Fig. 5). This can be avoided by using a continuous piecewise quadratic interpolation of the bulk velocity on the surface. This leads to better behaved approximations of the surface pressure. Although one can still prove (10.18) and its generalization for the modified versions of (10.17) and (10.17a–e), (10.25) if $\rho_\Gamma = 0$, one can no longer show (10.19) and (10.20). This can lead to poor surface area conservation for $d = 3$ in practice, see Barrett et al. (2016a, Remark 4.1) for more details.

Finally, we state a fully discrete equivalent of (10.17). Let the closed polyhedral hypersurface Γ^0 be an approximation of $\Gamma(0)$, and let $\vec{\kappa}_{\Gamma^0}^0 \in \underline{V}(\Gamma^0)$ be an approximation to its mean curvature vector. If $\rho_\Gamma > 0$, let $\vec{U}_{\Gamma^0}^0 \in \underline{V}(\Gamma^0)$ be an approximation to $(\vec{u}_0)|_{\Gamma^0}$. We also recall the time interval partitioning (4.5). Then, for $m = 0, \dots, M - 1$, find

$\vec{U}^{m+1} \in \mathbb{U}^m$, $P^{m+1} \in \widehat{\mathbb{P}}^m$, $P_\Gamma^{m+1} \in V(\Gamma^m)$, $\vec{X}^{m+1} \in \underline{V}(\Gamma^m)$, $\vec{\kappa}^{m+1} \in \underline{V}(\Gamma^m)$ and $\vec{F}_\Gamma^{m+1} \in \underline{V}(\Gamma^m)$ such that

$$\begin{aligned} & 2 \left(\mu^m \underline{D}(\vec{U}^{m+1}), \underline{D}(\vec{\xi}) \right) - \left(P^{m+1}, \nabla \cdot \vec{\xi} \right) + \rho_\Gamma \left\langle \frac{\vec{U}^{m+1} - \vec{U}_{\Gamma^m}^m}{\Delta t_m}, \vec{\xi} \right\rangle_{\Gamma^m}^h \\ & + 2 \mu_\Gamma \left\langle \underline{D}_s(\vec{\pi}_{\Gamma^m} \vec{U}^{m+1}), \underline{D}_s(\vec{\pi}_{\Gamma^m} \vec{\xi}) \right\rangle_{\Gamma^m} - \left\langle P_\Gamma^{m+1}, \nabla_s \cdot (\vec{\pi}_{\Gamma^m} \vec{\xi}) \right\rangle_{\Gamma^m} \\ & = \alpha \left\langle \vec{F}_\Gamma^{m+1}, \vec{\xi} \right\rangle_{\Gamma^m}^h \quad \forall \vec{\xi} \in \mathbb{U}^m, \end{aligned} \quad (10.26a)$$

$$\left(\nabla \cdot \vec{U}^{m+1}, \varphi \right) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}}^m, \quad (10.26b)$$

$$\left\langle \nabla_s \cdot (\vec{\pi}_{\Gamma^m} \vec{U}^{m+1}), \eta \right\rangle_{\Gamma^m} = 0 \quad \forall \eta \in V(\Gamma^m), \quad (10.26c)$$

$$\left\langle \frac{\vec{X}^{m+1} - \text{id}}{\Delta t_m}, \vec{\chi} \right\rangle_{\Gamma^m}^h = \left\langle \vec{U}^{m+1}, \vec{\chi} \right\rangle_{\Gamma^m}^h \quad \forall \vec{\chi} \in \underline{V}(\Gamma^m), \quad (10.26d)$$

$$\left\langle \vec{\kappa}^{m+1}, \vec{\eta} \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m), \quad (10.26e)$$

$$\begin{aligned} & \left\langle \vec{F}_\Gamma^{m+1}, \vec{\chi} \right\rangle_{\Gamma^m}^h = \left\langle \nabla_s \vec{\kappa}^{m+1}, \nabla_s \vec{\chi} \right\rangle_{\Gamma^m} + \left\langle \nabla_s \cdot \vec{\kappa}_{\Gamma^m}^m, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^m} \\ & + \frac{1}{2} \left\langle |\kappa_{\Gamma^m}^m|^2, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma^m} - 2 \left\langle \nabla_s \vec{\kappa}_{\Gamma^m}^m, \underline{D}_s(\vec{\chi}) \right\rangle_{\Gamma^m} \quad \forall \vec{\chi} \in \underline{V}(\Gamma^m), \end{aligned} \quad (10.26f)$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$, $\vec{\kappa}_{\Gamma^{m+1}}^{m+1} = \vec{\kappa}^{m+1} \circ (\vec{X}^{m+1})^{-1} \in \underline{V}(\Gamma^{m+1})$ and $\vec{U}_{\Gamma^{m+1}}^{m+1} = \vec{\pi}_{\Gamma^m} \left[\vec{U}_{\Gamma^m}^{m+1} \right] \circ (\vec{X}^{m+1})^{-1} \in \underline{V}(\Gamma^{m+1})$.

The cases in which one or both of $\varkappa$ and β are different from zero can be handled in a similar way. Moreover, on using the techniques from §8.2, the approximations introduced above can also be generalized to the case of Navier–Stokes flow in the bulk. In addition, a fully discrete equivalent of the approach mentioned in Remark 10.4(i) ensures good volume conservation in practice. We refer to Barrett et al. (2016a, 2017b) for more details. Moreover, on assuming a discrete version of the LBB condition (10.16), one can prove that there exists a unique solution to (10.26) and to the corresponding fully discrete approximation of (10.17a–e), (10.25), as well as to their extensions discussed above. The necessary techniques can be found in the proofs of Barrett et al. (2016a, Theorem 5.1) and Barrett et al. (2017b, Theorem 5.1). Finally, we observe that the linear systems resulting from (10.26) and its extensions can be solved with the help of a Schur complement approach, on combining the techniques presented in Remark 8.6 and Remark 9.18. We refer to Barrett et al. (2016a, §6) and Barrett et al. (2017b, §6) for more details.

In Figure 7 we show a numerical simulation for an extension of the scheme (10.26) to Navier–Stokes flow in the bulk. The domain Ω is chosen to have a constriction, and the chosen boundary conditions model a Poiseuille-type flow.

