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FINITE ELEMENT APPROXIMATION FOR THE DYNAMICS OF FLUIDIC TWO-PHASE BIOMEMBRANES

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Abstract. Biomembranes and vesicles consisting of multiple phases can attain a multitude of shapes, undergoing complex shape transitions. We study a Cahn–Hilliard model on an evolving hypersurface coupled to Navier–Stokes equations on the surface and in the surrounding medium to model these phenomena. The evolution is driven by a curvature energy, modelling the elasticity of the membrane, and by a Cahn–Hilliard type energy, modelling line energy effects. A stable semidiscrete finite element approximation is introduced and, with the help of a fully discrete method, several phenomena occurring for two-phase membranes are computed.

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1. Introduction

In lipid bilayer membranes a large variety of different shapes and complex shape transition behaviour can be observed. Biological membranes are composed of several components, and lateral separation into different phases or domains have been studied in experiments. Mathematical models for biological membranes treat them as a deformable inextensible fluidic surface governed by bending energies, which involve the curvature of the membrane. If different phases occur, these bending energies will depend on the individual phases, and the local shape of the membrane will depend on the phase present locally. It has also been observed that the interfacial energy of the phase boundaries on the membrane can have a pronounced effect on the membrane shape, and might lead to effects like budding and fission. We refer to [11] for experimental studies and to [10, 18, 31, 33, 45] for further information on membranes with different fluid phases.

There has been a huge interest in the modelling of (two-phase) biomembranes. Both equilibrium shapes, as well as the evolution of membranes, have been studied intensively. However, a model taking the fluidic behaviour of the membrane, the curvature elasticity, the interfacial line energy and the phase separation in a time dependent model into account is missing so far. It is the goal of this paper to present such a model and –which will be the main contribution of this paper– to come up with a stable (semidiscrete) numerical approximation scheme for the resulting equations. The model will be based on an elastic bending energy of Canham–Evans–Helfrich type and a Ginzburg–Landau energy modelling the interfacial energy. Through their first variation these energy contributions lead to driving forces for the evolution, which is given by a surface

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Navier–Stokes system, coupled to bulk dissipation of an ambient fluid, and a convective Cahn–Hilliard type equation, which is formulated on the evolving membrane. The fluid part of the model goes back to the work [1], whereas an evolution based on a Canham–Evans–Helfrich energy coupled to a Ginzburg–Landau energy on the surface has been studied in the context of gradient flows by [24–26, 29, 30, 35, 36]. However, a coupling, which will give the natural dynamics on the interface, is stated here for the first time, and we will show that physically reasonable energy dissipation inequalities hold. Here the dissipation has contributions stemming from viscous friction in the bulk and on the surface, and from dissipation due to diffusion on the membrane.

For the elastic energy we consider the classical Canham–Evans–Helfrich energy

$$\int_\Gamma \tfrac{1}{2}\,\alpha\,(\varkappa-\overline{\varkappa})^2 + \alpha^G\,\mathcal{K}\;\mathrm{d}\mathcal{H}^{d-1}\,, \tag{1.1}$$

where $\Gamma\subset\mathbb{R}^d$, $d=2,3$, is a hypersurface without boundary, $\alpha>0$ and α^G are the bending and Gaussian bending rigidities, $\varkappa$ is the mean curvature, $\overline{\varkappa}$ is the spontaneous curvature, which can be caused by local inhomogeneities within the membrane, $\mathcal{K}$ is the Gaussian curvature and $\mathcal{H}^{d-1}$ is the $(d-1)$-dimensional surface Hausdorff measure. As discussed in [38], the most general form of a curvature energy density that is at most quadratic in the principal curvatures and is also symmetric in the principal curvatures has the form $\frac{1}{2}\,\alpha\,\varkappa^2+\alpha^G\,\mathcal{K}+\alpha_1\,\varkappa+\alpha_2$, which leads to (1.1) by choosing $\alpha_1=-\alpha\,\overline{\varkappa}$ and $\alpha_2=\frac{1}{2}\,\alpha\,\overline{\varkappa}^2$. In the case $d=2$ the most general form which is at most quadratic in the curvature is $\frac{1}{2}\,\alpha\,\varkappa^2+\alpha_1\,\varkappa+\alpha_2$. Hence throughout this paper we set $\alpha^G=0$ in the case $d=2$.

We also introduce an order parameter $\mathfrak{c}$, which takes the values ±1 in the two different phases, and this parameter is related to the composition of the 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

$$\beta\int_\Gamma \tfrac{1}{2}\,\gamma\,|\nabla_s\,\mathfrak{c}|^2+\gamma^{-1}\,\Psi(\mathfrak{c})\;\mathrm{d}\mathcal{H}^{d-1}\,,$$

where $\beta>0$ is related to the line tension coefficient and γ is a multiple of the interfacial thickness of the diffusional layer separating the two phases. Furthermore, ∇_s is the surface gradient and Ψ is a double well potential.

In the different phases α, $\overline{\varkappa}$ and α^G will take different values, and we will interpolate these values obtaining functions $\alpha(\mathfrak{c})>0$, $\overline{\varkappa}(\mathfrak{c})$ and $\alpha^G(\mathfrak{c})$. The total energy will hence have the form

$$E(\Gamma,\mathfrak{c})=\int_\Gamma b(\varkappa,\mathfrak{c})+\alpha^G(\mathfrak{c})\,\mathcal{K}+\beta\,b_{GL}(\mathfrak{c})\;\mathrm{d}\mathcal{H}^{d-1}\,, \tag{1.2a}$$

where

$$b(\varkappa,\mathfrak{c})=\tfrac{1}{2}\,\alpha(\mathfrak{c})\,(\varkappa-\overline{\varkappa}(\mathfrak{c}))^2 \quad\text{and}\quad b_{GL}(\mathfrak{c})=\tfrac{1}{2}\,\gamma\,|\nabla_s\,\mathfrak{c}|^2+\gamma^{-1}\,\Psi(\mathfrak{c})\,. \tag{1.2b}$$

We recall that we assume $\alpha^G=0$ in the case $d=2$. In the case $d=3$, and if α^G is constant, then the contribution $\int_\Gamma \alpha^G(\mathfrak{c})\,\mathcal{K}\;\mathrm{d}\mathcal{H}^2$ is constant for a fixed topological type, which is a consequence of the Gauss–Bonnet theorem for closed surfaces,

$$\int_\Gamma \mathcal{K}\;\mathrm{d}\mathcal{H}^2=2\,\pi\,m(\Gamma)\,, \tag{1.3}$$

where $m(\Gamma)\in\mathbb{Z}$ denotes the Euler characteristic of Γ. However, if α^G is inhomogeneous, this term plays a role, which was discussed for example in [31] in the context of two-phase membranes. Here we also mention that the contributions $\frac{1}{2}\int_\Gamma \alpha(\mathfrak{c})\,\varkappa^2\;\mathrm{d}\mathcal{H}^2+\int_\Gamma \alpha^G(\mathfrak{c})\,\mathcal{K}\;\mathrm{d}\mathcal{H}^2$ to the energy $E(\Gamma,\mathfrak{c})$ are positive semidefinite with respect to the principal curvatures if $\alpha^G(s)\in[-2\,\alpha(s),0]$ for all $s\in\mathbb{R}$. On account of the Gauss–Bonnet theorem, (1.3), we hence obtain that the energy $E(\Gamma,\mathfrak{c})$ can be bounded from below if $\alpha^G(s)\geq\alpha^G_{\max}-2\,\alpha(s)$ for all $s\in\mathbb{R}$, which will hold whenever

$$\alpha_{\min}\geq\tfrac{1}{2}\,(\alpha^G_{\max}-\alpha^G_{\min})\,, \tag{1.4}$$

where $\alpha_{\min} = \min_{s\in\mathbb{R}} \alpha(s)$, and similarly for $\alpha^G_{\min}$, $\alpha^G_{\max}$. We note that this constraint is likely to have implications for the existence and regularity theory of gradient and related flows for $E(\Gamma, \mathfrak{c})$ in the case $d = 3$.

The energy (1.2a) represents a phase field approximation of a two-phase membrane curvature energy with line tension. In the limit $\gamma \to 0$ the diffusive interface disappears and a sharp interface limit is obtained. Sharp interface limits of phase field approaches to two-phase membranes have been studied with the help of formal asymptotics in [25] in the case of a C^1–limiting surface, and rigorously in [29] for axisymmetric two-phase membranes allowing for tangent discontinuities at interfaces. Later in [30] a rigorous convergence result for the axisymmetric situation in the C^1–case was also shown.

For the fluid part of the model we generalize the model from [1] to the two-phase phase field energy (1.2a). Here we only outline the main aspects of the model, with the precise details being given in Section 2. In particular, we consider a closed evolving membrane $(\Gamma(t))_{t\in[0,T]}$, with $T > 0$ being a fixed time, which separates a given domain Ω into regions $\Omega_+(t)$ and $\Omega_-(t) := \Omega \setminus \overline{\Omega}_+(t)$. We will assume that the classical Navier–Stokes equations, with density ρ and viscosity μ hold in $\Omega_-(t)$ and $\Omega_+(t)$. In the absence of mass transfer to/from the interface from/to the bulk it is natural to assume that the normal components of the velocity $\vec{u}$ in $\Omega_\pm(t)$ is continuous across the interface, see e.g. [42, p. 675] and [13, p. 137]. Moreover, we assume a no-slip condition of the velocity $\vec{u}$ at the interface, which means that the tangential components of the bulk velocity are also continuous across the interface, see e.g. [42, p. 293]. Hence the material on the interface is moved with the trace of the bulk velocity $\vec{u}\,|_{\Gamma(t)}$. In addition, and analogously to [1], we require an incompressible surface Navier–Stokes equation to hold on $\Gamma(t)$, with density ρ_Γ and surface viscosity μ_Γ. Here the main driving force for the surface Navier–Stokes equation is given by $\vec{f}_\Gamma = -\delta E/\delta\Gamma$, the first variation of the total energy of $\Gamma(t)$ with respect to Γ.

The overall model is completed by an appropriate evolution law for the species concentration on the membrane. To this end, we consider the following Cahn–Hilliard dynamics on $\Gamma(t)$

$$\vartheta\, \partial_t^\bullet\, \mathfrak{c} = \Delta_s\, \mathfrak{m}\,, \tag{1.5a}$$

$$\mathfrak{m} = -\beta\,\gamma\,\Delta_s\,\mathfrak{c} + \beta\,\gamma^{-1}\,\Psi'(\mathfrak{c}) + \tfrac{\partial}{\partial\mathfrak{c}}\,b(\varkappa,\mathfrak{c}) + (\alpha^G)'(\mathfrak{c})\,\mathcal{K}\,, \tag{1.5b}$$

where $\partial_t^\bullet$ is a material time derivative, $\mathfrak{m}$ denotes the chemical potential, $\Delta_s = \nabla_s\,.\,\nabla_s$ is the Laplace–Beltrami operator and $\vartheta \in \mathbb{R}_{>0}$ is a kinetic coefficient. We note here that $\mathfrak{m} = \delta E/\delta\mathfrak{c}$ is the first variation of the total energy with respect to $\mathfrak{c}$, see Sections 2, 3 and the Appendix for more details. Equation (1.5a) is a convection-diffusion equation for the species concentration on an evolving surface driven by the chemical potential $\mathfrak{m}$. For more information on the Cahn–Hilliard equation we refer to [22, 39]. We note that the Cahn–Hilliard equation on an evolving surface was studied in [23], including its finite element approximation.

It turns out that the overall model with suitable boundary conditions, e.g. $\vec{u} = 0$ on $\partial\Omega$, fulfils, in the case where the outer forces are zero, the following dissipation identity

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}&\left(\tfrac12\int_\Omega \rho\,|\vec{u}|^2\,\mathrm{d}\mathcal{L}^d + \tfrac12\int_{\Gamma(t)} \rho_\Gamma\,|\vec{u}|^2\,\mathrm{d}\mathcal{H}^{d-1} + E(\Gamma(t),\mathfrak{c}(t))\right)\\ &+ 2\int_\Omega \mu\,|\underline{\underline{D}}(\vec{u})|^2\,\mathrm{d}\mathcal{L}^d + 2\,\mu_\Gamma\int_{\Gamma(t)} |\underline{\underline{D}}_s(\vec{u})|^2\,\mathrm{d}\mathcal{H}^{d-1} + \vartheta^{-1}\int_{\Gamma(t)} |\nabla_s\,\mathfrak{m}|^2\,\mathrm{d}\mathcal{H}^{d-1} = 0\,,\end{aligned} \tag{1.6}$$

which is consistent with the second law of thermodynamics in its isothermal formulation. Here $\underline{\underline{D}}(\vec{u})$ and $\underline{\underline{D}}_s(\vec{u})$ are rate-of-deformation tensors in the bulk and on the surface, and so the fourth and fifth terms in (1.6) describe dissipation by viscous friction in the bulk and on the surface. In addition, the last term in (1.6) models dissipation due to diffusion of molecules on the surface. We also note that the introduced model conserves the volume of the bulk phases, the surface area and the total species concentration on the surface, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t}\,|\Omega^-(t)| = \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{H}^{d-1}(\Gamma(t)) = \frac{\mathrm{d}}{\mathrm{d}t}\int_{\Gamma(t)} \mathfrak{c}(t)\,\mathrm{d}\mathcal{H}^{d-1} = 0\,. \tag{1.7}$$

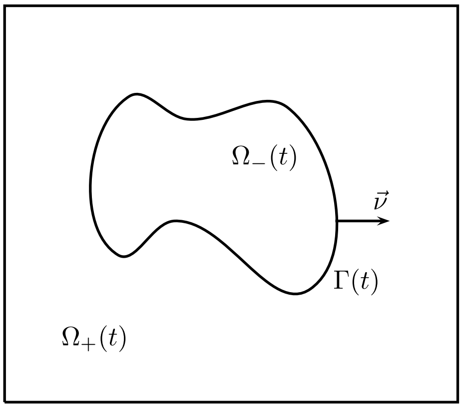

FIGURE 1. The domain Ω in the case $d = 2$.

In particular, in contrast to other works, no artificial Lagrange multipliers are needed to conserve the enclosed volume, the total surface area and the total species concentration.

It is one of the main goals of this contribution to introduce and analyze a numerical method that fulfils discrete variants of the dissipation identity and of the conservation properties (1.7), see the results in Theorem 4.2 and Theorem 4.3, below.

Let us now discuss related works on two-phase membranes. The interest in two-phase membranes increased due to the fascinating works [10,11], as experiments seem to validate earlier theories from [31,33] on two-phase membranes, and showed an amazing multitude of complex shapes and patterns. There have been many studies on two-phase axisymmetric two-phase membranes, both from an analytical and from a numerical point of view, see [14,15,28–31], and the references therein. However, only very few works study general shapes of two-phase membranes from a theoretical or computational point of view. In this context we refer to [16,24–26,34–37, 44,46]. But we note that none of the above mentioned contributions considered a stability analysis for their numerical approximations. We combine aspects of some of these approaches with the dynamics studied in [1], and we generalize computational approaches of the present authors for one-phase membranes, see e.g. [6,7], to numerically compute evolving two-phase membranes.

The outline of the paper is as follows. In the following section we introduce the model with all its details. In Section 3 we introduce a weak formulation, which is then discretized in space in Section 4. We then also show that this scheme decreases the total energy and obeys the relevant global conservation properties. In Section 5 we introduce a fully discrete scheme and show existence and uniqueness of a fully discrete solution assuming an LBB condition. In Section 6 we comment on the methods used to solve the fully discrete systems. In Section 7 we present several numerical computations in two and three spatial dimensions, illustrating the properties of the numerical approach and showing the complex interplay between the curvature functional, the Ginzburg–Landau energy and the Navier–Stokes dynamics. In the Appendix we finally state the details of the derivation of the model, and we show that the weak formulation we introduce is consistent with the strong formulation for smooth solutions.