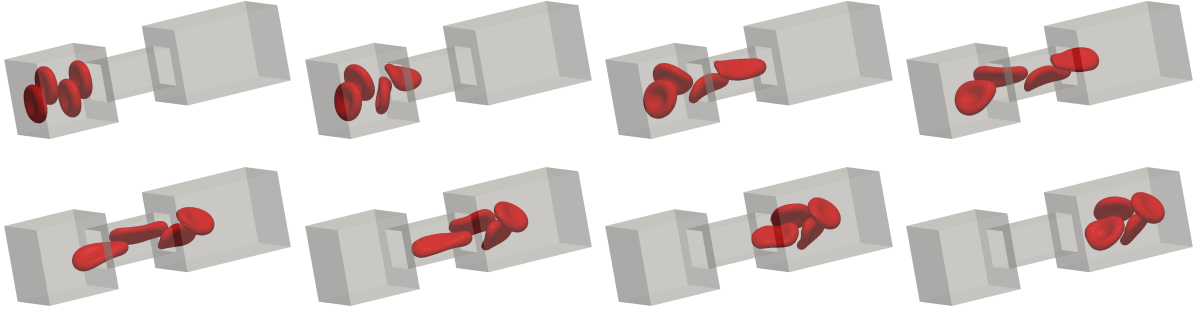


Figure 7: Visualization of the numerical experiment shown in Barrett et al. (2016a, Fig. 12). The snapshots are taken at times $t = 0, 0.5, 1, 1.5, 2, 2.5, 3, 4$.

10.4 Two-phase biomembranes

It is also possible to consider two-phase biomembranes. In this case we can introduce an order parameter $\mathbf{c}$, which takes the values ± 1 in the two different phases, and this parameter is related to the composition of a chemical species within the membrane. On the surface we then use a phase field model to approximate the interfacial energy by the Ginzburg–Landau functional

$$\varsigma \int_{\Gamma} \frac{1}{2} \varepsilon |\nabla_s \mathbf{c}|^2 + \varepsilon^{-1} \Psi(\mathbf{c}) \, d\mathcal{H}^{d-1}.$$

Here Ψ is a double well potential, $\varsigma > 0$ is related to the tension of the interface between the two phases on the membrane, often called line tension in the special case $d = 3$, and $\varepsilon > 0$ is related to the interfacial thickness of a diffuse layer between the two phases.

In the different phases α , $\overline{\alpha}$ and α^G , cf. (10.1), will take different values, and we will interpolate these values obtaining functions $\alpha(\mathbf{c}) > 0$, $\overline{\alpha}(\mathbf{c})$ and $\alpha^G(\mathbf{c})$. The total energy, in the absence of ADE effects, will hence have the form

$$E(\Gamma, \mathbf{c}) = \int_{\Gamma} b(\boldsymbol{\kappa}, \mathbf{c}) + \alpha^G(\mathbf{c}) \mathcal{K} + \varsigma b_{GL}(\mathbf{c}) \, d\mathcal{H}^{d-1}, \quad (10.27)$$

where

$$b(\boldsymbol{\kappa}, \mathbf{c}) = \frac{1}{2} \alpha(\mathbf{c}) (\boldsymbol{\kappa} - \overline{\alpha}(\mathbf{c}))^2 \quad \text{and} \quad b_{GL}(\mathbf{c}) = \frac{1}{2} \varepsilon |\nabla_s \mathbf{c}|^2 + \varepsilon^{-1} \Psi(\mathbf{c}).$$

In Barrett et al. (2017d) the present authors generalized the model for the dynamics of fluidic biomembranes to the two-phase case in the absence of ADE effects. Let us state here some basic ingredients. One now has to introduce an appropriate evolution law for the species concentration, $\mathbf{c}$, on the membrane. To this end, we considered the following Cahn–Hilliard dynamics on $\Gamma(t)$

$$\vartheta \partial_t^\bullet \mathbf{c} = \Delta_s \mathbf{m}, \quad \mathbf{m} = -\varsigma \varepsilon \Delta_s \mathbf{c} + \varsigma \varepsilon^{-1} \Psi'(\mathbf{c}) + (\partial_{\mathbf{c}} b)(\boldsymbol{\kappa}, \mathbf{c}) + (\alpha^G)'(\mathbf{c}) \mathcal{K},$$

where $\partial_t^\bullet$ is the material time derivative as defined in (10.5), $\mathbf{m}$ denotes the chemical potential and $\vartheta \in \mathbb{R}_{>0}$ is a kinetic coefficient. We note here that $\mathbf{m} = \frac{\delta}{\delta \mathbf{c}} E(\Gamma, \mathbf{c})$ is the

first variation of the total energy with respect to $\mathbf{c}$. In addition, the force $\vec{f}_\Gamma$ in (10.3b) needs to be modified to take into account the concentration $\mathbf{c}$. The generalized force is given by minus the first variation of the energy (10.27) with respect to Γ , i.e.

$$\begin{aligned}\vec{f}_\Gamma &= -\frac{\delta}{\delta\Gamma} E(\Gamma, \mathbf{c}) \\ &= \left[-\Delta_s [\alpha(\mathbf{c}) (\chi - \bar{\chi}(\mathbf{c}))] - \alpha(\mathbf{c}) (\chi - \bar{\chi}(\mathbf{c})) |\nabla_s \vec{\nu}|^2 + b(\chi, \mathbf{c}) \chi \right. \\ &\quad \left. - \nabla_s \cdot ([\chi \mathbf{Id} + \nabla_s \vec{\nu}] \nabla_s \alpha^G(\mathbf{c})) \right] \vec{\nu} + [(\partial_c b)(\chi, \mathbf{c}) + (\alpha^G)'(\mathbf{c}) \mathcal{K}] \nabla_s \mathbf{c} \\ &\quad + \varsigma [b_{GL}(\mathbf{c}) \chi \vec{\nu} + \nabla_s b_{GL}(\mathbf{c}) - \varepsilon \nabla_s \cdot ((\nabla_s \mathbf{c}) \otimes (\nabla_s \mathbf{c}))],\end{aligned}$$

where we note that

$$(\partial_c b)(\chi, \mathbf{c}) = \frac{1}{2} \alpha'(\mathbf{c}) (\chi - \bar{\chi}(\mathbf{c}))^2 - \alpha(\mathbf{c}) (\chi - \bar{\chi}(\mathbf{c})) \bar{\chi}'(\mathbf{c}).$$

We observe that in contrast to situations where the energy density does not depend on a species concentration, we now have tangential contributions to $\vec{f}_\Gamma$, which gives rise to a Marangoni-type effect. These equations now have to be coupled to (10.2) and (10.3). A stable semidiscrete formulation of the resulting total system has been derived in Barrett et al. (2017d), where also several numerical computations showing the influence of the occurrence of the two different phases on the evolution of the membrane are shown.

10.5 Alternative numerical approaches

Let us now mention other contributions that take local incompressibility and/or fluid effects into account in the evolution of vesicles and membranes. In Bonito et al. (2011) a fluid-membrane system, in which forces resulting from the Willmore energy act on an interior flow, has been studied. Local incompressibility conditions on the membrane have been addressed by Salac and Miksis (2011); Laadhari et al. (2014); Gera and Salac (2018) within a level set context, by Jamet and Misbah (2007); Aland et al. (2014) with the help of a phase field approach and by Hu et al. (2014); Heintz (2015) using an immersed boundary method. Moreover, Rahimi and Arroyo (2012); Rodrigues et al. (2015) presented numerical results using a surface Stokes system without taking the bulk fluid flow into account. There the volume conservation is enforced by a global Lagrange multiplier. Arroyo et al. (2010) simultaneously take surface and bulk viscosity effects in the fluidic membrane evolution into account. Their numerical results are in an axisymmetric setting.

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References

- M. Agnese and R. Nürnberg. Fitted finite element discretization of two-phase Stokes flow. *Internat. J. Numer. Methods Fluids*, 82(11):709–729, 2016.

- M. Agnese and R. Nürnberg. Fitted front tracking methods for two-phase incompressible Navier–Stokes flow: Eulerian and ALE finite element discretizations, 2019. (submitted for publication).
- I. Agricola and T. Friedrich. *Global Analysis: Differential Forms in Analysis, Geometry, and Physics*, volume 52 of *Graduate Studies in Mathematics*. Amer. Math. Soc., Providence, RI, 2002.
- S. Aland, S. Egerer, J. Lowengrub, and A. Voigt. Diffuse interface models of locally inextensible vesicles in a viscous fluid. *J. Comput. Phys.*, 277:32–47, 2014.
- S. Aland, A. Hahn, C. Kahle, and R. Nürnberg. Comparative simulations of Taylor flow with surfactants based on sharp- and diffuse-interface methods. In D. Bothe and A. Reusken, editors, *Transport Processes at Fluidic Interfaces*, pages 639–679. Birkhäuser, Berlin, 2017.
- R. F. Almgren. Variational algorithms and pattern formation in dendritic solidification. *J. Comput. Phys.*, 106(2):337–354, 1993.
- L. Alvarez, F. Guichard, P.-L. Lions, and J.-M. Morel. Axioms and fundamental equations of image processing. *Arch. Rational Mech. Anal.*, 123(3):199–257, 1993.
- H. Amann and J. Escher. *Analysis III*. Birkhäuser, Basel, 2009.
- M. Arroyo and A. DeSimone. Relaxation dynamics of fluid membranes. *Phys. Rev. E*, 79(3):031915, 2009.
- M. Arroyo, A. DeSimone, and L. Heltai. The role of membrane viscosity in the dynamics of fluid membranes. arXiv:1007.4934, 2010. URL <http://arxiv.org/abs/1007.4934>.
- E. Bänsch. Finite element discretization of the Navier–Stokes equations with a free capillary surface. *Numer. Math.*, 88(2):203–235, 2001.
- E. Bänsch and A. Schmidt. Simulation of dendritic crystal growth with thermal convection. *Interfaces Free Bound.*, 2(1):95–115, 2000.
- E. Bänsch and A. Schmidt. Free boundary problems in fluids and materials. In *Handbook of Numerical Analysis, Vol. XXI & XXII*. Elsevier, 2019. (to appear).
- E. Bänsch, P. Morin, and R. H. Nochetto. Surface diffusion of graphs: variational formulation, error analysis, and simulation. *SIAM J. Numer. Anal.*, 42(2):773–799, 2004.
- E. Bänsch, P. Morin, and R. H. Nochetto. A finite element method for surface diffusion: the parametric case. *J. Comput. Phys.*, 203(1):321–343, 2005.
- J. W. Barrett, K. Deckelnick, and V. Styles. Numerical analysis for a system coupling curve evolution to reaction diffusion on the curve. *SIAM J. Numer. Anal.*, 55(2):1080–1100, 2017a.
- J. W. Barrett and C. M. Elliott. A finite element method on a fixed mesh for the Stefan problem with convection in a saturated porous medium. In K. W. Morton and M. J. Baines, editors, *Numerical Methods for Fluid Dynamics*, pages 389–409. Academic Press (London), 1982.
- J. W. Barrett, H. Garcke, and R. Nürnberg. A parametric finite element method for fourth order geometric evolution equations. *J. Comput. Phys.*, 222(1):441–462, 2007a.
- J. W. Barrett, H. Garcke, and R. Nürnberg. On the variational approximation of combined second and fourth order geometric evolution equations. *SIAM J. Sci. Comput.*, 29(3):1006–1041, 2007b.
- J. W. Barrett, H. Garcke, and R. Nürnberg. On the parametric finite element approximation of evolving hypersurfaces in $\mathbb{R}^3$. *J. Comput. Phys.*, 227(9):4281–4307, 2008a.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Numerical approximation of anisotropic geometric evolution equations in the plane. *IMA J. Numer. Anal.*, 28(2):292–330, 2008b.
- J. W. Barrett, H. Garcke, and R. Nürnberg. A variational formulation of anisotropic geometric evolution equations in higher dimensions. *Numer. Math.*, 109(1):1–44, 2008c.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Parametric approximation of Willmore flow and related geometric evolution equations. *SIAM J. Sci. Comput.*, 31(1):225–253, 2008d.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Parametric approximation of surface clusters driven by isotropic and anisotropic surface energies. *Interfaces Free Bound.*, 12(2):187–234, 2010a.