2. Notation and governing equations

In this section we formulate the model, which was sketched in the Introduction, with all its details. Let $\Omega \subset \mathbb{R}^d$ be a given domain, where $d = 2$ or $d = 3$. We seek a time dependent interface $(\Gamma(t))_{t\in[0,T]}$, $\Gamma(t) \subset \Omega$, which for all $t \in [0, T]$ separates Ω into a domain $\Omega_+(t)$, occupied by the outer phase, and a domain $\Omega_-(t) := \Omega \setminus \overline{\Omega}_+(t)$, which is occupied by the inner phase, see Figure 1 for an illustration. For later use, we assume that $(\Gamma(t))_{t\in[0,T]}$ is an evolving hypersurface without boundary that is parameterized by $\vec{x}(\cdot, t) : \Upsilon \to \mathbb{R}^d$, where $\Upsilon \subset \mathbb{R}^d$ is a given reference manifold, i.e. $\Gamma(t) = \vec{x}(\Upsilon, t)$. Then

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

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

Let $\rho(t) = \rho_+\, \mathcal{X}_{\Omega_+(t)} + \rho_-\, \mathcal{X}_{\Omega_-(t)}$, with $\rho_\pm \in \mathbb{R}_{\geq 0}$, denote the fluid densities. Here and throughout $\mathcal{X}_\mathcal{A}$ defines the characteristic function for a set $\mathcal{A}$. Denoting by $\vec{u} : \Omega \times [0, T] \to \mathbb{R}^d$ the fluid velocity and by $p : \Omega \times [0, T] \to \mathbb{R}$ the pressure, we define the stress tensor

$$\underline{\underline{\sigma}} = \mu\, (\nabla\, \vec{u} + (\nabla\, \vec{u})^T) - p\, \underline{\underline{\mathrm{Id}}} = 2\, \mu\, \underline{\underline{D}}(\vec{u}) - p\, \underline{\underline{\mathrm{Id}}}\,, \tag{2.2}$$

where $\underline{\underline{\mathrm{Id}}} \in \mathbb{R}^{d\times d}$ denotes the identity matrix, $\underline{\underline{D}}(\vec{u}) := \frac{1}{2}\,(\nabla\, \vec{u} + (\nabla\, \vec{u})^T)$ is the bulk rate-of-deformation tensor, with $\nabla\, \vec{u} = \left(\partial_{x_j}\, u_i\right)_{i,j=1}^d$, and $\mu(t) = \mu_+\, \mathcal{X}_{\Omega_+(t)} + \mu_-\, \mathcal{X}_{\Omega_-(t)}$, for $\mu_\pm \in \mathbb{R}_{>0}$, denotes the dynamic viscosities in the two phases. With $\vec{f} : \Omega \times [0, T] \to \mathbb{R}^d$ denoting a possible volume force, the incompressible Navier–Stokes equations in the two phases are given by (2.2) and

$$\rho\, (\vec{u}_t + (\vec{u} \,.\, \nabla)\, \vec{u}) - \nabla \,.\, \underline{\underline{\sigma}} = \rho\, \vec{f} \qquad \text{in } \Omega_\pm(t)\,, \tag{2.3a}$$

$$\nabla \,.\, \vec{u} = 0 \qquad \text{in } \Omega_\pm(t)\,, \tag{2.3b}$$

$$\vec{u} = \vec{g} \qquad \text{on } \partial_1\Omega\,, \tag{2.3c}$$

$$\underline{\underline{\sigma}}\, \vec{\mathrm{n}} = \vec{0} \qquad \text{on } \partial_2\Omega\,, \tag{2.3d}$$

where $\partial\Omega = \partial_1\Omega \cup \partial_2\Omega$, with $\partial_1\Omega \cap \partial_2\Omega = \emptyset$, denotes the boundary of Ω with outer unit normal $\vec{\mathrm{n}}$. Hence (2.3c) prescribes a possibly inhomogeneous Dirichlet condition for the velocity on $\partial_1\Omega$, which collapses to the standard no-slip condition when $\vec{g} = \vec{0}$, while (2.3d) prescribes a stress-free condition on $\partial_2\Omega$. Throughout this paper we assume that $\mathcal{H}^{d-1}(\partial_1\Omega) > 0$. We will also assume w.l.o.g. that $\vec{g}$ is extended so that $\vec{g} : \Omega \to \mathbb{R}^d$.

Following [1], on the free surface $\Gamma(t)$ we require the conditions

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

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

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

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

where $[\vec{u}]_-^+ := \vec{u}_+ - \vec{u}_-$ and $[\underline{\underline{\sigma}}\, \vec{\nu}]_-^+ := \underline{\underline{\sigma}}_+\, \vec{\nu} - \underline{\underline{\sigma}}_-\, \vec{\nu}$ denote the jumps in velocity and normal stress across the interface $\Gamma(t)$. Here and throughout, we employ the shorthand notation $\vec{a}_\pm := \vec{a}\,|_{\Omega_\pm(t)}$ for a function $\vec{a} : \Omega \times [0, T] \to \mathbb{R}^d$; and similarly for scalar and matrix-valued functions. Moreover, $\rho_\Gamma \in \mathbb{R}_{\geq 0}$ denotes the surface material density and the source term $\vec{f}_\Gamma = -\delta E/\delta\Gamma$ is the first variation of the total energy of $\Gamma(t)$ with respect to Γ, see (2.9) below. In addition,

$$\partial_t^\bullet\, \zeta = \zeta_t + \vec{u} \,.\, \nabla\, \zeta \tag{2.5}$$

denotes the material time derivative of ζ on $\Gamma(t)$, see e.g. [21, p. 324]. Furthermore, the surface stress tensor is given by

$$\underline{\underline{\sigma}}_\Gamma = 2\, \mu_\Gamma\, \underline{\underline{D}}_s(\vec{u}) - p_\Gamma\, \underline{\underline{\mathcal{P}}}_\Gamma \quad \text{on } \Gamma(t)\,, \tag{2.6}$$

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

$$\underline{\underline{\mathcal{P}}}_\Gamma = \underline{\underline{\mathrm{Id}}} - \vec{\nu} \otimes \vec{\nu} \quad \text{on } \Gamma(t)\,, \tag{2.7a}$$

and

$$\underline{\underline{D}}_s(\vec{u}) = \tfrac{1}{2}\,\underline{\underline{\mathcal{P}}}_\Gamma\,(\nabla_s\,\vec{u} + (\nabla_s\,\vec{u})^T)\,\underline{\underline{\mathcal{P}}}_\Gamma \quad \text{on } \Gamma(t)\,, \tag{2.7b}$$

with the surface gradient $\nabla_s = \underline{\underline{\mathcal{P}}}_\Gamma\,\nabla = (\partial_{s_1},\ldots,\partial_{s_d})$ on $\Gamma(t)$, and $\nabla_s\,\vec{u} = \left(\partial_{s_j}\,u_i\right)_{i,j=1}^d$. Finally, $\nabla_s\,.$ denotes the surface divergence on $\Gamma(t)$. The system (2.3a–d), (2.2), (2.4a–d), (2.6) is closed with the initial conditions

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

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

The source term $\vec{f}_\Gamma$ in (2.4b) plays a crucial role, and it is given by minus the first variation of the energy (1.2a) with respect to Γ, i.e.

$$\begin{aligned}\vec{f}_\Gamma &= -\frac{\delta}{\delta\Gamma}\,E(\Gamma,\mathfrak{c}) \\ &= \left[-\Delta_s\,[\alpha(\mathfrak{c})\,(\varkappa - \overline{\varkappa}(\mathfrak{c}))] - \alpha(\mathfrak{c})\,(\varkappa - \overline{\varkappa}(\mathfrak{c}))\,|\nabla_s\,\vec{\nu}|^2 + b(\varkappa,\mathfrak{c})\,\varkappa - \nabla_s\,.\,([\varkappa\,\underline{\underline{\mathrm{Id}}} + \nabla_s\,\vec{\nu}]\,\nabla_s\,\alpha^G(\mathfrak{c}))\right]\vec{\nu} \\ &\qquad + (b_{,\mathfrak{c}}(\varkappa,\mathfrak{c}) + (\alpha^G)'(\mathfrak{c})\,\mathcal{K})\,\nabla_s\,\mathfrak{c} + \beta\,[b_{GL}(\mathfrak{c})\,\varkappa\,\vec{\nu} + \nabla_s\,b_{GL}(\mathfrak{c}) - \gamma\,\nabla_s\,.\,((\nabla_s\,\mathfrak{c})\otimes(\nabla_s\,\mathfrak{c}))]\,,\end{aligned} \tag{2.9}$$

where we have defined

$$b_{,\mathfrak{c}}(\varkappa,\mathfrak{c}) = \tfrac{\partial}{\partial\mathfrak{c}}\,b(\varkappa,\mathfrak{c}) = \tfrac{1}{2}\,\alpha'(\mathfrak{c})\,(\varkappa - \overline{\varkappa}(\mathfrak{c}))^2 - \alpha(\mathfrak{c})\,(\varkappa - \overline{\varkappa}(\mathfrak{c}))\,\overline{\varkappa}'(\mathfrak{c})\,. \tag{2.10}$$

Throughout we assume that $\alpha, \alpha^G \in C^1(\mathbb{R})$, with $\alpha(s) > 0$ for all $s \in \mathbb{R}$. We refer to the Appendix for a detailed derivation of (2.9). In contrast to situations where the energy density does not depend on a species concentration, we now have tangential contributions to $\vec{f}_\Gamma$. In particular, the terms $(b_{,\mathfrak{c}}(\varkappa,\mathfrak{c}) + (\alpha^G)'(\mathfrak{c})\,\mathcal{K})\,\nabla_s\,\mathfrak{c} + \beta\,\nabla_s\,b_{GL}(\mathfrak{c}) - \beta\,\gamma\,\nabla_s\,.\,((\nabla_s\,\mathfrak{c})\otimes(\nabla_s\,\mathfrak{c}))$ give rise to a tangential flow and hence can induce a Marangoni-type effect.

The overall model we are going to study in this work is the coupled bulk and surface Navier–Stokes equations (2.3a–d), (2.2), (2.4a–d), (2.6), (2.8) together with the convective Cahn–Hilliard system (1.5a,b) on the evolving interface, suitably supplemented with initial conditions for $\mathfrak{c}$. Here the double well potential Ψ in (1.2b) and (1.5b) may be chosen, for example, as a quartic potential

$$\Psi(s) = \tfrac{1}{4}\,(s^2 - 1)^2\,, \tag{2.11a}$$

or as the obstacle potential

$$\Psi(s) := \begin{cases} \tfrac{1}{2}\left(1 - s^2\right) & \text{if } |s| \leq 1, \\ \infty & \text{if } |s| > 1, \end{cases} \tag{2.11b}$$

which restricts $\mathfrak{c} \in [-1,1]$. For the analysis we will always assume that $\Psi \in C^1(\mathbb{R})$ for ease of exposition, but we will use (2.11b) for our fully discrete approximations.

As stated previously, $\varkappa$ in (2.9) denotes the so-called mean curvature of $\Gamma(t)$, i.e. the sum of the principal curvatures $\varkappa_i$, $i = 1,\ldots,d-1$, of $\Gamma(t)$, where we have adopted the sign convention that $\varkappa$ is negative where $\Omega_-(t)$ is locally convex. In particular, it holds that

$$\Delta_s\,\vec{\mathrm{id}} = \varkappa\,\vec{\nu} =: \vec{\varkappa} \qquad \text{on } \Gamma(t)\,, \tag{2.12}$$

where $\vec{\mathrm{id}}$ is the identity function on $\mathbb{R}^d$. We recall that the second fundamental tensor for $\Gamma(t)$ is given by $\nabla_s\,\vec{\nu}$, and this appears in (2.9). Moreover, we note that $-\nabla_s\,\vec{\nu}(\vec{z})$, for any $\vec{z} \in \Gamma(t)$, is a symmetric linear map that has a zero eigenvalue with eigenvector $\vec\nu$, i.e.

$$(\nabla_s\,\vec\nu)^T = \nabla_s\,\vec\nu \quad \text{and} \quad (\nabla_s\,\vec\nu)\,\vec\nu = \vec 0\,, \tag{2.13}$$

and the remaining $(d-1)$ eigenvalues, $\varkappa_1,\ldots,\varkappa_{d-1}$, are the principal curvatures of Γ at $\vec z$; see e.g. [17, p. 152]. The mean curvature $\varkappa$ and the Gauss curvature $\mathcal{K}$ can now be stated as

$$\varkappa = -\operatorname{tr}(\nabla_s\,\vec\nu) = -\nabla_s\,.\,\vec\nu = \sum_{i=1}^{d-1}\varkappa_i \qquad \text{and} \qquad \mathcal{K} = \prod_{i=1}^{d-1}\varkappa_i\,, \tag{2.14}$$

which in the case $d=3$ immediately yields that

$$\mathcal{K} = \tfrac12\,(\varkappa^2 - |\nabla_s\,\vec\nu|^2)\,. \tag{2.15}$$

Finally, it is not difficult to show that the conditions (2.3b) enforce volume preservation for the phases, while (2.4c) leads to the conservation of the total surface area $\mathcal{H}^{d-1}(\Gamma(t))$, see (3.7) and (3.8) in Section 3 below for the relevant proofs. As an immediate consequence we obtain that a sphere $\Gamma(t)$ remain a sphere, and that a sphere $\Gamma(t)$ with a zero bulk velocity is a stationary solution.

3. Weak formulation

We begin by recalling the weak formulation of (2.3a–d), (2.2), (2.4a–d), (2.6) from [6] for the special case $\alpha\in\mathbb{R}_{>0}$, $\alpha^G = \overline\varkappa = \beta = 0$, i.e. when $E(\Gamma,\mathfrak{c})$ in (1.2a) is replaced by $\frac12\,\alpha\int_\Gamma \varkappa^2\,\mathrm{d}\mathcal{H}^{d-1}$. To this end, we introduce the following function spaces for a given $\vec a\in[H^1(\Omega)]^d$:

$$\begin{aligned}&\mathbb{U}(\vec a) := \{\vec\varphi\in[H^1(\Omega)]^d : \vec\varphi = \vec a \ \text{ on } \partial_1\Omega\}\,, \quad \mathbb{V}(\vec a) := L^2(0,T;\mathbb{U}(\vec a))\cap H^1(0,T;[L^2(\Omega)]^d)\,,\\ &\mathbb{V}_\Gamma(\vec a) := \{\vec\varphi\in\mathbb{V}(\vec a) : \vec\varphi|_{\Gamma_T}\in[H^1(\Gamma_T)]^d\}\,.\end{aligned} \tag{3.1a}$$

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

$$\widehat{\mathbb{P}} := \begin{cases}\{\eta\in\mathbb{P} : \int_\Omega \eta\,\mathrm{d}\mathcal{L}^d = 0\} & \text{if } \mathcal{H}^{d-1}(\partial_2\Omega) = 0\,,\\ \mathbb{P} & \text{if } \mathcal{H}^{d-1}(\partial_2\Omega) > 0\,.\end{cases} \tag{3.1b}$$

Here and throughout, $\mathcal{H}^{d-1}$ denotes the $(d-1)$-dimensional Hausdorff measure in $\mathbb{R}^d$, while $\mathcal{L}^d$ denotes the Lebesgue measure in $\mathbb{R}^d$. Moreover, we let $(\cdot,\cdot)$ and $\langle\cdot,\cdot\rangle_{\partial_2\Omega}$ denote the L^2–inner products on Ω and $\partial_2\Omega$, and similarly for $\langle\cdot,\cdot\rangle_{\Gamma(t)}$.

Similarly to (2.5) we define the following time derivative that follows the parameterization $\vec x(\cdot,t)$ of $\Gamma(t)$, rather than $\vec u$. In particular, we let

$$\partial_t^\circ\,\zeta = \zeta_t + \vec{\mathcal{V}}\,.\,\nabla\,\zeta \qquad \forall\,\zeta\in H^1(\Gamma_T)\,; \tag{3.2}$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\langle\chi,\zeta\rangle_{\Gamma(t)} = \langle\partial_t^\circ\,\chi,\zeta\rangle_{\Gamma(t)} + \langle\chi,\partial_t^\circ\,\zeta\rangle_{\Gamma(t)} + \left\langle\chi\,\zeta,\nabla_s\,.\,\vec{\mathcal{V}}\right\rangle_{\Gamma(t)} \qquad \forall\,\chi,\zeta\in H^1(\Gamma_T)\,, \tag{3.3}$$

see [21, Lem. 5.2].

On recalling (2.5) we obtain from (3.2) that $\partial_t^\circ = \partial_t^\bullet$ if

$$\vec{\mathcal{V}} = \vec u \qquad \text{on } \Gamma(t)\,. \tag{3.4}$$

Hence the most natural tangential velocity for the parameterization $\vec{x}(\cdot,t) : \Upsilon \to \Gamma(t)$ is the fluidic tangential velocity, and so our weak formulation will replace (2.4d) with (3.4). Recall that while the tangential velocity for the parameterization may be chosen arbitrarily on the continuous level, any particular choice will have important implications on the mesh quality on the discrete level. For the approximation of fluidic biomembranes, thanks to the surface incompressibility condition (2.4c), it turns out that the choice (3.4) in general leads to good meshes. See [6] for more details.

The weak formulation of (2.3a–d), (2.2), (2.4a–d), (2.6), with $E(\Gamma(t),\mathfrak{c}(t))$ replaced by $\frac12\,\alpha\,\langle \vec\varkappa, \vec\varkappa\rangle_{\Gamma(t)}$, from [6] is then given as follows. Find $\Gamma(t) = \vec{x}(\Upsilon,t)$ for $t\in[0,T]$ with $\vec{\mathcal{V}} \in [L^2(\Gamma_T)]^d$ and $\vec{\mathcal{V}}(\cdot,t) \in [H^1(\Gamma(t)]^d$ for almost all $t\in(0,T)$, and functions $\vec u \in \mathbb{V}_\Gamma(\vec g)$, $p \in L^2(0,T;\widehat{\mathbb{P}})$, $p_\Gamma \in L^2(\Gamma_T)$, $\vec\varkappa \in [H^1(\Gamma_T)]^d$ and $\vec f_\Gamma \in [L^2(\Gamma_T)]^d$ such that the initial conditions (2.8) hold and such that for almost all $t\in(0,T)$ it holds that

$$
\begin{aligned}
&\tfrac12 \left[\frac{\mathrm d}{\mathrm dt}(\rho\,\vec u,\vec\xi) + (\rho\,\vec u_t,\vec\xi) - (\rho\,\vec u,\vec\xi_t) + (\rho,[(\vec u\,.\,\nabla)\,\vec u]\,.\,\vec\xi - [(\vec u\,.\,\nabla)\,\vec\xi]\,.\,\vec u) + \rho_+\left\langle \vec u\,.\,\mathrm{n}, \vec u\,.\,\vec\xi\right\rangle_{\partial_2\Omega}\right] \\
&\qquad + 2\,(\mu\,\underline{\underline{D}}(\vec u),\underline{\underline{D}}(\vec\xi)) - (p,\nabla\,.\,\vec\xi) + \rho_\Gamma\left\langle \partial_t^\circ\,\vec u,\vec\xi\right\rangle_{\Gamma(t)} + 2\,\mu_\Gamma\left\langle \underline{\underline{D}}_s(\vec u),\underline{\underline{D}}_s(\vec\xi)\right\rangle_{\Gamma(t)} - \left\langle p_\Gamma,\nabla_s\,.\,\vec\xi\right\rangle_{\Gamma(t)} \\
&\quad = (\rho\,\vec f,\vec\xi) + \left\langle \vec f_\Gamma,\vec\xi\right\rangle_{\Gamma(t)} \qquad \forall\ \vec\xi \in \mathbb{V}_\Gamma(\vec 0)\,,
\end{aligned} \tag{3.5a}
$$

$$(\nabla\,.\,\vec u,\varphi) = 0 \qquad \forall\ \varphi\in\widehat{\mathbb{P}}\,, \tag{3.5b}$$

$$\langle\nabla_s\,.\,\vec u,\eta\rangle_{\Gamma(t)} = 0 \qquad \forall\ \eta\in L^2(\Gamma(t))\,, \tag{3.5c}$$

$$\left\langle \vec{\mathcal{V}} - \vec u,\vec\chi\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec\chi\in[L^2(\Gamma(t))]^d\,, \tag{3.5d}$$

as well as

$$\langle\vec\varkappa,\vec\eta\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec{\mathrm{id}},\nabla_s\,\vec\eta\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec\eta\in[H^1(\Gamma(t))]^d\,, \tag{3.6a}$$

$$
\begin{aligned}
\left\langle \vec f_\Gamma,\vec\chi\right\rangle_{\Gamma(t)} &= \alpha\,\langle\nabla_s\,\vec\varkappa,\nabla_s\,\vec\chi\rangle_{\Gamma(t)} + \alpha\,\langle\nabla_s\,.\,\vec\varkappa,\nabla_s\,.\,\vec\chi\rangle_{\Gamma(t)} + \tfrac12\,\alpha\,\langle|\vec\varkappa|^2,\nabla_s\,.\,\vec\chi\rangle_{\Gamma(t)} \\
&\qquad - 2\,\alpha\left\langle(\nabla_s\,\vec\varkappa)^T,\underline{\underline{D}}_s(\vec\chi)\,(\nabla_s\,\vec{\mathrm{id}})^T\right\rangle_{\Gamma(t)} \qquad \forall\ \vec\chi\in[H^1(\Gamma(t))]^d\,,
\end{aligned} \tag{3.6b}
$$

where in (3.5d) we have recalled (2.1) and (3.4). We also note that (3.6a) is the weak form of (2.12).

For the case $\vec g = \vec 0$, it was shown in [6] that choosing $\vec\xi = \vec u \in \mathbb{V}_\Gamma(\vec 0)$ in (3.5a), $\varphi = p(\cdot,t)\in\widehat{\mathbb{P}}$ in (3.5b), $\eta = p_\Gamma(\cdot,t)\in L^2(\Gamma(t))$, $\vec\chi = \vec f_\Gamma$ in (3.5d) and $\vec\chi = \vec{\mathcal{V}}$ in (3.6b) yields that

$$
\begin{aligned}
&\tfrac12\,\frac{\mathrm d}{\mathrm dt}\left(\|\rho^{\frac12}\,\vec u\|_0^2 + \rho_\Gamma\,\langle\vec u,\vec u\rangle_{\Gamma(t)} + \alpha\,\langle\vec\varkappa,\vec\varkappa\rangle_{\Gamma(t)}\right) + 2\,\|\mu^{\frac12}\,\underline{\underline{D}}(\vec u)\|_0^2 + 2\,\mu_\Gamma\,\langle\underline{\underline{D}}_s(\vec u),\underline{\underline{D}}_s(\vec u)\rangle_{\Gamma(t)} + \tfrac12\,\rho_+\,\langle\vec u\,.\,\mathrm{n},|\vec u|^2\rangle_{\partial_2\Omega} \\
&\quad = (\rho\,\vec f,\vec u)\,.
\end{aligned}
$$

Moreover, we recall from [6] that it follows from (3.3) and (3.5c,d) that

$$\frac{\mathrm d}{\mathrm dt}\,\mathcal{H}^{d-1}(\Gamma(t)) = \frac{\mathrm d}{\mathrm dt}\,\langle 1,1\rangle_{\Gamma(t)} = \left\langle 1,\nabla_s\,.\,\vec{\mathcal{V}}\right\rangle_{\Gamma(t)} = \langle 1,\nabla_s\,.\,\vec u\rangle_{\Gamma(t)} = 0\,, \tag{3.7}$$

while [17, Lemma 2.1], (3.5b,d) and (3.1b) imply that

$$\frac{\mathrm d}{\mathrm dt}\mathcal{L}^d(\Omega_-(t)) = \left\langle\vec{\mathcal{V}},\vec\nu\right\rangle_{\Gamma(t)} = \langle\vec u,\vec\nu\rangle_{\Gamma(t)} = \int_{\Omega_-(t)} \nabla\,.\,\vec u\;\mathrm d\mathcal{L}^d = 0\,. \tag{3.8}$$

We remark that very recently, in [5, 7] the present authors have extended the weak formulation (3.6a,b) for the energy $\frac{1}{2}\,\alpha\,\langle \varkappa^2, 1\rangle_{\Gamma(t)}$ to energies of the form $\frac{1}{2}\,\alpha\,\langle (\varkappa-\overline{\varkappa})^2, 1\rangle_{\Gamma(t)}$, with $\overline{\varkappa} \in \mathbb{R}$. In the remainder of this section, we will extend (3.6a,b) to deal with the general two-phase energy $E(\Gamma, \mathfrak{c})$ as in (1.2a).

3.1. Reformulation of $E(\Gamma(t), \mathfrak{c}(t))$

We recall that in the case $d = 2$, we always assume that $\alpha^G = 0$. In the case $d = 3$, on the other hand, we have from (2.15) that

$$\left\langle \alpha^G(\mathfrak{c}), \mathcal{K}\right\rangle_{\Gamma(t)} = \tfrac{1}{2}\left\langle \alpha^G(\mathfrak{c}), |\vec\varkappa|^2 - |\underline{\underline{w}}|^2\right\rangle_{\Gamma(t)}, \tag{3.9}$$

where $\underline{\underline{w}} \in [H^1(\Gamma(t))]^{d\times d}$ is such that for all $\underline{\underline{\zeta}} \in [H^1(\Gamma(t))]^{d\times d}$

$$\left\langle \underline{\underline{w}}, \underline{\underline{\zeta}}\right\rangle_{\Gamma(t)} = \left\langle \nabla_s\,\vec\nu, \underline{\underline{\zeta}}\right\rangle_{\Gamma(t)} = -\left\langle \vec\nu, \underline{\underline{\zeta}}\,\vec\varkappa + \nabla_s\,.\,\underline{\underline{\zeta}}\right\rangle_{\Gamma(t)}. \tag{3.10}$$

Here we have recalled from [21, Theorem 2.10] that

$$\langle \nabla_s\,\zeta, \vec\eta\rangle_{\Gamma(t)} + \langle \zeta, \nabla_s\,.\,\vec\eta\rangle_{\Gamma(t)} = \langle \nabla_s\,.\,(\zeta\,\vec\eta), 1\rangle_{\Gamma(t)} = -\,\langle \zeta\,\varkappa\,\vec\nu, \vec\eta\rangle_{\Gamma(t)} \qquad \forall\ \zeta \in H^1(\Gamma(t)),\ \vec\eta \in [H^1(\Gamma(t))]^d\,. \tag{3.11}$$

Hence the total energy $E(\Gamma(t), \mathfrak{c}(t))$, on recalling (1.2a,b) and (2.12), can be rewritten as

$$E(\Gamma(t), \mathfrak{c}(t)) = \int_\Gamma \tfrac{1}{2}\,\alpha(\mathfrak{c})\,|\vec\varkappa - \overline{\varkappa}(\mathfrak{c})\,\vec\nu|^2 + \tfrac{1}{2}\,\alpha^G(\mathfrak{c})\,(|\vec\varkappa|^2 - |\underline{\underline{w}}|^2) + \beta\,b_{GL}(\mathfrak{c})\;\mathrm{d}\mathcal{H}^{d-1}\,, \tag{3.12}$$

and it is this reformulation on which our weak formulation, and hence our stable semidiscrete finite element approximation, will be based.

3.2. The first variation of $E(\Gamma(t), \mathfrak{c}(t))$

In this section we would like to derive a weak formulation for the first variation of $E(\Gamma(t), \mathfrak{c}(t))$ with respect to $\Gamma(t) = \vec x(\Upsilon, t)$. To this end, for a given $\vec\chi \in [H^1(\Gamma(t))]^d$ and for $\varepsilon \in (0, \varepsilon_0)$, where $\varepsilon_0 \in \mathbb{R}_{>0}$, let $\vec\Phi(\cdot, \varepsilon)$ be a family of transformations such that

$$\Gamma_\varepsilon(t) := \{\vec\Phi(\vec z, \varepsilon) : \vec z \in \Gamma(t)\}\,, \quad \text{where} \quad \vec\Phi(\vec z, 0) = \vec z \text{ and } \tfrac{\partial\vec\Phi}{\partial\varepsilon}(\vec z, 0) = \vec\chi(\vec z) \quad \forall\ \vec z \in \Gamma(t)\,. \tag{3.13}$$

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

$$\begin{aligned}\left[\frac{\delta}{\delta\Gamma}\,\mathcal{H}^{d-1}(\Gamma(t))\right](\vec\chi) &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\,\mathcal{H}^{d-1}(\Gamma_\varepsilon(t))\mid_{\varepsilon=0} = \lim_{\varepsilon\to0}\tfrac{1}{\varepsilon}\left[\mathcal{H}^{d-1}(\Gamma_\varepsilon(t)) - \mathcal{H}^{d-1}(\Gamma(t))\right] = \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec\chi\right\rangle_{\Gamma(t)}\\ &= \langle 1, \nabla_s\,.\,\vec\chi\rangle_{\Gamma(t)}\,,\end{aligned} \tag{3.14}$$

see e.g. the proof of Lemma 1 in [20]. For any quantity w, that is naturally defined on $\Gamma_\varepsilon(t)$, we define

$$\partial_\varepsilon^0\,w(\vec z) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon} w_\varepsilon(\vec\Phi(\vec z, \varepsilon))\mid_{\varepsilon=0} \qquad \forall\ \vec z \in \Gamma(t)\,, \tag{3.15}$$

and similarly for $\partial_\varepsilon^0\,\vec w$ and $\partial_\varepsilon^0\,\underline{\underline{w}}$. A common example is $\vec\nu_\varepsilon$, the outer normal on $\Gamma_\varepsilon(t)$. In cases where $w \in L^\infty(\Gamma(t))$ is meaningful only on $\Gamma(t)$, we let $w_\varepsilon \in L^\infty(\Gamma_\varepsilon(t))$ be such that

$$w_\varepsilon(\vec\Phi(\vec z, \varepsilon)) = w(\vec z) \qquad \forall\ \vec z \in \Gamma(t)\,, \tag{3.16}$$

which immediately implies that for such w it holds that $\partial_\varepsilon^0 w = 0$. Once again, we extend (3.16) also to vector- and tensor-valued functions. For later use we note that generalized variants of (3.14) also hold. Similarly to (3.3) it holds that

$$\left[\frac{\delta}{\delta\Gamma}\langle w, v\rangle_{\Gamma(t)}\right](\vec\chi) = \left\langle \partial_\varepsilon^0 w, v\right\rangle_{\Gamma(t)} + \left\langle w, \partial_\varepsilon^0 v\right\rangle_{\Gamma(t)} + \langle w\, v, \nabla_s \,.\, \vec\chi\rangle_{\Gamma(t)} \quad \forall\, w, v \in L^\infty(\Gamma(t))\,. \tag{3.17}$$

Similarly, it holds that

$$\left[\frac{\delta}{\delta\Gamma}\langle \vec w, \vec\nu\rangle_{\Gamma(t)}\right](\vec\chi) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\langle \vec w_\varepsilon, \vec\nu_\varepsilon\rangle_{\Gamma_\varepsilon(t)}\mid_{\varepsilon=0} = \left\langle \partial_\varepsilon^0 \vec w, \vec\nu\right\rangle_{\Gamma(t)} + \left\langle \vec w, \partial_\varepsilon^0 \vec\nu\right\rangle_{\Gamma(t)} + \langle \vec w \,.\, \vec\nu, \nabla_s \,.\, \vec\chi\rangle_{\Gamma(t)}$$
$$\forall\, \vec w \in [L^\infty(\Gamma(t))]^d\,, \tag{3.18}$$

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

$$\partial_\varepsilon^0 \vec\nu = -[\nabla_s \vec\chi]^T \vec\nu \quad \text{on} \quad \Gamma(t) \quad \Rightarrow \quad \partial_t^\circ \vec\nu = -[\nabla_s \vec{\mathcal{V}}]^T \vec\nu \quad \text{on} \quad \Gamma(t)\,, \tag{3.19}$$

see [41, Lemma 9]. Next we note that for $\vec\eta \in [H^1(\Gamma(t))]^d$ it holds that

$$\begin{aligned}
\left[\frac{\delta}{\delta\Gamma}\left\langle \nabla_s \vec{\mathrm{id}}, \nabla_s \vec\eta\right\rangle_{\Gamma(t)}\right](\vec\chi) &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\langle \nabla_s \vec{\mathrm{id}}, \nabla_s \vec\eta_\varepsilon\right\rangle_{\Gamma_\varepsilon(t)}\mid_{\varepsilon=0}\\
&= \langle \nabla_s \,.\, \vec\eta, \nabla_s \,.\, \vec\chi\rangle_{\Gamma(t)} + \sum_{l,\,m=1}^{d}\left[\langle (\vec\nu)_l\, (\vec\nu)_m \,\nabla_s\, (\vec\eta)_m, \nabla_s\, (\vec\chi)_l\rangle_{\Gamma(t)} - \langle (\nabla_s)_m\, (\vec\eta)_l, (\nabla_s)_l\, (\vec\chi)_m\rangle_{\Gamma(t)}\right]\\
&= \langle \nabla_s \vec\eta, \nabla_s \vec\chi\rangle_{\Gamma(t)} + \langle \nabla_s \,.\, \vec\eta, \nabla_s \,.\, \vec\chi\rangle_{\Gamma(t)} - 2\left\langle (\nabla_s \vec\eta)^T, \underline{\underline{D}}_s(\vec\chi)\,(\nabla_s \vec{\mathrm{id}})^T\right\rangle_{\Gamma(t)}\,,
\end{aligned} \tag{3.20}$$

where $\partial_\varepsilon^0 \vec\eta = \vec 0$. We refer to Lemma 2 and the proof of Lemma 3 in [20] for a proof of (3.20). Here we observe that our notation is such that $\nabla_s \vec\chi = (\nabla_\Gamma \vec\chi)^T$, with $\nabla_\Gamma \vec\chi = (\partial_{s_i} \chi_j)_{i,j=1}^d$ defined as in [20]. Moreover, it holds, on noting (2.7a), that

$$\nabla_s \vec\chi\, \underline{\underline{\mathcal{P}}}_\Gamma = \nabla_s \vec\chi \quad \Rightarrow \quad \underline{\underline{\mathcal{P}}}_\Gamma\, (\nabla_s \vec\chi)^T = (\nabla_s \vec\chi)^T \tag{3.21a}$$

and

$$2\,(\nabla_s \vec\eta)^T : \underline{\underline{D}}_s(\vec\chi)\,(\nabla_s \vec\phi)^T = (\nabla_s \vec\eta)^T : [\nabla_s \vec\chi + (\nabla_s \vec\chi)^T]\,(\nabla_s \vec\phi)^T\,, \tag{3.21b}$$

which yields that the last term on the right hand side in (3.20) can be rewritten as in [20].