- J. W. Barrett, H. Garcke, and R. Nürnberg. Numerical approximation of gradient flows for closed curves in $\mathbb{R}^d$. *IMA J. Numer. Anal.*, 30(1):4–60, 2010b.
- J. W. Barrett, H. Garcke, and R. Nürnberg. On stable parametric finite element methods for the Stefan problem and the Mullins–Sekerka problem with applications to dendritic growth. *J. Comput. Phys.*, 229(18):6270–6299, 2010c.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Finite element approximation of coupled surface and grain boundary motion with applications to thermal grooving and sintering. *European J. Appl. Math.*, 21(6):519–556, 2010d.
- J. W. Barrett, H. Garcke, and R. Nürnberg. The approximation of planar curve evolutions by stable fully implicit finite element schemes that equidistribute. *Numer. Methods Partial Differential Equations*, 27(1):1–30, 2011.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Numerical computations of faceted pattern formation in snow crystal growth. *Phys. Rev. E*, 86(1):011604, 2012a.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Parametric approximation of isotropic and anisotropic elastic flow for closed and open curves. *Numer. Math.*, 120(3):489–542, 2012b.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Elastic flow with junctions: Variational approximation and applications to nonlinear splines. *Math. Models Methods Appl. Sci.*, 22(11):1250037, 2012c.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Finite element approximation of one-sided Stefan problems with anisotropic, approximately crystalline, Gibbs–Thomson law. *Adv. Differential Equations*, 18(3-4):383–432, 2013a.
- J. W. Barrett, H. Garcke, and R. Nürnberg. On the stable discretization of strongly anisotropic phase field models with applications to crystal growth. *ZAMM Z. Angew. Math. Mech.*, 93(10-11):719–732, 2013b.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Eliminating spurious velocities with a stable approximation of viscous incompressible two-phase Stokes flow. *Comput. Methods Appl. Mech. Engrg.*, 267:511–530, 2013c.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Stable phase field approximations of anisotropic solidification. *IMA J. Numer. Anal.*, 34(4):1289–1327, 2014a.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Phase field models versus parametric front tracking methods: Are they accurate and computationally efficient? *Commun. Comput. Phys.*, 15(2):506–555, 2014b.
- J. W. Barrett, H. Garcke, and R. Nürnberg. A stable parametric finite element discretization of two-phase Navier–Stokes flow. *J. Sci. Comp.*, 63(1):78–117, 2015a.
- J. W. Barrett, H. Garcke, and R. Nürnberg. On the stable numerical approximation of two-phase flow with insoluble surfactant. *M2AN Math. Model. Numer. Anal.*, 49(2):421–458, 2015b.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Stable finite element approximations of two-phase flow with soluble surfactant. *J. Comput. Phys.*, 297:530–564, 2015c.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Stable numerical approximation of two-phase flow with a Boussinesq–Scriven surface fluid. *Commun. Math. Sci.*, 13(7):1829–1874, 2015d.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Numerical computations of the dynamics of fluidic membranes and vesicles. *Phys. Rev. E*, 92(5):052704, 2015e.
- J. W. Barrett, H. Garcke, and R. Nürnberg. A stable numerical method for the dynamics of fluidic biomembranes. *Numer. Math.*, 134(4):783–822, 2016a.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Computational parametric Willmore flow with spontaneous curvature and area difference elasticity effects. *SIAM J. Numer. Anal.*, 54(3):1732–1762, 2016b.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Finite element approximation for the dynamics of asymmetric fluidic biomembranes. *Math. Comp.*, 86(305):1037–1069, 2017b.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Stable variational approximations of boundary

- value problems for Willmore flow with Gaussian curvature. *IMA J. Numer. Anal.*, 37(4): 1657–1709, 2017c.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Finite element approximation for the dynamics of fluidic two-phase biomembranes. *M2AN Math. Model. Numer. Anal.*, 51(6):2319–2366, 2017d.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Gradient flow dynamics of two-phase biomembranes: Sharp interface variational formulation and finite element approximation. *SMAI J. Comput. Math.*, 4:151–195, 2018.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Variational discretization of axisymmetric curvature flows. *Numer. Math.*, 141(3):791–837, 2019a.
- J. W. Barrett, H. Garcke, and R. Nürnberg. Finite element methods for fourth order axisymmetric geometric evolution equations. *J. Comput. Phys.*, 376:733–766, 2019b.
- S. Bartels. Nonlinear plates. In *Handbook of Numerical Analysis, Vol. XXI & XXII*. Elsevier, 2019. (to appear).
- S. Bartels, G. Dolzmann, R. H. Nochetto, and A. Raisch. Finite element methods for director fields on flexible surfaces. *Interfaces Free Bound.*, 14(2):231–272, 2012.
- A. Bartezzaghi, L. Dedè, and A. Quarteroni. Biomembrane modeling with isogeometric analysis. *Comput. Methods Appl. Mech. Engrg.*, 347:103–119, 2019.
- L. Beirão da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L. D. Marini, and A. Russo. Basic principles of virtual element methods. *Math. Models Methods Appl. Sci.*, 23(1):199–214, 2013.
- G. Bellettini, M. Novaga, and M. Paolini. Facet-breaking for three-dimensional crystals evolving by mean curvature. *Interfaces Free Bound.*, 1(1):39–55, 1999.
- M. Beneš. Diffuse-interface treatment of the anisotropic mean-curvature flow. *Appl. Math.*, 48(6):437–453, 2003.
- A. I. Bobenko and P. Schröder. Discrete Willmore flow. In J. Fujii, editor, *ACM SIGGRAPH 2005 Courses*, SIGGRAPH ’05, New York, NY, 2005. ACM.
- D. Boffi. Three-dimensional finite element methods for the Stokes problem. *SIAM J. Numer. Anal.*, 34(2):664–670, 1997.
- A. Bonito, R. H. Nochetto, and M. S. Pauletti. Parametric FEM for geometric biomembranes. *J. Comput. Phys.*, 229(9):3171–3188, 2010.
- A. Bonito, R. H. Nochetto, and M. S. Pauletti. Dynamics of biomembranes: effect of the bulk fluid. *Math. Model. Nat. Phenom.*, 6(5):25–43, 2011.
- A. Bonito, A. Demlow, and R. H. Nochetto. Numerical methods for the Laplace–Beltrami operator. In *Handbook of Numerical Analysis, Vol. XXI & XXII*. Elsevier, 2019. (to appear).
- D. Bothe and J. Prüss. On the two-phase Navier–Stokes equations with Boussinesq–Scriven surface fluid. *J. Math. Fluid Mech.*, 12(1):133–150, 2010.
- E. Bretin, S. Masnou, and E. Oudet. Phase-field approximations of the Willmore functional and flow. *Numer. Math.*, 131(1):115–171, 2015.
- M. Burger. Numerical simulation of anisotropic surface diffusion with curvature-dependent energy. *J. Comput. Phys.*, 203(2):602–625, 2005.
- M. Burger, F. Haußer, C. Stöcker, and A. Voigt. A level set approach to anisotropic flows with curvature regularization. *J. Comput. Phys.*, 225(1):183–205, 2007.
- G. Caginalp and J.-T. Lin. A numerical analysis of an anisotropic phase field model. *IMA J. Appl. Math.*, 39(1):51–66, 1987.
- J. W. Cahn and J. E. Taylor. Surface motion by surface diffusion. *Acta Metall. Mater.*, 42: 1045–1063, 1994.
- P. B. Canham. The minimum energy of bending as a possible explanation of the biconcave shape of the human red blood cell. *J. Theor. Biol.*, 26(1):61–81, 1970.
- P. G. Ciarlet. *The Finite Element Method for Elliptic Problems*. North-Holland Publishing Co., Amsterdam, 1978. Studies in Mathematics and its Applications, Vol. 4.