As $\nabla_s \vec{\mathrm{id}} = \underline{\underline{\mathcal{P}}}_\Gamma$, one can deduce from (2.7a), (3.20) and (3.17) that for sufficiently smooth $\vec\eta$

$$\partial_\varepsilon^0\,(\nabla_s \,.\, \vec\eta) = \partial_\varepsilon^0\,(\nabla_s \vec{\mathrm{id}} : \nabla_s \vec\eta) = \nabla_s \vec\eta : \nabla_s \vec\chi - 2\,(\nabla_s \vec\eta)^T : \underline{\underline{D}}_s(\vec\chi)\,(\nabla_s \vec{\mathrm{id}})^T = [\nabla_s \vec\chi - 2\,\underline{\underline{D}}_s(\vec\chi)] : \nabla_s \vec\eta \quad \text{a.e. on } \Gamma(t)\,, \tag{3.22}$$

where $\partial_\varepsilon^0 \vec\eta = \vec 0$. From (3.22) we can also derive that for sufficiently smooth w

$$\partial_\varepsilon^0\,(\nabla_s\, w) = [\nabla_s \vec\chi - 2\,\underline{\underline{D}}_s(\vec\chi)]\,\nabla_s\, w \quad \text{a.e. on } \Gamma(t)\,, \tag{3.23}$$

where $\partial_\varepsilon^0 w = 0$. In addition, it follows from (3.23) that

$$\partial_\varepsilon^0\,|\nabla_s\, w|^2 = 2\,\nabla_s\, w \,.\, \partial_\varepsilon^0\,(\nabla_s\, w) = -2\,\nabla_s\, w \,.\, (\nabla_s \vec\chi\, \nabla_s\, w) = -2\,(\nabla_s\, w \otimes \nabla_s\, w) : \nabla_s \vec\chi \quad \text{a.e. on } \Gamma(t)\,, \tag{3.24}$$

where $\partial_\varepsilon^0 w = 0$.

Remark 3.1. We note from (3.22) that the last term in (3.20) can be simplified to

$$-2\left\langle \nabla_s\,\vec\eta, \underline{\underline{D}}_s(\vec\chi)\right\rangle_{\Gamma(t)}.$$

However, to be consistent with our approximations in [5], we prefer the form used in (3.20).

It is straightforward to derive results for the time derivative of the considered quantities from the collected first variations above. For example, it follows from (3.20) that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec\eta\right\rangle_{\Gamma(t)} = \left\langle \nabla_s\,.\,\vec\eta, \nabla_s\,.\,\vec{\mathcal{V}}\right\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec\eta, \nabla_s\,\vec{\mathcal{V}}\right\rangle_{\Gamma(t)} - 2\left\langle (\nabla_s\,\vec\eta)^T, \underline{\underline{D}}_s(\vec{\mathcal{V}})\,(\nabla_s\,\vec{\mathrm{id}})^T\right\rangle_{\Gamma(t)}$$
$$\forall\ \vec\eta \in \{\vec\xi \in [H^1(\Gamma_T)]^d : \partial_t^\circ\,\vec\xi = \vec 0\}\,. \quad (3.25)$$

On recalling (3.6a), (3.10) and (2.13), we now consider the first variation of (3.12) subject to the side constraints

$$\langle \vec\varkappa^\star, \vec\eta\rangle_{\Gamma(t)} + \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec\eta\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec\eta \in [H^1(\Gamma(t))]^d\,, \quad (3.26a)$$

$$\left\langle \underline{\underline{w}}^\star, \underline{\underline{\zeta}}\right\rangle_{\Gamma(t)} + \tfrac12\left\langle \vec\nu, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\,\vec\varkappa^\star + \nabla_s\,.\,[\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \underline{\underline{\zeta}} \in [H^1(\Gamma(t))]^{d\times d}\,. \quad (3.26b)$$

Here we use the symmetric formulation in (3.26b), because its discretized form will then ensure that the discrete approximations to $\underline{\underline{w}}^\star$ are also symmetric, since

$$\left\langle (\underline{\underline{w}}^\star)^T, \underline{\underline{\zeta}}\right\rangle_{\Gamma(t)} = \left\langle \underline{\underline{w}}^\star, \underline{\underline{\zeta}}^T\right\rangle_{\Gamma(t)} = \left\langle \underline{\underline{w}}^\star, \underline{\underline{\zeta}}\right\rangle_{\Gamma(t)} \qquad \forall\ \underline{\underline{\zeta}} \in [H^1(\Gamma(t))]^{d\times d}\,. \quad (3.27)$$

On recalling (3.12), we define the Lagrangian

$$L(\Gamma, \vec\varkappa^\star, \vec y, \underline{\underline{w}}^\star, \underline{\underline{z}}, \mathfrak{c}) = \tfrac12\left\langle \alpha(\mathfrak{c})\,|\vec\varkappa^\star - \overline{\varkappa}(\mathfrak{c})\,\vec\nu|^2, 1\right\rangle_{\Gamma(t)} + \tfrac12\left\langle \alpha^G(\mathfrak{c}), |\vec\varkappa^\star|^2 - |\underline{\underline{w}}^\star|^2\right\rangle_{\Gamma(t)} + \beta\,\langle b_{GL}(\mathfrak{c}), 1\rangle_{\Gamma(t)}$$
$$- \langle \vec\varkappa^\star, \vec y\rangle_{\Gamma(t)} - \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec y\right\rangle_{\Gamma(t)} - \langle \underline{\underline{w}}^\star, \underline{\underline{z}}\rangle_{\Gamma(t)} - \tfrac12\left\langle \vec\nu, [\underline{\underline{z}} + \underline{\underline{z}}^T]\,\vec\varkappa^\star + \nabla_s\,.\,[\underline{\underline{z}} + \underline{\underline{z}}^T]\right\rangle_{\Gamma(t)}, \quad (3.28)$$

where $\vec y \in [H^1(\Gamma(t))]^d$ and $\underline{\underline{z}} \in [H^1(\Gamma(t))]^{d\times d}$ are Lagrange multipliers for (3.26a,b). In order to compute the direction of steepest descent, $\vec f_\Gamma$, of $E(\Gamma(t), \mathfrak{c}(t))$, with respect to $\Gamma(t)$ and subject to the constraints (3.26a,b), we set the variations of $L(\Gamma, \vec\varkappa^\star, \vec y, \underline{\underline{w}}^\star, \underline{\underline{z}}, \mathfrak{c})$ with respect to $\vec\varkappa^\star$, $\vec y$, $\underline{\underline{w}}^\star$ and $\underline{\underline{z}}$ to zero, and we use the variation with respect to $\mathfrak{c}$ to define the Cahn–Hilliard dynamics. Moreover, we obtain on using the formal calculus of PDE constrained optimization, see e.g. [43], that

$$\left[\frac{\delta}{\delta\Gamma}\,L\right](\vec\chi) = \lim_{\varepsilon\to0}\tfrac1\varepsilon\left[L(\Gamma_\varepsilon, \vec\varkappa^\star_\varepsilon, \vec y_\varepsilon, \underline{\underline{w}}^\star_\varepsilon, \underline{\underline{z}}_\varepsilon, \mathfrak{c}_\varepsilon) - L(\Gamma, \vec\varkappa^\star, \vec y, \underline{\underline{w}}^\star, \underline{\underline{z}}, \mathfrak{c})\right] = -\left\langle \vec f_\Gamma, \vec\chi\right\rangle_{\Gamma(t)}, \quad (3.29a)$$

$$\left[\frac{\delta}{\delta\vec\varkappa^\star}\,L\right](\vec\xi) = \lim_{\varepsilon\to0}\tfrac1\varepsilon\left[L(\Gamma, \vec\varkappa^\star + \varepsilon\,\vec\xi, \vec y, \underline{\underline{w}}^\star, \underline{\underline{z}}, \mathfrak{c}) - L(\Gamma, \vec\varkappa^\star, \vec y, \underline{\underline{w}}^\star, \underline{\underline{z}}, \mathfrak{c})\right] = 0\,, \quad (3.29b)$$

$$\left[\frac{\delta}{\delta\vec y}\,L\right](\vec\eta) = \lim_{\varepsilon\to0}\tfrac1\varepsilon\left[L(\Gamma, \vec\varkappa^\star, \vec y + \varepsilon\,\vec\eta, \underline{\underline{w}}^\star, \underline{\underline{z}}, \mathfrak{c}) - L(\Gamma, \vec\varkappa^\star, \vec y, \underline{\underline{w}}^\star, \underline{\underline{z}}, \mathfrak{c})\right] = 0\,, \quad (3.29c)$$

$$\left[\frac{\delta}{\delta\underline{\underline{w}}^\star}\,L\right](\underline{\underline{\phi}}) = \lim_{\varepsilon\to0}\tfrac1\varepsilon\left[L(\Gamma, \vec\varkappa^\star, \vec y, \underline{\underline{w}}^\star + \varepsilon\,\underline{\underline{\phi}}, \underline{\underline{z}}, \mathfrak{c}) - L(\Gamma, \vec\varkappa^\star, \vec y, \underline{\underline{w}}^\star, \underline{\underline{z}}, \mathfrak{c})\right] = 0\,, \quad (3.29d)$$

$$\left[\frac{\delta}{\delta\underline{\underline{z}}}\,L\right](\underline{\underline{\zeta}}) = \lim_{\varepsilon\to0}\tfrac1\varepsilon\left[L(\Gamma, \vec\varkappa^\star, \vec y, \underline{\underline{w}}^\star, \underline{\underline{z}} + \varepsilon\,\underline{\underline{\zeta}}, \mathfrak{c}) - L(\Gamma, \vec\varkappa^\star, \vec y, \underline{\underline{w}}^\star, \underline{\underline{z}}, \mathfrak{c})\right] = 0\,, \quad (3.29e)$$

$$\left[\frac{\delta}{\delta\mathfrak{c}}\,L\right](\xi) = \lim_{\varepsilon\to 0}\tfrac{1}{\varepsilon}\left[L(\Gamma,\vec\varkappa^\star,\vec y,\underline{\underline{w}}^\star,\underline{\underline{z}},\mathfrak{c}+\varepsilon\,\xi) - L(\Gamma,\vec\varkappa^\star,\vec y,\underline{\underline{w}}^\star,\underline{\underline{z}},\mathfrak{c})\right] = \langle\mathfrak{m},\xi\rangle_{\Gamma(t)}\,, \tag{3.29f}$$

where $\vec\varkappa^\star_\varepsilon$, $\vec y_\varepsilon \in [H^1(\Gamma_\varepsilon(t))]^d$, $\underline{\underline{w}}^\star_\varepsilon$, $\underline{\underline{z}}_\varepsilon \in [H^1(\Gamma_\varepsilon(t))]^{d\times d}$, $\mathfrak{c}_\varepsilon \in H^1(\Gamma_\varepsilon(t))$ are defined as in (3.16), and where $\mathfrak{m}$ defines the chemical potential. We note that (3.29c,e) immediately yield (3.26a,b), which means that we can recover $\vec\varkappa^\star$ and $\underline{\underline{w}}^\star$ in terms of $\Gamma(t)$ again. In particular, combining (3.11) and (3.26a) yields, on recalling (2.12) that $\vec\varkappa^\star = \vec\varkappa$. In addition, it then follows from (3.26b) and (3.10) that $\underline{\underline{w}}^\star = \underline{\underline{w}} = \nabla_s\,\vec\nu$. On recalling (1.2b), (3.17)–(3.20), (3.22) and (3.24) this yields that

$$\begin{aligned}
&\left\langle \vec f_\Gamma,\vec\chi\right\rangle_{\Gamma(t)} - \langle\nabla_s\,\vec y,\nabla_s\,\vec\chi\rangle_{\Gamma(t)} - \langle\nabla_s\,.\,\vec y,\nabla_s\,.\,\vec\chi\rangle_{\Gamma(t)} + 2\left\langle(\nabla_s\,\vec y)^T,\underline{\underline{D}}_s(\vec\chi)\,(\nabla_s\,\vec{\mathrm{id}})^T\right\rangle_{\Gamma(t)}\\
&\quad+\tfrac12\left\langle\alpha(\mathfrak{c})\,|\vec\varkappa-\overline{\varkappa}(\mathfrak{c})\,\vec\nu|^2 - 2\,\vec y\,.\,\vec\varkappa,\nabla_s\,.\,\vec\chi\right\rangle_{\Gamma(t)} + \left\langle\alpha(\mathfrak{c})\,\overline{\varkappa}(\mathfrak{c})\,(\vec\varkappa-\overline{\varkappa}(\mathfrak{c})\,\vec\nu),[\nabla_s\,\vec\chi]^T\,\vec\nu\right\rangle_{\Gamma(t)}\\
&\quad+\beta\,\langle b_{GL}(\mathfrak{c}),\nabla_s\,.\,\vec\chi\rangle_{\Gamma(t)} - \beta\,\gamma\,\langle(\nabla_s\,\mathfrak{c})\otimes(\nabla_s\,\mathfrak{c}),\nabla_s\,\vec\chi\rangle_{\Gamma(t)} + \tfrac12\left\langle\alpha^G(\mathfrak{c})\,(|\vec\varkappa|^2 - |\underline{\underline{w}}|^2),\nabla_s\,.\,\vec\chi\right\rangle_{\Gamma(t)}\\
&\quad-\left\langle\underline{\underline{w}}:\underline{\underline{z}},\nabla_s\,.\,\vec\chi\right\rangle_{\Gamma(t)} - \tfrac12\left\langle\vec\nu\,.\,([\underline{\underline{z}}+\underline{\underline{z}}^T]\,\vec\varkappa + \nabla_s\,.\,[\underline{\underline{z}}+\underline{\underline{z}}^T]),\nabla_s\,.\,\vec\chi\right\rangle_{\Gamma(t)} - \sum_{i=1}^d\left\langle\nu_i\,\nabla_s\,\vec z_i,\nabla_s\,\vec\chi - 2\,\underline{\underline{D}}_s(\vec\chi)\right\rangle_{\Gamma(t)}\\
&\quad+\tfrac12\left\langle[\underline{\underline{z}}+\underline{\underline{z}}^T]\,\vec\varkappa + \nabla_s\,.\,[\underline{\underline{z}}+\underline{\underline{z}}^T],[\nabla_s\,\vec\chi]^T\,\vec\nu\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec\chi\in[H^1(\Gamma(t))]^d\,, &&\text{(3.30a)}\\
&\left\langle\alpha(\mathfrak{c})\,(\vec\varkappa-\overline{\varkappa}(\mathfrak{c})\,\vec\nu) + \alpha^G(\mathfrak{c})\,\vec\varkappa - \tfrac12\,[\underline{\underline{z}}+\underline{\underline{z}}^T]\,\vec\nu - \vec y,\vec\xi\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec\xi\in[H^1(\Gamma(t))]^d\,, &&\text{(3.30b)}\\
&\underline{\underline{z}} = -\alpha^G(\mathfrak{c})\,\underline{\underline{w}}\,, &&\text{(3.30c)}\\
&\langle\vec\varkappa,\vec\eta\rangle_{\Gamma(t)} + \left\langle\nabla_s\,\vec{\mathrm{id}},\nabla_s\,\vec\eta\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec\eta\in[H^1(\Gamma(t))]^d\,, &&\text{(3.30d)}\\
&\left\langle\underline{\underline{w}},\underline{\underline{\zeta}}\right\rangle_{\Gamma(t)} + \tfrac12\left\langle\vec\nu,[\underline{\underline{\zeta}}+\underline{\underline{\zeta}}^T]\,\vec\varkappa + \nabla_s\,.\,[\underline{\underline{\zeta}}+\underline{\underline{\zeta}}^T]\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \underline{\underline{\zeta}}\in[H^1(\Gamma(t))]^{d\times d}\,. &&\text{(3.30e)}
\end{aligned}$$

The above is coupled to (3.5a–d) subject to the initial conditions (2.8). Here we have introduced $\vec z_i = \frac12\,[\underline{\underline{z}}+\underline{\underline{z}}^T]\,\vec e_i$, $i = 1\to d$, as well as $\nu_i = \vec\nu\,.\,\vec e_i$, $i = 1\to d$. Finally, on recalling (1.5a), and on using (3.11), (3.3), (3.2), (2.5) and (3.5c,d), a weak form of the Cahn–Hilliard dynamics is given by

$$\begin{aligned}
&\vartheta\,\frac{\mathrm{d}}{\mathrm{d}t}\,\langle\mathfrak{c},\eta\rangle_{\Gamma(t)} + \langle\nabla_s\,\mathfrak{m},\nabla_s\,\eta\rangle_{\Gamma(t)} = 0 \quad \forall\ \eta\in\{\xi\in H^1(\Gamma_T) : \partial_t^\circ\,\xi = 0\}\,, &&\text{(3.31a)}\\
&\langle\mathfrak{m},\xi\rangle_{\Gamma(t)} = \beta\,\gamma\,\langle\nabla_s\,\mathfrak{c},\nabla_s\,\xi\rangle_{\Gamma(t)} + \beta\,\gamma^{-1}\,\langle\Psi'(\mathfrak{c}),\xi\rangle_{\Gamma(t)} + \tfrac12\left\langle\alpha'(\mathfrak{c})\,|\vec\varkappa-\overline{\varkappa}(\mathfrak{c})\,\vec\nu|^2 - 2\,\overline{\varkappa}'(\mathfrak{c})\,\alpha(\mathfrak{c})\,(\vec\varkappa-\overline{\varkappa}(\mathfrak{c})\,\vec\nu)\,.\,\vec\nu,\xi\right\rangle_{\Gamma(t)}\\
&\qquad+\tfrac12\left\langle(\alpha^G)'(\mathfrak{c})\,(|\vec\varkappa|^2 - |\underline{\underline{w}}|^2),\xi\right\rangle_{\Gamma(t)} \qquad \forall\ \xi\in H^1(\Gamma(t))\,, &&\text{(3.31b)}\\
&\mathfrak{c}(\cdot,0) = \mathfrak{c}_0 \qquad \text{on } \Gamma_0\,, &&\text{(3.31c)}
\end{aligned}$$

with $\mathfrak{c}_0 : \Gamma_0 \to \mathbb{R}$ given initial data, recall (2.8). Here we note that (3.31b) is well-posed for nonconstant α, α^G and $\overline{\varkappa}$ only in the case $\beta > 0$, which is why we assume that β is positive throughout the manuscript. In addition, we observe that choosing $\eta = 1$ in (3.31a) yields that

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\langle\mathfrak{c},1\rangle_{\Gamma(t)} = 0\,. \tag{3.32}$$

Remark 3.2. With regards to (3.30b) we note from (3.30c) and (2.13), as $\underline{\underline{w}} = \nabla_s\,\vec\nu = (\nabla_s\,\vec\nu)^T$, it holds that $\underline{\underline{z}} = -\alpha^G(\mathfrak{c})\,\underline{\underline{w}} = -\alpha^G(\mathfrak{c})\,\nabla_s\,\vec\nu$, and so $\underline{\underline{z}}\,\vec\nu = \underline{\underline{z}}^T\,\vec\nu = \vec 0$. For further simplifications we refer to the Appendix.

We note the following LBB-type condition:

$$\inf_{(\varphi,\eta)\in\widehat{\mathbb{P}}\times L^2(\Gamma(t))} \sup_{\vec\xi\in\mathbb{U}_{\Gamma(t)}(\vec 0)} \frac{(\varphi, \nabla\,.\,\vec\xi) + \left\langle \eta, \nabla_s\,.\,\vec\xi\right\rangle_{\Gamma(t)}}{(\|\varphi\|_0 + \|\eta\|_{0,\Gamma(t)})\,(\|\vec\xi\|_1 + \|\underline{\underline{\mathcal{P}}}_\Gamma\,\vec\xi\,|_{\Gamma(t)}\,\|_{1,\Gamma(t)})} \geq C > 0\,, \tag{3.33}$$

which we also refer to as the LBB$_\Gamma$ condition. Here we have defined the space $\mathbb{U}_{\Gamma(t)}(\vec 0) := \{\vec\xi \in \mathbb{U}(\vec 0) : \underline{\underline{\mathcal{P}}}_\Gamma\,\vec\xi\,|_{\Gamma(t)}\in [H^1(\Gamma(t))]^d\}$, and let $\|\vec\eta\|^2_{1,\Gamma(t)} := \langle\vec\eta,\vec\eta\rangle_{\Gamma(t)} + \langle\nabla_s\,\vec\eta,\nabla_s\,\vec\eta\rangle_{\Gamma(t)}$. In the case that the smooth hypersurface $\Gamma(t)$ is not a sphere, then (3.33) is shown to hold if $\partial_1\Omega = \partial\Omega$ is a smooth boundary in [32, p. 15]. See also the discussion around (2.11a,b) in [6].

Overall the weak formulation for the free boundary problem (2.3a–d), (2.2), (2.4a–d), (2.6), (1.5a,b), (2.8), (3.31c) that we consider in this paper is given by

$$\text{(P)} \qquad\qquad (3.5\text{a–d}),\ (3.30\text{a–e}),\ (3.31\text{a–c}),\ (2.8). \tag{3.34}$$

Remark 3.3. We note that in the case $d = 2$ we do not consider Gaussian curvature terms, i.e. we assume that $\alpha^G(\mathfrak{c}) = 0$. Then (3.30a) simplifies to

$$\begin{aligned}
&\left\langle \vec f_\Gamma, \vec\chi\right\rangle_{\Gamma(t)} - \langle\nabla_s\,\vec y, \nabla_s\,\vec\chi\rangle_{\Gamma(t)} - \langle\nabla_s\,.\,\vec y, \nabla_s\,.\,\vec\chi\rangle_{\Gamma(t)} + 2\left\langle(\nabla_s\,\vec y)^T, \underline{\underline{D}}_s(\vec\chi)\,(\nabla_s\,\vec{\rm id})^T\right\rangle_{\Gamma(t)} \\
&\quad + \tfrac12\left\langle\alpha(\mathfrak{c})\,|\vec\varkappa - \overline\varkappa(\mathfrak{c})\,\vec\nu|^2 - 2\,\vec y\,.\,\vec\varkappa, \nabla_s\,.\,\vec\chi\right\rangle_{\Gamma(t)} + \left\langle\alpha(\mathfrak{c})\,\overline\varkappa(\mathfrak{c})\,(\vec\varkappa - \overline\varkappa(\mathfrak{c})\,\vec\nu), [\nabla_s\,\vec\chi]^T\,\vec\nu\right\rangle_{\Gamma(t)} \\
&\quad + \beta\,\langle b_{GL}(\mathfrak{c}), \nabla_s\,.\,\vec\chi\rangle_{\Gamma(t)} - \beta\,\gamma\left\langle(\partial_s\,\mathfrak{c})^2, \nabla_s\,.\,\vec\chi\right\rangle_{\Gamma(t)} = 0 \qquad \forall\ \vec\chi \in [H^1(\Gamma(t))]^d\,.
\end{aligned} \tag{3.35}$$

Clearly, the last two terms in (3.35) can be absorbed by the surface pressure p_Γ in (3.5a). Hence, for constant α and constant $\overline\varkappa$, the evolution of the interface is totally independent of the Cahn–Hilliard system. Of course, for $d = 3$ even for constant α, $\overline\varkappa$ and α^G, the line tension term $\beta\,\gamma\,\langle(\nabla_s\,\mathfrak{c})\otimes(\nabla_s\,\mathfrak{c}), \nabla_s\,\vec\chi\rangle_{\Gamma(t)}$ in (3.30a) means that nonconstant values of $\mathfrak{c}$ do have an influence on the membrane evolution.

4. Semidiscrete finite element approximation

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

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

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

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

Our approximation to the velocity and pressure on $\mathcal{T}^h$ will be based on standard finite element spaces $\mathbb{U}^h(\vec g) \subset \mathbb{U}(\vec I^h_k\,\vec g)$, for some $k \geq 2$, and $\mathbb{P}^h(t) \subset \mathbb{P}$, recall (3.1a,b). Here, for the former we assume from now on that $\vec g \in [C(\overline\Omega)]^d$. We require also the space $\widehat{\mathbb{P}}^h(t) := \mathbb{P}^h(t)\cap\widehat{\mathbb{P}}$. Here, in general, we will choose pairs of velocity/pressure finite element spaces that satisfy the LBB inf-sup condition, see e.g. [27, p. 114]. For example, we may choose the lowest order Taylor-Hood element P2–P1 for $d = 2$ and $d = 3$, the P2–P0 element or the P2–(P1+P0) element for $d = 2$ on setting $\mathbb{U}^h(\vec{g}) = [S_2^h]^d \cap \mathbb{U}(\vec{I}_2^h\,\vec{g})$, and $\mathbb{P}^h = S_1^h$, S_0^h or $S_1^h + S_0^h$, respectively.

The parametric finite element spaces in order to approximate e.g. $\vec{\varkappa}$ and $\mathfrak{c}$ are defined as follows. Similarly to [2], we introduce the following discrete spaces, based on the work of Dziuk, [19]. Let $\Gamma^h(t) \subset \mathbb{R}^d$ be a $(d-1)$-dimensional *polyhedral surface*, i.e. a union of non-degenerate $(d-1)$-simplices with no hanging vertices (see [17, p. 164] for $d = 3$), approximating the closed surface $\Gamma(t)$. In particular, let $\Gamma^h(t) = \bigcup_{j=1}^{J_\Gamma} \overline{\sigma_j^h(t)}$, where $\{\sigma_j^h(t)\}_{j=1}^{J_\Gamma}$ is a family of mutually disjoint open $(d-1)$-simplices with vertices $\{\vec{q}_k^h(t)\}_{k=1}^{K_\Gamma}$. Then let

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

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

$$
\chi_k^h(\vec{q}_l^h(t),t) = \delta_{kl} \qquad \forall\, k,l \in \{1,\dots,K_\Gamma\}\,, t \in [0,T]\,. \tag{4.1}
$$

We require that $\Gamma^h(t) = \vec{X}^h(\Gamma^h(0),t)$ with $\vec{X}^h \in \underline{V}(\Gamma^h(0))$, and that $\vec{q}_k^h \in [H^1(0,T)]^d$, $k = 1,\dots,K_\Gamma$. For later purposes, we also introduce $\pi^h(t) : C(\Gamma^h(t)) \to W(\Gamma^h(t))$, the standard interpolation operator at the nodes $\{\vec{q}_k^h(t)\}_{k=1}^{K_\Gamma}$, and similarly $\vec{\pi}^h(t) : [C(\Gamma^h(t))]^d \to \underline{V}(\Gamma^h(t))$.

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

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

In order to derive a stable (semidiscrete) numerical method, it is crucial to consider numerical integration in the discrete energy, see (4.11) below. Hence, for piecewise continuous functions v, w, with possible jumps across the edges of $\{\sigma_j^h(t)\}_{j=1}^{J_\Gamma}$, we introduce the mass lumped inner product $\langle\cdot,\cdot\rangle_{\Gamma^h(t)}^h$ as

$$
\langle \eta, \phi\rangle_{\Gamma^h(t)}^h = \sum_{j=1}^{J} \langle \eta, \phi\rangle_{\sigma_j^h(t)}^h := \sum_{j=1}^{J} \tfrac{1}{d}\,\mathcal{H}^{d-1}(\sigma_j^h(t)) \sum_{k=1}^{d} (\eta\,\phi)((\vec{q}_{j_k}^h(t))^-)\,, \tag{4.2}
$$

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

Following [21, (5.23)], we define the discrete material velocity for $\vec{z} \in \Gamma^h(t)$ by

$$
\vec{\mathcal{V}}^h(\vec{z},t) := \sum_{k=1}^{K_\Gamma} \left[\frac{\mathrm{d}}{\mathrm{d}t}\,\vec{q}_k^h(t)\right] \chi_k^h(\vec{z},t)\,. \tag{4.3}
$$

For later use, we also introduce the finite element spaces

$$
W_T(\Gamma_T^h) := \{\phi \in C(\Gamma_T^h) : \phi(\cdot,t) \in W(\Gamma^h(t)) \quad \forall\, t \in [0,T]\,, \quad \phi(\vec{q}_k^h(t),t) \in H^1(0,T) \quad \forall\, k \in \{1,\dots,K\}\}\,,
$$

where $\Gamma_T^h := \bigcup_{t\in[0,T]} \Gamma^h(t) \times \{t\}$, as well as the vector- and tensor-valued analogues $\underline{V}_T(\Gamma_T^h)$ and $\underline{\underline{V}}_T(\Gamma_T^h)$. In a similar fashion, we introduce $W_T(\sigma_{j,T}^h)$ via

$$
W_T(\sigma_{j,T}^h) := \{\phi \in C(\overline{\sigma_{j,T}^h}) : \phi(\cdot,t) \text{ is linear} \quad \forall\, t \in [0,T]\,, \quad \phi(\vec{q}_{j_k}^h(t),t) \in H^1(0,T) \quad k = 1,\dots,d\}\,,
$$

where $\{\vec{q}^h_{j_k}(t)\}_{k=1}^d$ are the vertices of $\sigma^h_j(t)$, and where $\sigma^h_{j,T} := \bigcup_{t\in[0,T]} \sigma^h_j(t) \times \{t\}$, for $j \in \{1,\ldots,J\}$.

Then, similarly to (3.2), we define the discrete material derivatives on $\Gamma^h(t)$ element-by-element via the equations

$$(\partial_t^{\circ,h}\,\phi)\,|_{\sigma^h_j(t)} = (\phi_t + \vec{\mathcal{V}}^h\,.\,\nabla\,\phi)\,|_{\sigma^h_j(t)} \qquad \forall\ \phi \in W_T(\sigma^h_{j,T})\,,\ j \in \{1,\ldots,J\}\,.$$

Moreover, similarly to (3.13), for any given $\vec{\chi} \in \underline{V}(\Gamma^h(t))$ we introduce

$$\Gamma^h_\varepsilon(t) := \{\vec{\Phi}^h(\vec{z},\varepsilon) : \vec{z} \in \Gamma^h(t)\}\,, \quad \text{where} \quad \vec{\Phi}^h(\vec{z},0) = \vec{z} \quad \text{and} \quad \tfrac{\partial\vec{\Phi}^h}{\partial\varepsilon}(\vec{z},0) = \vec{\chi}(\vec{z}) \quad \forall\ \vec{z} \in \Gamma^h(t)\,, \tag{4.4}$$

as well as $\partial_\varepsilon^{0,h}$ defined by (3.15) with $\Gamma(t)$ and $\vec{\Phi}$ replaced by $\Gamma^h(t)$ and $\vec{\Phi}^h$, respectively. We also introduce

$$\mathbb{V}^h_{\Gamma^h}(\vec{g}) := \{\vec{\phi} \in H^1(0,T;\mathbb{U}^h(\vec{g})) : \exists\,\vec{\chi} \in \underline{V}_T(\Gamma^h_T), \text{ s.t. } \vec{\chi}(\cdot,t) = \vec{\pi}^h\,[\vec{\phi}|_{\Gamma^h(t)}]\ \forall\ t \in [0,T]\}\,. \tag{4.5}$$

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

$$\partial_t^{\circ,h}\,\chi^h_k = 0 \quad \forall\ k \in \{1,\ldots,K_\Gamma\}\,, \tag{4.6}$$

see [21, Lem. 5.5]. It follows directly from (4.6) that

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

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

We recall from [21, Lem. 5.6] that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\sigma^h_j(t)} \zeta\ \mathrm{d}\mathcal{H}^{d-1} = \int_{\sigma^h_j(t)} \partial_t^{\circ,h}\,\zeta + \zeta\,\nabla_s\,.\,\vec{\mathcal{V}}^h\ \mathrm{d}\mathcal{H}^{d-1} \quad \forall\ \zeta \in W_T(\sigma^h_{j,T})\,, j \in \{1,\ldots,J_\Gamma\}\,. \tag{4.7}$$