- CIBC, 2016. Cleaver: A MultiMaterial Tetrahedral Meshing Library and Application. Scientific Computing and Imaging Institute (SCI), Download from: www.sci.utah.edu/cibc/software.
- U. Clarenz, U. Diewald, G. Dziuk, M. Rumpf, and R. Rusu. A finite element method for surface restoration with smooth boundary conditions. *Comput. Aided Geom. Design*, 21(5):427–445, 2004.
- U. Clarenz, F. Haußer, M. Rumpf, A. Voigt, and U. Weikard. On level set formulations for anisotropic mean curvature flow and surface diffusion. In *Multiscale Modeling in Epitaxial Growth*, volume 149 of *Internat. Ser. Numer. Math.*, pages 227–237. Birkhäuser, Basel, 2005.
- B. D. Coleman, R. S. Falk, and M. Moakher. Space-time finite element methods for surface diffusion with applications to the theory of the stability of cylinders. *SIAM J. Sci. Comput.*, 17(6):1434–1448, 1996.
- T. A. Davis. Algorithm 832: UMFPACK V4.3—an unsymmetric-pattern multifrontal method. *ACM Trans. Math. Software*, 30(2):196–199, 2004.
- T. A. Davis. Algorithm 915, SuiteSparseQR: Multifrontal multithreaded rank-revealing sparse QR factorization. *ACM Trans. Math. Software*, 38(1):1–22, 2011.
- J.-M. Debierre, A. Karma, F. Celestini, and R. Guérin. Phase-field approach for faceted solidification. *Phys. Rev. E*, 68(4):041604, 2003.
- K. Deckelnick and G. Dziuk. On the approximation of the curve shortening flow. In C. Bandle, J. Bemelmans, M. Chipot, J. S. J. Paulin, and I. Shafrir, editors, *Calculus of Variations, Applications and Computations (Pont-à-Mousson, 1994)*, volume 326 of *Pitman Res. Notes Math. Ser.*, pages 100–108. Longman Sci. Tech., Harlow, 1995.
- K. Deckelnick and G. Dziuk. Discrete anisotropic curvature flow of graphs. *M2AN Math. Model. Numer. Anal.*, 33(6):1203–1222, 1999.
- K. Deckelnick and G. Dziuk. Error analysis of a finite element method for the Willmore flow of graphs. *Interfaces Free Bound.*, 8(1):21–46, 2006.
- K. Deckelnick and G. Dziuk. Error analysis for the elastic flow of parametrized curves. *Math. Comp.*, 78(266):645–671, 2009.
- K. Deckelnick and F. Schieweck. Error analysis for the approximation of axisymmetric Willmore flow by C^1 -finite elements. *Interfaces Free Bound.*, 12(4):551–574, 2010.
- K. Deckelnick, G. Dziuk, and C. M. Elliott. Error analysis of a semidiscrete numerical scheme for diffusion in axially symmetric surfaces. *SIAM J. Numer. Anal.*, 41(6):2161–2179, 2003.
- K. Deckelnick, G. Dziuk, and C. M. Elliott. Computation of geometric partial differential equations and mean curvature flow. *Acta Numer.*, 14:139–232, 2005a.
- K. Deckelnick, G. Dziuk, and C. M. Elliott. Fully discrete finite element approximation for anisotropic surface diffusion of graphs. *SIAM J. Numer. Anal.*, 43(3):1112–1138, 2005b.
- K. Deckelnick, J. Katz, and F. Schieweck. A C^1 -finite element method for the Willmore flow of two-dimensional graphs. *Math. Comp.*, 84(296):2617–2643, 2015.
- A. Dedner, R. Klöforn, M. Nolte, and M. Ohlberger. A Generic Interface for Parallel and Adaptive Scientific Computing: Abstraction Principles and the DUNE-FEM Module. *Computing*, 90(3–4):165–196, 2010.
- D. M. DeTurck. Deforming metrics in the direction of their Ricci tensors. *J. Differential Geom.*, 18(1):157–162, 1983.
- M. P. do Carmo. *Differential Geometry of Curves and Surfaces*. Prentice-Hall Inc., Englewood Cliffs, N. J., 1976.
- M. Droske and M. Rumpf. A level set formulation for Willmore flow. *Interfaces Free Bound.*, 6(3):361–378, 2004.
- Q. Du and X. Feng. The phase field method for geometric moving interfaces and their numerical approximations. In *Handbook of Numerical Analysis, Vol. XXI & XXII*. Elsevier, 2019. (to appear).