Moreover, on recalling (4.2), we have that

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\langle \eta,\zeta\rangle^h_{\sigma^h_j(t)} = \left\langle \partial_t^{\circ,h}\,\eta,\zeta\right\rangle^h_{\sigma^h_j(t)} + \left\langle \eta,\partial_t^{\circ,h}\,\zeta\right\rangle^h_{\sigma^h_j(t)} + \left\langle \eta\,\zeta,\nabla_s\,.\,\vec{\mathcal{V}}^h\right\rangle^h_{\sigma^h_j(t)} \quad \forall\ \eta,\zeta \in W_T(\sigma^h_{j,T})\,, j \in \{1,\ldots,J_\Gamma\}\,. \tag{4.8}$$

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

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

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

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

Similarly to (2.7a,b), we introduce

$$\underline{\underline{\mathcal{P}}}_{\Gamma^h} = \underline{\underline{\mathrm{Id}}} - \vec{\nu}^h \otimes \vec{\nu}^h \quad \text{on } \Gamma^h(t)\,, \tag{4.9a}$$

and

$$\underline{\underline{D}}_s^h(\vec\eta) = \tfrac12\,\underline{\underline{\mathcal{P}}}_{\Gamma^h}\,(\nabla_s\,\vec\eta + (\nabla_s\,\vec\eta)^T)\,\underline{\underline{\mathcal{P}}}_{\Gamma^h} \quad \text{on } \Gamma^h(t)\,, \tag{4.9b}$$

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

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

where for $k=1,\ldots,K^h_\Gamma$ we define $\Theta^h_k := \{j : \vec q^h_k(t) \in \overline{\sigma^h_j(t)}\}$ and set

$$\Lambda^h_k(t) := \cup_{j\in\Theta^h_k}\overline{\sigma^h_j(t)}\,.$$

For later use we note that

$$\left\langle \vec z, w\,\vec\nu^h\right\rangle^h_{\Gamma^h(t)} = \left\langle \vec z, w\,\vec\omega^h\right\rangle^h_{\Gamma^h(t)} \qquad \forall\ \vec z \in \underline{V}(\Gamma^h(t))\,,\ w \in W(\Gamma^h(t))\,, \tag{4.10}$$

and so, in particular, $\left\langle \vec z, \vec\nu^h\right\rangle_{\Gamma^h(t)} = \left\langle \vec z, \vec\nu^h\right\rangle^h_{\Gamma^h(t)} = \left\langle \vec z, \vec\omega^h\right\rangle^h_{\Gamma^h(t)}$ for all $\vec z \in \underline{V}(\Gamma^h(t))$.

In what follows we will introduce a finite element approximation for the weak formulation (P), recall (3.34). By repeating on the discrete level the steps in §3.2, we will now derive a discrete analogue of (3.30a–e).

Similarly to the continuous setting in (3.12) and (3.26a,b), we consider the first variation of the discrete energy

$$E^h(\Gamma^h(t),\mathfrak{C}^h(t)) = \tfrac12\left\langle \alpha(\mathfrak{C}^h), |\vec\kappa^h - \overline{\varkappa}(\mathfrak{C}^h)\,\vec\nu^h|^2\right\rangle^h_{\Gamma^h(t)} + \tfrac12\left\langle \alpha^G(\mathfrak{C}^h), |\vec\kappa^h|^2 - |\underline{\underline{W}}^h|^2\right\rangle^h_{\Gamma^h(t)} + \beta\left\langle b_{GL}(\mathfrak{C}^h), 1\right\rangle^h_{\Gamma^h(t)}\,, \tag{4.11}$$

where $\vec\kappa^h \in \underline{V}(\Gamma^h(t))$ and $\underline{\underline{W}}^h \in \underline{\underline{V}}(\Gamma^h(t))$ have to satisfy side constraints

$$\left\langle \vec\kappa^h, \vec\eta\right\rangle^h_{\Gamma^h(t)} + \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec\eta\right\rangle_{\Gamma^h(t)} = 0 \qquad \forall\ \vec\eta \in \underline{V}(\Gamma^h(t))\,, \tag{4.12a}$$

$$\left\langle \underline{\underline{W}}^h, \underline{\underline{\zeta}}\right\rangle^h_{\Gamma^h(t)} + \tfrac12\left\langle \vec\nu^h, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\,\vec\kappa^h + \nabla_s\,.\,[\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\right\rangle^h_{\Gamma^h(t)} = 0 \qquad \forall\ \underline{\underline{\zeta}} \in \underline{\underline{V}}(\Gamma^h(t))\,. \tag{4.12b}$$

Similarly to (3.28), we define the Lagrangian

$$\begin{aligned} &L^h(\Gamma^h, \vec\kappa^h, \vec Y^h, \underline{\underline{W}}^h, \underline{\underline{Z}}^h, \mathfrak{C}^h) \\ &\quad = \tfrac12\left\langle \alpha(\mathfrak{C}^h), |\vec\kappa^h - \overline{\varkappa}(\mathfrak{C}^h)\,\vec\nu^h|^2\right\rangle^h_{\Gamma^h(t)} + \tfrac12\left\langle \alpha^G(\mathfrak{C}^h), |\vec\kappa^h|^2 - |\underline{\underline{W}}^h|^2\right\rangle^h_{\Gamma^h(t)} + \beta\left\langle b_{GL}(\mathfrak{C}^h), 1\right\rangle^h_{\Gamma^h(t)} - \left\langle \vec\kappa^h, \vec Y^h\right\rangle^h_{\Gamma^h(t)} \\ &\qquad - \left\langle \nabla_s\,\vec{\mathrm{id}}, \nabla_s\,\vec Y^h\right\rangle_{\Gamma^h(t)} - \left\langle \underline{\underline{W}}^h, \underline{\underline{Z}}^h\right\rangle^h_{\Gamma^h(t)} - \tfrac12\left\langle \vec\nu^h, [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T]\,\vec\kappa^h + \nabla_s\,.\,[\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T]\right\rangle^h_{\Gamma^h(t)}\,, \end{aligned}$$

where $\vec\kappa^h \in \underline{V}(\Gamma^h(t))$, $\underline{\underline{W}}^h \in \underline{\underline{V}}(\Gamma^h(t))$, $\mathfrak{C}^h \in W(\Gamma^h(t))$, with $\vec Y^h \in \underline{V}(\Gamma^h(t))$ and $\underline{\underline{Z}}^h \in \underline{\underline{V}}(\Gamma^h(t))$ being Lagrange multipliers for (4.12a,b), respectively. Similarly to (3.30a–c), on recalling the formal calculus of PDE constrained optimization, we obtain the gradient $\vec F^h_\Gamma \in \underline{V}(\Gamma^h(t))$ of $E^h(\Gamma^h(t),\mathfrak{C}^h(t))$ with respect to $\Gamma^h(t)$ subject to the side constraints (4.12a,b) by setting $[\frac{\delta}{\delta\Gamma^h}\,L^h](\vec\chi) = -\left\langle \vec F^h_\Gamma, \vec\chi\right\rangle^h_{\Gamma^h(t)}$ for $\vec\chi \in \underline{V}(\Gamma^h(t))$, where we have recalled the definition (4.4), and by setting the remaining variations with respect to $\vec\kappa^h$, $\vec Y^h$, $\underline{\underline{W}}^h$ and $\underline{\underline{Z}}^h$ to zero. On noting (1.2b), (4.10) and the variation analogue of (4.8), as well as the obvious discrete variants of (3.17)–(3.20), (3.22) and (3.24), we then obtain that

$$\left\langle \vec{F}^h_\Gamma, \vec\chi \right\rangle^h_{\Gamma^h(t)} - \left\langle \nabla_s \vec{Y}^h, \nabla_s \vec\chi \right\rangle_{\Gamma^h(t)} - \left\langle \nabla_s \,.\, \vec{Y}^h, \nabla_s \,.\, \vec\chi \right\rangle_{\Gamma^h(t)} + \tfrac12 \left\langle \alpha(\mathfrak{C}^h)\, |\vec\kappa^h - \overline{\varkappa}(\mathfrak{C}^h)\,\vec\nu^h|^2 - 2\,\vec{Y}^h \,.\, \vec\kappa^h, \nabla_s \,.\, \vec\chi \right\rangle^h_{\Gamma^h(t)}$$
$$+ 2 \left\langle (\nabla_s \vec{Y}^h)^T, \underline{\underline{D}}^h_s(\vec\chi)\,(\nabla_s \vec{\rm id})^T \right\rangle_{\Gamma^h(t)} + \left\langle \alpha(\mathfrak{C}^h)\,\overline{\varkappa}(\mathfrak{C}^h)\,(\vec\kappa^h - \overline{\varkappa}(\mathfrak{C}^h)\,\vec\nu^h), [\nabla_s \vec\chi]^T\,\vec\nu^h \right\rangle^h_{\Gamma^h(t)}$$
$$+ \beta \left\langle b_{GL}(\mathfrak{C}^h), \nabla_s \,.\, \vec\chi \right\rangle^h_{\Gamma^h(t)} - \beta\,\gamma \left\langle (\nabla_s \mathfrak{C}^h) \otimes (\nabla_s \mathfrak{C}^h), \nabla_s \vec\chi \right\rangle_{\Gamma^h(t)} + \tfrac12 \left\langle \alpha^G(\mathfrak{C}^h)\,(|\vec\kappa^h|^2 - |\underline{\underline{W}}^h|^2), \nabla_s \,.\, \vec\chi \right\rangle^h_{\Gamma^h(t)}$$
$$- \left\langle \underline{\underline{W}}^h : \underline{\underline{Z}}^h, \nabla_s \,.\, \vec\chi \right\rangle^h_{\Gamma^h(t)} - \tfrac12 \left\langle \vec\nu^h \,.\, ([\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T]\,\vec\kappa^h + \nabla_s \,.\, [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T]), \nabla_s \,.\, \vec\chi \right\rangle^h_{\Gamma^h(t)}$$
$$- \sum_{i=1}^d \left\langle \nu^h_i\, \nabla_s \vec{Z}^h_i, \nabla_s \vec\chi - 2\,\underline{\underline{D}}^h_s(\vec\chi) \right\rangle_{\Gamma^h(t)} + \tfrac12 \left\langle [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T]\,\vec\kappa^h + \nabla_s \,.\, [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T], [\nabla_s \vec\chi]^T\,\vec\nu^h \right\rangle^h_{\Gamma^h(t)}$$
$$= 0 \qquad \forall\ \vec\chi \in \underline{V}(\Gamma^h(t))\,, \tag{4.13a}$$

$$\left\langle \alpha(\mathfrak{C}^h)\,(\vec\kappa^h - \overline{\varkappa}(\mathfrak{C}^h)\,\vec\nu^h) + \alpha^G(\mathfrak{C}^h)\,\vec\kappa^h - \tfrac12\,[\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T]\,\vec\nu^h - \vec{Y}^h, \vec\xi \right\rangle^h_{\Gamma^h(t)} = 0 \qquad \forall\ \vec\xi \in \underline{V}(\Gamma^h(t))\,, \tag{4.13b}$$

$$\underline{\underline{Z}}^h = \underline{\underline{\pi}}^h[-\alpha^G(\mathfrak{C}^h)\,\underline{\underline{W}}^h]\,, \tag{4.13c}$$

as well as (4.12a,b) from the variations with respect to $\vec{Y}^h$ and $\underline{\underline{Z}}^h$. Here we have introduced $\vec{Z}^h_i = \frac12\,[\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T]\,\vec{e}_i$, $i = 1 \to d$, as well as $\nu^h_i = \vec\nu^h \,.\, \vec{e}_i$, $i = 1 \to d$. Similarly to (3.27) it clearly follows from (4.12b) that

$$(\underline{\underline{W}}^h)^T = \underline{\underline{W}}^h \quad \Rightarrow \quad (\underline{\underline{Z}}^h)^T = \underline{\underline{Z}}^h\,, \tag{4.14}$$

and so many terms in (4.13a,b) can be simplified. We will perform these simplifications when we introduce the semidiscrete finite element approximation, see (4.16a–d), (4.17a–d) below. The Cahn–Hilliard dynamics are defined by

$$\vartheta\,\frac{\rm d}{{\rm d}t} \left\langle \mathfrak{C}^h, \chi^h_k \right\rangle^h_{\Gamma^h(t)} + \left\langle \nabla_s \mathfrak{M}^h, \nabla_s \chi^h_k \right\rangle_{\Gamma^h(t)} = 0 \qquad \forall\ k \in \{1, \ldots, K_\Gamma\}\,, \tag{4.15a}$$
$$\left\langle \mathfrak{M}^h, \xi \right\rangle^h_{\Gamma^h(t)} = \beta\,\gamma \left\langle \nabla_s \mathfrak{C}^h, \nabla_s \xi \right\rangle_{\Gamma^h(t)} + \beta\,\gamma^{-1} \left\langle \Psi'(\mathfrak{C}^h), \xi \right\rangle^h_{\Gamma^h(t)} + \tfrac12 \left\langle (\alpha^G)'(\mathfrak{C}^h)\,(|\vec\kappa^h|^2 - |\underline{\underline{W}}^h|^2), \xi \right\rangle^h_{\Gamma^h(t)}$$
$$+ \tfrac12 \left\langle \alpha'(\mathfrak{C}^h)\,|\vec\kappa^h - \overline{\varkappa}(\mathfrak{C}^h)\,\vec\nu^h|^2 - 2\,\overline{\varkappa}'(\mathfrak{C}^h)\,\alpha(\mathfrak{C}^h)\,(\vec\kappa^h - \overline{\varkappa}(\mathfrak{C}^h)\,\vec\nu^h) \,.\, \vec\nu^h, \xi \right\rangle^h_{\Gamma^h(t)} \qquad \forall\ \xi \in W(\Gamma^h(t))\,, \tag{4.15b}$$

where, similarly to the continuous setting (3.31a,b), we have defined $\mathfrak{M}^h \in W(\Gamma^h(t))$ by $\left\langle \mathfrak{M}^h, \xi \right\rangle^h_{\Gamma^h(t)} = [\frac{\delta}{\delta \mathfrak{C}^h}\, L^h](\xi)$ for all $\xi \in W(\Gamma^h(t))$.

Overall, we then obtain the following semidiscrete continuous-in-time finite element approximation, which is the semidiscrete analogue of the weak formulation (P), recall (3.34). Given $\Gamma^h(0)$, $\vec{U}^h(\cdot, 0) \in \mathbb{U}^h(\vec{g})$ and $\mathfrak{C}^h(\cdot, 0) \in W(\Gamma^h(0))$, find $(\Gamma^h(t))_{t\in(0,T]}$ such that $\vec{\rm id}\,|_{\Gamma^h(\cdot)} \in \underline{V}_T(\Gamma^h_T)$, with $\vec{\mathcal{V}}^h = \partial_t^{\circ,h}\,\vec{\rm id}\,|_{\Gamma^h(t)} \in \underline{V}(\Gamma^h(t))$ for all $t \in (0, T]$, and $\vec{U}^h \in \mathbb{V}^h_{\Gamma^h}(\vec{g})$, $\mathfrak{C}^h \in W_T(\Gamma^h_T)$, and, for all $t \in (0, T]$, $P^h(t) \in \widehat{\mathbb{P}}^h(t)$, $P^h_\Gamma(T) \in W(\Gamma^h(t))$, $\underline{\underline{W}}^h(t) \in \underline{\underline{V}}(\Gamma^h(t))$ and $\vec\kappa^h(t)$, $\vec{Y}^h(t)$, $\vec{F}^h_\Gamma(t) \in \underline{V}(\Gamma^h(t))$, $\mathfrak{M}^h \in W(\Gamma^h(t))$ such that (4.15a,b) holds, as well as

$$\tfrac12 \left[\frac{\rm d}{{\rm d}t} \left(\rho^h\,\vec{U}^h, \vec\xi \right) + \left(\rho^h\,\vec{U}^h_t, \vec\xi \right) - (\rho^h\,\vec{U}^h, \vec\xi_t) + \rho_+ \left\langle \vec{U}^h \,.\, \vec{\rm n}, \vec{U}^h \,.\, \vec\xi \right\rangle_{\partial_2\Omega} \right] + 2 \left(\mu^h\,\underline{\underline{D}}(\vec{U}^h), \underline{\underline{D}}(\vec\xi) \right)$$
$$+ \tfrac12 \left(\rho^h, [(\vec{U}^h \,.\, \nabla)\,\vec{U}^h] \,.\, \vec\xi - [(\vec{U}^h \,.\, \nabla)\,\vec\xi] \,.\, \vec{U}^h \right) - \left(P^h, \nabla \,.\, \vec\xi \right) + \rho_\Gamma \left\langle \partial_t^{\circ,h}\,\vec\pi^h\,\vec{U}^h, \vec\xi \right\rangle^h_{\Gamma^h(t)}$$
$$+ 2\,\mu_\Gamma \left\langle \underline{\underline{D}}^h_s(\vec\pi^h\,\vec{U}^h), \underline{\underline{D}}^h_s(\vec\pi^h\,\vec\xi) \right\rangle_{\Gamma^h(t)} - \left\langle P^h_\Gamma, \nabla_s \,.\, (\vec\pi^h\,\vec\xi) \right\rangle_{\Gamma^h(t)} = \left(\rho^h\,\vec{f}^h, \vec\xi \right) + \left\langle \vec{F}^h_\Gamma, \vec\xi \right\rangle^h_{\Gamma^h(t)}$$

$$\forall\, \vec\xi \in H^1(0,T;\mathbb{U}^h(\vec 0))\,, \tag{4.16a}$$

$$\left(\nabla\,.\,\vec U^h, \varphi\right) = 0 \qquad \forall\ \varphi \in \widehat{\mathbb{P}}^h(t)\,, \tag{4.16b}$$

$$\left\langle \nabla_s\,.\,(\vec\pi^h\,\vec U^h), \eta\right\rangle_{\Gamma^h(t)} = 0 \qquad \forall\ \eta \in W(\Gamma^h(t))\,, \tag{4.16c}$$

$$\left\langle \vec{\mathcal{V}}^h, \vec\chi\right\rangle_{\Gamma^h(t)}^h = \left\langle \vec U^h, \vec\chi\right\rangle_{\Gamma^h(t)}^h \qquad \forall\ \vec\chi \in \underline{V}(\Gamma^h(t))\,, \tag{4.16d}$$

where we recall (4.3), and

$$\langle \vec\kappa^h, \vec\eta\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s\,\vec{\rm id}, \nabla_s\,\vec\eta\right\rangle_{\Gamma^h(t)} = 0 \quad \forall\ \vec\eta \in \underline{V}(\Gamma^h(t))\,, \tag{4.17a}$$

$$\left\langle \underline{\underline{W}}^h, \underline{\underline{\zeta}}\right\rangle_{\Gamma^h(t)}^h + \tfrac12 \left\langle \vec\nu^h, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\,\vec\kappa^h + \nabla_s\,.\,[\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\right\rangle_{\Gamma^h(t)}^h = 0 \qquad \forall\ \underline{\underline{\zeta}} \in \underline{\underline{V}}(\Gamma^h(t))\,, \tag{4.17b}$$

$$\left\langle \alpha(\mathfrak{C}^h)\,(\vec\kappa^h - \overline{\varkappa}(\mathfrak{C}^h)\,\vec\nu^h) + \alpha^G(\mathfrak{C}^h)\,(\vec\varkappa + \underline{\underline{W}}^h\,\vec\nu^h) - \vec Y^h, \vec\xi\right\rangle_{\Gamma^h(t)}^h = 0 \qquad \forall\ \vec\xi \in \underline{V}(\Gamma^h(t))\,, \tag{4.17c}$$

$$\begin{aligned}
\left\langle \vec F_\Gamma^h, \vec\chi\right\rangle_{\Gamma^h(t)}^h &= \left\langle \nabla_s\,\vec Y^h, \nabla_s\,\vec\chi\right\rangle_{\Gamma^h(t)} + \left\langle \nabla_s\,.\,\vec Y^h, \nabla_s\,.\,\vec\chi\right\rangle_{\Gamma^h(t)} - 2\left\langle (\nabla_s\,\vec Y^h)^T, \underline{\underline{D}}_s^h(\vec\chi)\,(\nabla_s\,\vec{\rm id})^T\right\rangle_{\Gamma^h(t)} \\
&\quad - \tfrac12 \left\langle [\alpha(\mathfrak{C}^h)\,|\vec\kappa^h - \overline{\varkappa}(\mathfrak{C}^h)\,\vec\nu^h|^2 - 2\,\vec Y^h\,.\,\vec\kappa^h], \nabla_s\,.\,\vec\chi\right\rangle_{\Gamma^h(t)}^h - \langle \alpha(\mathfrak{C}^h)\,\overline{\varkappa}(\mathfrak{C}^h)\,\vec\kappa^h, [\nabla_s\,\vec\chi]^T\,\vec\nu^h\rangle_{\Gamma^h(t)}^h \\
&\quad - \beta\,\langle b_{GL}(\mathfrak{C}^h), \nabla_s\,.\,\vec\chi\rangle_{\Gamma^h(t)}^h + \beta\,\gamma\,\langle (\nabla_s\,\mathfrak{C}^h)\otimes(\nabla_s\,\mathfrak{C}^h), \nabla_s\,\vec\chi\rangle_{\Gamma^h(t)} \\
&\quad - \tfrac12 \langle \alpha^G(\mathfrak{C}^h)\,(|\vec\kappa^h|^2 + |\underline{\underline{W}}^h|^2), \nabla_s\,.\,\vec\chi\rangle_{\Gamma^h(t)}^h + \langle \vec\nu^h\,.\,(\underline{\underline{Z}}^h\,\vec\kappa^h + \nabla_s\,.\,\underline{\underline{Z}}^h), \nabla_s\,.\,\vec\chi\rangle_{\Gamma^h(t)}^h \\
&\quad + \sum_{i=1}^d \left\langle \nu_i^h\,\nabla_s\,\vec Z_i^h, \nabla_s\,\vec\chi - 2\,\underline{\underline{D}}_s^h(\vec\chi)\right\rangle_{\Gamma^h(t)} - \langle \underline{\underline{Z}}^h\,\vec\kappa^h + \nabla_s\,.\,\underline{\underline{Z}}^h, [\nabla_s\,\vec\chi]^T\,\vec\nu^h\rangle_{\Gamma^h(t)}^h \qquad \forall\ \vec\chi \in \underline{V}(\Gamma^h(t))\,,
\end{aligned} \tag{4.17d}$$

where $\underline{\underline{Z}}^h = \underline{\underline{\pi}}^h[-\alpha^G(\mathfrak{C}^h)\,\underline{\underline{W}}^h]$ and $\vec Z_i^h = \underline{\underline{Z}}^h\,\vec e_i$, $i = 1 \to d$. In addition, we have noted (4.14) and that $\alpha(\mathfrak{C}^h)\,\overline{\varkappa}^2(\mathfrak{C}^h)\,\vec\nu^h\,.\,[\nabla_s\,\vec\chi]^T\,\vec\nu^h = 0$ on $\Gamma^h(t)$. Here we have defined $\vec f^h(\cdot,t) := \vec I_2^h\,\vec f(\cdot,t)$, where here and throughout we assume that $\vec f \in L^2(0,T;[C(\overline\Omega)]^d)$. We note that in the special case of uniform α and $\overline{\varkappa}$, and if $\alpha^G = \beta = 0$, the scheme (4.16a–d), (4.17a–d) collapses to the semidiscrete approximation (4.15a–g), with $\beta = 0$, from [7].

The following lemma is crucial in establishing a direct discrete analogue of (1.6).

Lemma 4.1. *Let* $\{(\Gamma^h, \vec U^h, P^h, P_\Gamma^h, \vec\kappa^h, \vec Y^h, \vec F_\Gamma^h, \underline{\underline{W}}^h, \underline{\underline{Z}}^h, \mathfrak{C}^h, \mathfrak{M}^h)(t)\}_{t\in[0,T]}$ *be a solution to* (4.15a,b), (4.16a–d), (4.17a–d). *In addition, we assume that* $\vec\kappa^h \in \underline{V}_T(\Gamma_T^h)$ *and* $\underline{\underline{W}}^h \in \underline{\underline{V}}_T(\Gamma_T^h)$. *Then*

$$\frac{\rm d}{{\rm d}t}\,E^h(\Gamma^h(t), \mathfrak{C}^h(t)) = -\left\langle \vec F_\Gamma^h, \vec{\mathcal{V}}^h\right\rangle_{\Gamma^h(t)}^h + \left\langle \mathfrak{M}^h, \partial_t^{\circ,h}\,\mathfrak{C}^h\right\rangle_{\Gamma^h(t)}^h. \tag{4.18}$$

Proof. Taking the time derivatives of (4.12a,b), where we choose discrete test functions $\vec\eta$ and $\underline{\underline{\zeta}}$ such that $\partial_t^{\circ,h}\,\vec\eta = \vec 0$ and $\partial_t^{\circ,h}\,\underline{\underline{\zeta}} = \underline{\underline{0}}$, respectively, yields that

$$\begin{aligned}
&\left\langle \partial_t^{\circ,h}\,\vec\kappa^h, \vec\eta\right\rangle_{\Gamma^h(t)}^h + \left\langle \vec\kappa^h\,.\,\vec\eta, \nabla_s\,.\,\vec{\mathcal{V}}^h\right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s\,.\,\vec{\mathcal{V}}^h, \nabla_s\,.\,\vec\eta\right\rangle_{\Gamma^h(t)} + \left\langle \nabla_s\,\vec{\mathcal{V}}^h, \nabla_s\,\vec\eta\right\rangle_{\Gamma^h(t)} \\
&\qquad - 2\left\langle \underline{\underline{D}}_s^h(\vec{\mathcal{V}}^h)\,(\nabla_s\,\vec{\rm id})^T, (\nabla_s\,\vec\eta)^T\right\rangle_{\Gamma^h(t)} = 0\,,
\end{aligned} \tag{4.19a}$$

$$\left\langle \partial_t^{\circ,h}\,\underline{\underline{W}}^h, \underline{\underline{\zeta}}\right\rangle_{\Gamma^h(t)}^h + \left\langle \underline{\underline{W}}^h : \underline{\underline{\zeta}}, \nabla_s\,.\,\vec{\mathcal{V}}^h\right\rangle_{\Gamma^h(t)}^h + \tfrac12 \left\langle \partial_t^{\circ,h}\,\vec\nu^h, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\,\vec\kappa^h + \nabla_s\,.\,[\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\right\rangle_{\Gamma^h(t)}^h$$

$$+ \tfrac{1}{2} \left\langle \vec{\nu}^h \,.\, ([\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\, \vec{\kappa}^h + \nabla_s \,.\, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]), \nabla_s \,.\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)}$$

$$+ \sum_{i=1}^{d} \left\langle \nu_i^h \,\nabla_s \,\vec{\zeta}_i, \nabla_s \,\vec{\mathcal{V}}^h - 2\,\underline{\underline{D}}^h_s(\vec{\mathcal{V}}^h) \right\rangle_{\Gamma^h(t)} + \tfrac{1}{2} \left\langle \vec{\nu}^h, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\, \partial_t^{\circ,h}\, \vec{\kappa}^h \right\rangle^h_{\Gamma^h(t)} = 0\,, \tag{4.19b}$$

where $\vec{\zeta}_i = \frac{1}{2}\,[\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\,\vec{e}_i$, $i = 1,\ldots,d$. Here we have noted $\vec{\kappa}^h \in \underline{V}_T(\Gamma^h_T)$, $\underline{\underline{W}}^h \in \underline{\underline{V}}_T(\Gamma^h_T)$, (4.8) and the discrete versions of (3.25) and (3.22). Choosing $\vec{\chi} = \vec{\mathcal{V}}^h$ in (4.13a), $\vec{\eta} = \vec{Y}^h$ in (4.19a) $\underline{\underline{\zeta}} = \underline{\underline{Z}}^h$ in (4.19b) and combining yields, on recalling (4.8) and the discrete variants of (3.19) and (3.24), that

$$\begin{aligned}
- \left\langle \vec{F}^h_\Gamma, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} &= \tfrac{1}{2} \left\langle \alpha(\mathfrak{c}^h)\, |\vec{\kappa}^h - \overline{\varkappa}(\mathfrak{c}^h)\,\vec{\nu}^h|^2, \nabla_s \,.\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} - \left\langle \alpha(\mathfrak{c}^h)\,\overline{\varkappa}(\mathfrak{c}^h)\,(\vec{\kappa}^h - \overline{\varkappa}(\mathfrak{c}^h)\,\vec{\nu}^h), \partial_t^{\circ,h}\,\vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} \\
&\quad + \left\langle \partial_t^{\circ,h}\,\vec{\kappa}^h, \vec{Y}^h \right\rangle^h_{\Gamma^h(t)} + \beta \left\langle b_{GL}(\mathfrak{c}^h), \nabla_s \,.\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} - \beta\,\gamma \left\langle (\nabla_s\,\mathfrak{c}^h) \otimes (\nabla_s\,\mathfrak{c}^h), \nabla_s\,\vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)} \\
&\quad + \tfrac{1}{2} \left\langle \alpha^G(\mathfrak{c}^h)\,(|\vec{\kappa}^h|^2 - |\underline{\underline{W}}^h|^2), \nabla_s \,.\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} + \left\langle \partial_t^{\circ,h}\,\underline{\underline{W}}^h, \underline{\underline{Z}}^h \right\rangle^h_{\Gamma^h(t)} + \tfrac{1}{2} \left\langle \vec{\nu}^h, [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T]\,\partial_t^{\circ,h}\,\vec{\kappa}^h \right\rangle^h_{\Gamma^h(t)} \\
&= \tfrac{1}{2} \left\langle \alpha(\mathfrak{c}^h)\, |\vec{\kappa}^h - \overline{\varkappa}(\mathfrak{c}^h)\,\vec{\nu}^h|^2, \nabla_s \,.\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} - \left\langle \alpha(\mathfrak{c}^h)\,\overline{\varkappa}(\mathfrak{c}^h)\,(\vec{\kappa}^h - \overline{\varkappa}(\mathfrak{c}^h)\,\vec{\nu}^h), \partial_t^{\circ,h}\,\vec{\nu}^h \right\rangle^h_{\Gamma^h(t)} \\
&\quad + \left\langle \alpha(\mathfrak{c}^h)\,(\vec{\kappa}^h - \overline{\varkappa}(\mathfrak{c}^h)\,\vec{\nu}^h) + \alpha^G(\mathfrak{c}^h)\,\vec{\kappa}^h, \partial_t^{\circ,h}\,\vec{\kappa}^h \right\rangle^h_{\Gamma^h(t)} - \beta\,\gamma \left\langle (\nabla_s\,\mathfrak{c}^h) \otimes (\nabla_s\,\mathfrak{c}^h), \nabla_s\,\vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)} \\
&\quad + \beta \left\langle b_{GL}(\mathfrak{c}^h), \nabla_s \,.\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} + \tfrac{1}{2} \left\langle \alpha^G(\mathfrak{c}^h)\,(|\vec{\kappa}^h|^2 - |\underline{\underline{W}}^h|^2), \nabla_s \,.\, \vec{\mathcal{V}}^h \right\rangle^h_{\Gamma^h(t)} - \left\langle \alpha^G(\mathfrak{c}^h)\,\partial_t^{\circ,h}\,\underline{\underline{W}}^h, \underline{\underline{W}}^h \right\rangle^h_{\Gamma^h(t)} \\
&= \frac{\mathrm{d}}{\mathrm{d}t} \left[\tfrac{1}{2} \left\langle \alpha(\mathfrak{c}^h), |\vec{\kappa}^h - \overline{\varkappa}(\mathfrak{c}^h)\,\vec{\nu}^h|^2 \right\rangle^h_{\Gamma^h(t)} + \tfrac{1}{2} \left\langle \alpha^G(\mathfrak{c}^h), |\vec{\kappa}^h|^2 - |\underline{\underline{W}}^h|^2 \right\rangle^h_{\Gamma^h(t)} + \beta \left\langle b_{GL}(\mathfrak{c}^h), 1 \right\rangle^h_{\Gamma^h(t)} \right] \\
&\quad - \tfrac{1}{2} \left\langle \alpha'(\mathfrak{c}^h)\, |\vec{\kappa}^h - \overline{\varkappa}(\mathfrak{c}^h)\,\vec{\nu}^h|^2 - 2\,\overline{\varkappa}'(\mathfrak{c}^h)\,\alpha(\mathfrak{c}^h)\,(\vec{\kappa}^h - \overline{\varkappa}(\mathfrak{c}^h)\,\vec{\nu}^h) \,.\, \vec{\nu}^h, \partial_t^{\circ,h}\,\mathfrak{c}^h \right\rangle^h_{\Gamma^h(t)} \\
&\quad - \tfrac{1}{2} \left\langle (\alpha^G)'(\mathfrak{c}^h)\,(|\vec{\kappa}^h|^2 - |\underline{\underline{W}}^h|^2), \partial_t^{\circ,h}\,\mathfrak{c}^h \right\rangle^h_{\Gamma^h(t)} - \beta\,\gamma \left\langle \nabla_s\,\mathfrak{c}^h, \nabla_s\,\partial_t^{\circ,h}\,\mathfrak{c}^h \right\rangle_{\Gamma^h(t)} - \beta\,\gamma^{-1} \left\langle \Psi'(\mathfrak{c}^h), \partial_t^{\circ,h}\,\mathfrak{c}^h \right\rangle^h_{\Gamma^h(t)} \\
&= \frac{\mathrm{d}}{\mathrm{d}t} E^h(\Gamma^h(t), \mathfrak{c}^h(t)) - \left\langle \mathfrak{M}^h, \partial_t^{\circ,h}\,\mathfrak{c}^h \right\rangle^h_{\Gamma^h(t)}
\end{aligned} \tag{4.20}$$

where we have noted (4.13b,c) and (4.15b), as well as $\mathfrak{c}^h \in W_T(\Gamma^h_T)$. This yields the desired result (4.18). □

In the following theorem we derive discrete analogues of (1.6), (3.7) and (3.32) for the scheme (4.15a,b), (4.16a–d), (4.17a–d).