- Q. Du, C. Liu, R. Ryham, and X. Wang. A phase field formulation of the Willmore problem. *Nonlinearity*, 18(3):1249–1267, 2005.
- G. Dziuk. An algorithm for evolutionary surfaces. *Numer. Math.*, 58(6):603–611, 1991.
- G. Dziuk. Convergence of a semi-discrete scheme for the curve shortening flow. *Math. Models Methods Appl. Sci.*, 4:589–606, 1994.
- G. Dziuk. Discrete anisotropic curve shortening flow. *SIAM J. Numer. Anal.*, 36:1808–1830, 1999a.
- G. Dziuk. Numerical schemes for the mean curvature flow of graphs. In *Variations of domain and free-boundary problems in solid mechanics (Paris, 1997)*, volume 66 of *Solid Mech. Appl.*, pages 63–70. Kluwer Acad. Publ., Dordrecht, 1999b.
- G. Dziuk. Computational parametric Willmore flow. *Numer. Math.*, 111(1):55–80, 2008.
- G. Dziuk and C. M. Elliott. Finite element methods for surface PDEs. *Acta Numer.*, 22:289–396, 2013.
- G. Dziuk, E. Kuwert, and R. Schätzle. Evolution of elastic curves in $\mathbb{R}^n$: existence and computation. *SIAM J. Math. Anal.*, 33(5):1228–1245, 2002.
- C. Eck, H. Garcke, and P. Knabner. *Mathematical modeling*. Springer Undergraduate Mathematics Series. Springer, Cham, 2017.
- C. M. Elliott and H. Fritz. On approximations of the curve shortening flow and of the mean curvature flow based on the DeTurck trick. *IMA J. Numer. Anal.*, 37(2):543–603, 2017.
- C. M. Elliott and H. Garcke. Diffusional phase transitions in multicomponent systems with a concentration dependent mobility matrix. *Phys. D*, 109:242–256, 1997.
- C. M. Elliott and B. Stinner. Modeling and computation of two phase geometric biomembranes using surface finite elements. *J. Comput. Phys.*, 229(18):6585–6612, 2010.
- C. M. Elliott and B. Stinner. Computation of two-phase biomembranes with phase dependent material parameters using surface finite elements. *Commun. Comput. Phys.*, 13(2):325–360, 2013.
- H. C. Elman, D. J. Silvester, and A. J. Wathen. *Finite elements and fast iterative solvers: with applications in incompressible fluid dynamics*. Numerical Mathematics and Scientific Computation. Oxford University Press, New York, 2005.
- J. Escher, Y. Giga, and K. Ito. On a limiting motion and self-intersections of curves moved by the intermediate surface diffusion flow. *Nonlinear Anal.*, 47(6):3717–3728, 2001.
- S. Esedoğlu, A. Rätz, and M. Röger. Colliding interfaces in old and new diffuse-interface approximations of Willmore-flow. *Commun. Math. Sci.*, 12(1):125–147, 2014.
- M. Gage and R. S. Hamilton. The heat equation shrinking convex plane curves. *J. Differential Geom.*, 23(1):69–96, 1986.
- S. Ganesan and L. Tobiska. Arbitrary Lagrangian–Eulerian finite-element method for computation of two-phase flows with soluble surfactants. *J. Comput. Phys.*, 231(9):3685–3702, 2012.
- S. Ganesan, G. Matthies, and L. Tobiska. On spurious velocities in incompressible flow problems with interfaces. *Comput. Methods Appl. Mech. Engrg.*, 196(7):1193–1202, 2007.
- H. Garcke. Curvature driven interface evolution. *Jahresber. Dtsch. Math.-Ver.*, 115(2):63–100, 2013.
- H. Garcke, B. Stoth, and B. Nestler. Anisotropy in multi-phase systems: a phase field approach. *Interfaces Free Bound.*, 1(2):175–198, 1999.
- H. Garcke, M. Hinze, and C. Kahle. A stable and linear time discretization for a thermodynamically consistent model for two-phase incompressible flow. *Appl. Numer. Math.*, 99:151–171, 2016.
- P. Gera and D. Salac. Modeling of multicomponent three-dimensional vesicles. *Comput. & Fluids*, 172:362–383, 2018.
- C. Geuzaine and J.-F. Remacle. Gmsh: A 3-D finite element mesh generator with built-in pre-

- and post-processing facilities. *Internat. J. Numer. Methods Engrg.*, 79(11):1309–1331, 2009.
- Y. Giga. *Surface Evolution Equations*. Birkhäuser, Basel, 2006.
- D. Gilbarg and N. S. Trudinger. *Elliptic Partial Differential Equations of Second Order*, volume 224 of *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*. Springer-Verlag, Berlin, second edition, 1983.
- V. Girault and P.-A. Raviart. *Finite element methods for Navier–Stokes equations*, volume 5 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, 1986. Theory and algorithms.
- C. Gräser, R. Kornhuber, and U. Sack. Time discretizations of anisotropic Allen–Cahn equations. *IMA J. Numer. Anal.*, 33:1226–1244, 2013.
- J. Gravner and D. Griffeath. Modeling snow-crystal growth: A three-dimensional mesoscopic approach. *Phys. Rev. E*, 79(1):011601–1–18, 2009.
- S. Groß and A. Reusken. An extended pressure finite element space for two-phase incompressible flows with surface tension. *J. Comput. Phys.*, 224(1):40–58, 2007.
- G. Grün and F. Klingbeil. Two-phase flow with mass density contrast: Stable schemes for a thermodynamic consistent and frame-indifferent diffuse-interface model. *J. Comput. Phys.*, 257:708–725, 2014.
- F. Haußer and A. Voigt. A discrete scheme for regularized anisotropic surface diffusion: a 6th order geometric evolution equation. *Interfaces Free Bound.*, 7:353–369, 2005.
- C.-J. Heine. Isoparametric finite element approximation of curvature on hypersurfaces, 2004. Preprint, University Freiburg.
- A. Heintz. A numerical method for simulation dynamics of incompressible lipid membranes in viscous fluid. *J. Comput. Appl. Math.*, 289:87–100, 2015.
- W. Helfrich. Elastic properties of lipid bilayers: Theory and possible experiments. *Z. Naturforsch.*, 28c:693–703, 1973.
- K. Hildebrandt, K. Polthier, and M. Wardetzky. On the convergence of metric and geometric properties of polyhedral surfaces. *Geom. Dedicata*, 123:89–112, 2006.
- M. Hinze, R. Pinnau, M. Ulbrich, and S. Ulbrich. *Optimization with PDE constraints*, volume 23 of *Mathematical Modelling: Theory and Applications*. Springer-Verlag, New York, 2009.
- C. W. Hirt and B. D. Nichols. Volume of fluid (VOF) method for the dynamics of free boundaries. *J. Comput. Phys.*, 39(1):201–225, 1981.
- T. Y. Hou, J. S. Lowengrub, and M. J. Shelley. Removing the stiffness from interfacial flows with surface tension. *J. Comput. Phys.*, 114(2):312–338, 1994.
- W.-F. Hu, Y. Kim, and M.-C. Lai. An immersed boundary method for simulating the dynamics of three-dimensional axisymmetric vesicles in Navier–Stokes flows. *J. Comput. Phys.*, 257:670–686, 2014.
- G. Huisken. Flow by mean curvature of convex surfaces into spheres. *J. Differential Geom.*, 20(1):237–266, 1984.
- A. J. James and J. Lowengrub. A surfactant-conserving volume-of-fluid method for interfacial flows with insoluble surfactant. *J. Comput. Phys.*, 201(2):685–722, 2004.
- D. Jamet and C. Misbah. Towards a thermodynamically consistent picture of the phase-field model of vesicles: Local membrane incompressibility. *Phys. Rev. E*, 76(5):051907, 2007.
- D. Juric and G. Tryggvason. A front-tracking method for dendritic solidification. *J. Comput. Phys.*, 123(1):127–148, 1996.
- A. Karma and W.-J. Rappel. Quantitative phase-field modeling of dendritic growth in two and three dimensions. *Phys. Rev. E*, 57(4):4323–4349, Apr 1998.
- D. Kay, V. Styles, and R. Welford. Finite element approximation of a Cahn–Hilliard–Navier–Stokes system. *Interfaces Free Bound.*, 10(1):15–43, 2008.
- D. A. Kessler, J. Koplik, and H. Levine. Numerical simulation of two-dimensional snowflake growth. *Phys. Rev. A*, 30(5):2820–2823, Nov 1984.

- J. Kim, K. Kang, and J. Lowengrub. Conservative multigrid methods for Cahn–Hilliard fluids. *J. Comput. Phys.*, 193(2):511–543, 2004.
- M. Kimura. Accurate numerical scheme for the flow by curvature. *Appl. Math. Lett.*, 7(1):69–73, 1994.
- R. Kobayashi. Modeling and numerical simulations of dendritic crystal growth. *Phys. D*, 63(3–4):410–423, 1993.
- M. Köhne and D. Lengeler. Local well-posedness for relaxational fluid vesicle dynamics. *J. Evol. Equ.*, 18(4):1787–1818, 2018.
- B. Kovács, B. Li, and C. Lubich. A convergent evolving finite element algorithm for mean curvature flow of closed surfaces. arXiv:1805.06667, 2018. URL <https://arxiv.org/abs/1805.06667>.
- W. Kühnel. *Differential Geometry: Curves – Surfaces – Manifolds*, volume 77 of *Student Mathematical Library*. Amer. Math. Soc., Providence, RI, 2015.
- A. Laadhari, P. Saramito, and C. Misbah. Computing the dynamics of biomembranes by combining conservative level set and adaptive finite element methods. *J. Comput. Phys.*, 263:328–352, 2014.
- D. Lengeler. On a Stokes-type system arising in fluid vesicle dynamics. arXiv:1506.08991, 2015. URL <http://arxiv.org/abs/1506.08991>.
- D. Lengeler. Asymptotic stability of local Helfrich minimizers. *Interfaces Free Bound.*, 20(4):533–550, 2018.
- K. G. Libbrecht. The physics of snow crystals. *Rep. Progr. Phys.*, 68(4):855–895, 2005.
- K. G. Libbrecht. Physically derived rules for simulating faceted crystal growth using cellular automata. arXiv:0807.2616, 2008. URL <http://arxiv.org/abs/0807.2616>.
- C. Mantegazza. *Lecture notes on mean curvature flow*, volume 290 of *Progress in Mathematics*. Birkhäuser/Springer Basel AG, Basel, 2011.
- S. V. Matveev. *Lectures on algebraic topology*. EMS Series of Lectures in Mathematics. European Mathematical Society, Zürich, 2006.
- U. F. Mayer and G. Simonett. A numerical scheme for axisymmetric solutions of curvature-driven free boundary problems, with applications to the Willmore flow. *Interfaces Free Bound.*, 4(1):89–109, 2002.
- K. Mikula and D. Ševčovič. Evolution of plane curves driven by a nonlinear function of curvature and anisotropy. *SIAM J. Appl. Math.*, 61(5):1473–1501, 2001.
- K. Mikula, M. Remešíková, P. Sarkoci, and D. Ševčovič. Manifold evolution with tangential redistribution of points. *SIAM J. Sci. Comput.*, 36(4):A1384–A1414, 2014.
- W. W. Mullins. Theory of thermal grooving. *J. Appl. Phys.*, 28:333–339, 1957.
- B. Nestler. A 3D parallel simulator for crystal growth and solidification in complex alloy systems. *J. Cryst. Growth*, 275(1–2):e273–e278, 2005.
- J. C. C. Nitsche. Boundary value problems for variational integrals involving surface curvatures. *Quart. Appl. Math.*, 51(2):363–387, 1993.
- Z. Pan. *Simulation and Analysis of Coupled Surface and Grain Boundary Motion*. PhD thesis, University of British Columbia, Vancouver, 2008.
- Z. Pan and B. Wetton. A numerical method for coupled surface and grain boundary motion. *European J. Appl. Math.*, 19(3):311–327, 2008.
- P. Pozzi. Anisotropic curve shortening flow in higher codimension. *Math. Methods Appl. Sci.*, 30(11):1243–1281, 2007.
- P. Pozzi. Anisotropic mean curvature flow for two dimensional surfaces in higher codimension: a numerical scheme. *Interfaces Free Bound.*, 10(4):539–576, 2008.
- J. Prüss and G. Simonett. *Moving interfaces and quasilinear parabolic evolution equations*, volume 105 of *Monographs in Mathematics*. Birkhäuser/Springer, 2016.

- M. Rahimi and M. Arroyo. Shape dynamics, lipid hydrodynamics, and the complex viscoelasticity of bilayer membranes. *Phys. Rev. E*, 86(1):011932, 2012.
- C. A. Reiter. A local cellular model for snow crystal growth. *Chaos Soliton. Fract.*, 23(4):1111–1119, 2005.
- Y. Renardy and M. Renardy. PROST: a parabolic reconstruction of surface tension for the volume-of-fluid method. *J. Comput. Phys.*, 183(2):400–421, 2002.
- L. Rineau and M. Yvinec. 3D surface mesh generation. In *CGAL User and Reference Manual*. CGAL Editorial Board, 4.13 edition, 2018.
- D. S. Rodrigues, R. F. Ausas, F. Mut, and G. C. Buscaglia. A semi-implicit finite element method for viscous lipid membranes. *J. Comput. Phys.*, 298:565–584, 2015.
- A. R. Roosen and J. E. Taylor. Simulation of crystal growth with faceted interfaces. *Mater. Res. Soc. Symp. Proc.*, 237:25–36, 1991.
- R. E. Rusu. An algorithm for the elastic flow of surfaces. *Interfaces Free Bound.*, 7(3):229–239, 2005.
- D. Salac and M. Miksis. A level set projection model of lipid vesicles in general flows. *J. Comput. Phys.*, 230(22):8192–8215, 2011.
- G. Sapiro and A. Tannenbaum. On affine plane curve evolution. *J. Funct. Anal.*, 119(1):79–120, 1994.
- A. Schmidt. *Die Berechnung dreidimensionaler Dendriten mit Finiten Elementen*. PhD thesis, University Freiburg, Freiburg, 1993.
- A. Schmidt. Computation of three dimensional dendrites with finite elements. *J. Comput. Phys.*, 195(2):293–312, 1996.
- A. Schmidt. Approximation of crystalline dendrite growth in two space dimensions. In J. Kačur and K. Mikula, editors, *Proceedings of the Algoritmy’97 Conference on Scientific Computing (Zuberec)*, volume 67, pages 57–68, Bratislava, 1998. Slovak University of Technology.
- A. Schmidt and K. G. Siebert. *Design of Adaptive Finite Element Software: The Finite Element Toolbox ALBERTA*, volume 42 of *Lecture Notes in Computational Science and Engineering*. Springer-Verlag, Berlin, 2005.
- J. Schöberl. NETGEN: An advancing front 2D/3D-mesh generator based on abstract rules. *Comput. Vis. Sci.*, 1(1):41–52, 1997. sourceforge.net/projects/netgen-mesher/.
- L. E. Scriven. Dynamics of a fluid interface: Equation of motion for Newtonian surface fluids. *Chem. Eng. Sci.*, 12(2):98–108, 1960.
- U. Seifert. Configurations of fluid membranes and vesicles. *Adv. Phys.*, 46(1):13–137, 1997.
- J. A. Sethian. Curvature and the evolution of fronts. *Comm. Math. Phys.*, 101(4):487–499, 1985.
- J. A. Sethian. Level-set methods and geometric PDEs. In *Handbook of Numerical Analysis, Vol. XXI & XXII*. Elsevier, 2019. (to appear).
- J. A. Sethian and J. Strain. Crystal growth and dendritic solidification. *J. Comput. Phys.*, 98(2):231–253, 1992.
- J. C. Slattery, L. Sagis, and E.-S. Oh. *Interfacial transport phenomena*. Springer, New York, second edition, 2007.
- J. Strain. A boundary integral approach to unstable solidification. *J. Comput. Phys.*, 85(2):342–389, 1989.
- M. Sussman, P. Semerka, and S. Osher. A level set approach for computing solutions to incompressible two-phase flow. *J. Comput. Phys.*, 114(1):146–159, 1994.
- J. E. Taylor and J. W. Cahn. Linking anisotropic sharp and diffuse surface motion laws via gradient flows. *J. Statist. Phys.*, 77(1-2):183–197, 1994.
- J. E. Taylor, J. W. Cahn, and C. A. Handwerker. Geometric models of crystal growth. *Acta Metall. Mater.*, 40(7):1443–1474, 1992.
- R. Temam. *Navier–Stokes Equations*. Amer. Math. Soc., Providence, RI, 2001.

- S. Torabi, J. Lowengrub, A. Voigt, and S. Wise. A new phase-field model for strongly anisotropic systems. *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.*, 465(2105):1337–1359, 2009.
- F. Tröltzsch. *Optimal Control of Partial Differential Equations: Theory, Methods and Applications*, volume 112 of *Graduate Studies in Mathematics*. Amer. Math. Soc., Providence, RI, 2010.
- G. Tryggvason, B. Bunner, A. Esmaeeli, D. Juric, N. Al-Rawahi, W. Tauber, J. Han, S. Nas, and Y.-J. Jan. A front-tracking method for the computations of multiphase flow. *J. Comput. Phys.*, 169(2):708–759, 2001.
- S. Turek. Bubbles in fluid dynamics. In *Handbook of Numerical Analysis, Vol. XXI & XXII*. Elsevier, 2019. (to appear).
- S. O. Unverdi and G. Tryggvason. A front-tracking method for viscous, incompressible multi-fluid flows. *J. Comput. Phys.*, 100(1):25–37, 1992.
- S. W. Walker. Tetrahedralization of isosurfaces with guaranteed-quality by edge rearrangement (TIGER). *SIAM J. Sci. Comput.*, 35(1):A294–A326, 2013.
- S. W. Walker. *The Shapes of Things: A Practical Guide to Differential Geometry and the Shape Derivative*, volume 28 of *Advances in Design and Control*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2015.
- S. W. Walker. FELICITY: A MATLAB/C++ toolbox for developing finite element methods and simulation modeling. *SIAM J. Sci. Comput.*, 40(2):C234–C257, 2018.
- A. A. Wheeler, B. T. Murray, and R. J. Schaefer. Computation of dendrites using a phase field model. *Phys. D*, 66(1-2):243–262, 1993.
- J. Wloka. *Partial Differential Equations*. Cambridge University Press, Cambridge, 1987.
- E. Yokoyama. Formation of patterns during growth of snow crystals. *J. Cryst. Growth*, 128: 251–257, 1993.
- E. Zeidler. *Nonlinear Functional Analysis and its Applications IV, Applications to Mathematical Physics*. Springer-Verlag, Berlin, 1988.