Theorem 4.2. *Let the assumptions of* Lemma 4.1 *hold. Then, in the case* $\vec{g} = \vec{0}$, *it holds that*

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t} \left(\tfrac{1}{2}\, \|[\rho^h]^{\frac{1}{2}}\, \vec{U}^h\|_0^2 + \tfrac{1}{2}\,\rho_\Gamma \left\langle \vec{U}^h, \vec{U}^h \right\rangle^h_{\Gamma^h(t)} + E^h(\Gamma^h(t), \mathfrak{c}^h(t)) \right) + 2\,\mu_\Gamma \left\langle \underline{\underline{D}}^h_s(\vec{\pi}^h\,\vec{U}^h), \underline{\underline{D}}^h_s(\vec{\pi}^h\,\vec{U}^h) \right\rangle_{\Gamma^h(t)} \\
&\quad + 2\,\|[\mu^h]^{\frac{1}{2}}\, \underline{\underline{D}}(\vec{U}^h)\|_0^2 + \tfrac{1}{2}\,\rho_+ \left\langle \vec{U}^h \,.\, \mathrm{n}, |\vec{U}^h|^2 \right\rangle_{\partial_2\Omega} + \vartheta^{-1} \left\langle \nabla_s\,\mathfrak{M}^h, \nabla_s\,\mathfrak{M}^h \right\rangle_{\Gamma^h(t)} = (\rho^h\,\vec{f}^h, \vec{U}^h)\,.
\end{aligned} \tag{4.21}$$

Moreover, it holds that

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\langle \chi^h_k, 1 \right\rangle_{\Gamma^h(t)} = 0 \quad \forall\ k \in \{1,\ldots,K_\Gamma\} \tag{4.22a}$$

and hence that

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{H}^{d-1}(\Gamma^h(t)) = 0\,. \tag{4.22b}$$

Finally, we have that

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\langle \mathfrak{C}^h, 1 \right\rangle_{\Gamma^h(t)} = 0\,. \tag{4.22c}$$

Proof. Choosing $\vec\xi = \vec U^h$ in (4.16a), recall that $\vec g = \vec 0$, $\varphi = P^h$ in (4.16b) and $\eta = P^h_\Gamma$ in (4.16c) yields that

$$\begin{aligned}\tfrac12 \frac{\mathrm{d}}{\mathrm{d}t} \|[\rho^h]^{\frac12}\,\vec U^h\|_0^2 + 2\,\|[\mu^h]^{\frac12}\,\underline{\underline{D}}(\vec U^h)\|_0^2 + \rho_\Gamma \left\langle \partial_t^{\circ,h}\,\vec\pi^h\,\vec U^h, \vec U^h\right\rangle_{\Gamma^h(t)}^h + \tfrac12\,\rho_+ \left\langle \vec U^h \,.\, \mathrm{\vec n}, |\vec U^h|^2\right\rangle_{\partial_2\Omega} \\ + 2\,\mu_\Gamma \left\langle \underline{\underline{D}}{}_s^h(\vec\pi^h\,\vec U^h), \underline{\underline{D}}{}_s^h(\vec\pi^h\,\vec U^h)\right\rangle_{\Gamma^h(t)} = (\rho^h\,\vec f^h, \vec U^h) + \left\langle \vec F_\Gamma^h, \vec U^h\right\rangle_{\Gamma^h(t)}^h .\end{aligned} \tag{4.23}$$

In addition, we note that (4.8), (4.16d) and (4.16c) with $\eta = \pi^h\,[|\vec U^h\,|_{\Gamma^h(t)}\,|^2]$ imply that

$$\begin{aligned}\tfrac12\,\rho_\Gamma \frac{\mathrm{d}}{\mathrm{d}t} \left\langle \vec U^h, \vec U^h\right\rangle_{\Gamma^h(t)}^h &= \tfrac12\,\rho_\Gamma \left\langle \partial_t^{\circ,h}\,\pi^h\,[|\vec U^h|^2], 1\right\rangle_{\Gamma^h(t)}^h + \tfrac12\,\rho_\Gamma \left\langle \nabla_s \,.\, \vec{\mathcal{V}}^h, |\vec U^h|^2\right\rangle_{\Gamma^h(t)}^h \\ &= \rho_\Gamma \left\langle \partial_t^{\circ,h}\,\vec\pi^h\,\vec U^h, \vec U^h\right\rangle_{\Gamma^h(t)}^h + \tfrac12\,\rho_\Gamma \left\langle \nabla_s \,.\, (\vec\pi^h\,\vec U^h), |\vec\pi^h\,\vec U^h|^2\right\rangle_{\Gamma^h(t)} = \rho_\Gamma \left\langle \partial_t^{\circ,h}\,\vec\pi^h\,\vec U^h, \vec U^h\right\rangle_{\Gamma^h(t)}^h ,\end{aligned} \tag{4.24}$$

where we have recalled $\vec U^h \in \mathbb{V}^h_{\Gamma^h}(\vec g)$, see (4.5). Choosing $\vec\chi = \vec F^h_\Gamma$ in (4.16d), and combining with (4.18), yields that

$$\left\langle \vec F_\Gamma^h, \vec U^h\right\rangle_{\Gamma^h(t)}^h = \left\langle \vec F_\Gamma^h, \vec{\mathcal{V}}^h\right\rangle_{\Gamma^h(t)}^h = -\frac{\mathrm{d}}{\mathrm{d}t} E^h(\Gamma^h(t), \mathfrak{C}^h(t)) + \left\langle \mathfrak{M}^h, \partial_t^{\circ,h}\,\mathfrak{C}^h\right\rangle_{\Gamma^h(t)}^h . \tag{4.25}$$

Moreover, similarly to (4.24), it follows from (4.8), (4.6) and (4.16c,d), on recalling $\mathfrak{C}^h \in W_T(\Gamma^h_T)$, that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} \left\langle \mathfrak{C}^h, \chi_k^h\right\rangle_{\Gamma^h(t)}^h &= \left\langle \partial_t^{\circ,h}\,\mathfrak{C}^h, \chi_k^h\right\rangle_{\Gamma^h(t)}^h + \left\langle \mathfrak{C}^h\,\chi_k^h, \nabla_s \,.\, \vec{\mathcal{V}}^h\right\rangle_{\Gamma^h(t)}^h = \left\langle \partial_t^{\circ,h}\,\mathfrak{C}^h, \chi_k^h\right\rangle_{\Gamma^h(t)}^h + \left\langle \pi^h\,[\mathfrak{C}^h\,\chi_k^h], \nabla_s \,.\, \vec{\mathcal{V}}^h\right\rangle_{\Gamma^h(t)} \\ &= \left\langle \partial_t^{\circ,h}\,\mathfrak{C}^h, \chi_k^h\right\rangle_{\Gamma^h(t)}^h + \left\langle \pi^h\,[\mathfrak{C}^h\,\chi_k^h], \nabla_s \,.\, (\vec\pi^h\,\vec U^h)\right\rangle_{\Gamma^h(t)} = \left\langle \partial_t^{\circ,h}\,\mathfrak{C}^h, \chi_k^h\right\rangle_{\Gamma^h(t)}^h ,\end{aligned}$$

for $k = 1, \ldots, K_\Gamma$. Hence we obtain from (4.15a) that

$$-\left\langle \mathfrak{M}^h, \partial_t^{\circ,h}\,\mathfrak{C}^h\right\rangle_{\Gamma^h(t)}^h = \vartheta^{-1} \left\langle \nabla_s\,\mathfrak{M}^h, \nabla_s\,\mathfrak{M}^h\right\rangle_{\Gamma^h(t)} . \tag{4.26}$$

The desired result (4.21) now directly follows from combining (4.23), (4.24), (4.25) and (4.26).

Similarly to (3.7), it immediately follows from (4.7) and (4.6), on choosing $\eta = \chi_k^h$ in (4.16c), and on recalling from (4.16d) that $\vec{\mathcal{V}}^h = \vec\pi^h\,[\vec U^h\,|_{\Gamma^h(t)}]$, that

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

which proves the desired result (4.22a). Summing (4.22a) for all $k = 1, \ldots, K_\Gamma$ then yields the desired result (4.22b). Similarly, summing (4.15a) for $k = 1, \ldots, K_\Gamma$ yields the desired result (4.22c). □

We observe that it does not appear possible to prove a discrete analogue of (3.8) for the scheme (4.15a,b), (4.16a–d), (4.17a–d), even if the pressure space $\mathbb{P}^h(t)$ is enriched by the characteristic function of the inner phase, $\mathcal{X}_{\Omega_-^h(t)}$. Following the approach introduced in [6, 7], we enforce

$$\left\langle \vec U^h, \vec\omega^h\right\rangle_{\Gamma^h(t)}^h = 0\,, \tag{4.27}$$

which will lead to volume conservation for the two phases on the discrete level. As (4.27) cannot be interpreted in terms of enriching $\mathbb{P}^h(t)$, we enforce it separately with the help of a Lagrange multiplier, which we denote by $P^h_{\rm sing}$. We are now in a position to propose the following adaptation of (4.15a,b), (4.16a–d), (4.17a–d)

Given $\Gamma^h(0)$, $\vec U^h(\cdot,0) \in \mathbb{U}^h(\vec g)$ and $\mathfrak{C}^h(\cdot,0) \in W(\Gamma^h(0))$, find $(\Gamma^h(t))_{t\in(0,T]}$ such that $\vec{\rm id}\mid_{\Gamma^h(\cdot)} \in \underline{V}_T(\Gamma^h_T)$, with $\vec{\mathcal{V}}^h = \partial_t^{\circ,h}\,\vec{\rm id}\mid_{\Gamma^h(t)} \in \underline{V}(\Gamma^h(t))$ for all $t\in(0,T]$, and $\vec U^h \in \mathbb{V}^h_{\Gamma^h}(\vec g)$, $\mathfrak{C}^h \in W_T(\Gamma^h_T)$, and, for all $t\in(0,T]$, $P^h(t) \in \widehat{\mathbb{P}}^h(t)$, $P^h_{\rm sing}(t) \in \mathbb{R}$, $P^h_\Gamma(T) \in W(\Gamma^h(t))$, $\underline{\underline{W}}^h(t) \in \underline{\underline{V}}(\Gamma^h(t))$ and $\vec\kappa^h(t)$, $\vec Y^h(t)$, $\vec F^h_\Gamma(t) \in \underline{V}(\Gamma^h(t))$, $\mathfrak{M}^h \in W(\Gamma^h(t))$ such that (4.15a,b) holds, as well as

$$
\begin{aligned}
&\tfrac12\left[\frac{\rm d}{{\rm d}t}\left(\rho^h\,\vec U^h,\vec\xi\right)+\left(\rho^h\,\vec U^h_t,\vec\xi\right)-(\rho^h\,\vec U^h,\vec\xi_t)+\rho_+\left\langle \vec U^h\,.\,\vec{\rm n},\vec U^h\,.\,\vec\xi\right\rangle_{\partial_2\Omega}\right]\\
&\quad+2\left(\mu^h\,\underline{\underline{D}}(\vec U^h),\underline{\underline{D}}(\vec\xi)\right)+\tfrac12\left(\rho^h,[(\vec U^h\,.\,\nabla)\,\vec U^h]\,.\,\vec\xi-[(\vec U^h\,.\,\nabla)\,\vec\xi]\,.\,\vec U^h\right)-\left(P^h,\nabla\,.\,\vec\xi\right)\\
&\quad-P^h_{\rm sing}\left\langle\vec\omega^h,\vec\xi\right\rangle^h_{\Gamma^h(t)}+\rho_\Gamma\left\langle\partial_t^{\circ,h}\,\vec\pi^h\,\vec U^h,\vec\xi\right\rangle^h_{\Gamma^h(t)}+2\,\mu_\Gamma\left\langle\underline{\underline{D}}^h_s(\vec\pi^h\,\vec U^h),\underline{\underline{D}}^h_s(\vec\pi^h\,\vec\xi)\right\rangle_{\Gamma^h(t)}\\
&\quad-\left\langle P^h_\Gamma,\nabla_s\,.\,(\vec\pi^h\,\vec\xi)\right\rangle_{\Gamma^h(t)}=\left(\rho^h\,\vec f^h,\vec\xi\right)+\left\langle\vec F^h_\Gamma,\vec\xi\right\rangle^h_{\Gamma^h(t)}\qquad\forall\,\vec\xi\in H^1(0,T;\mathbb{U}^h(\vec 0))\,,
\end{aligned}
\tag{4.28a}
$$

$$
\left(\nabla\,.\,\vec U^h,\varphi\right)=0\qquad\forall\,\varphi\in\widehat{\mathbb{P}}^h(t)\qquad\text{and}\qquad\left\langle\vec U^h,\vec\omega^h\right\rangle^h_{\Gamma^h(t)}=0
\tag{4.28b}
$$

and (4.16c,d), (4.17a–d) hold. We now have the following result.

Theorem 4.3. *Let* $\{(\Gamma^h,\vec U^h,P^h,P^h_{\rm sing},P^h_\Gamma,\vec\kappa^h,\vec Y^h,\vec F^h_\Gamma,\underline{\underline{W}}^h,\underline{\underline{Z}}^h,\mathfrak{C}^h,\mathfrak{M}^h)(t)\}_{t\in[0,T]}$ *be a solution to* (4.15a,b), (4.28a,b), (4.16c,d), (4.17a–d). *In addition, we assume that* $\vec\kappa^h \in \underline{V}_T(\Gamma^h_T)$ *and* $\underline{\underline{W}}^h \in \underline{\underline{V}}_T(\Gamma^h_T)$. *Then* (4.21) *holds if* $\vec g = \vec 0$. *In addition,* (4.22a–c) *and*

$$
\frac{\rm d}{{\rm d}t}\,\mathcal{L}^d(\Omega^h_-(t))=0
\tag{4.29}
$$

hold.

Proof. The proofs for (4.21) and (4.22a–c) are analogous to the proofs in Theorem 4.2. In order to prove (4.29) we choose $\vec\chi=\vec\omega^h\in\underline{V}(\Gamma^h(t))$ in (4.16d) to yield that

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

where we have used [17, Lemma 2.1], (4.10) and (4.28b). □

5. Fully discrete finite element approximation

We consider the partitioning $t_m = m\,\tau$, $m=0,\ldots,M$, of $[0,T]$ into uniform time steps $\tau=T/M$. The time discrete spatial discretizations then directly follow from the finite element spaces introduced in §4, where in order to allow for adaptivity in space we consider bulk finite element spaces that change in time. For all $m\geq 0$, let $\mathcal{T}^m$ be a regular partitioning of Ω into disjoint open simplices o^m_j, $j=1,\ldots,J^m_\Omega$. Associated with $\mathcal{T}^m$ are the finite element spaces $S^m_k(\Omega)$ for $k\geq 0$. We introduce also $\vec I^m_k : [C(\overline\Omega)]^d \to [S^m_k(\Omega)]^d$, $k\geq 1$, the standard interpolation operators, and the standard projection operator $I^m_0 : L^1(\Omega)\to S^m_0(\Omega)$. The parametric finite element spaces are given by

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

for $m=0,\ldots,M-1$, and similarly for $\underline{\underline{V}}(\Gamma^m)$. Here $\Gamma^m=\bigcup_{j=1}^{J_\Gamma}\overline{\sigma^m_j}$, where $\{\sigma^m_j\}_{j=1}^{J_\Gamma}$ is a family of mutually disjoint open $(d-1)$-simplices with vertices $\{\vec q^m_k\}_{k=1}^{K_\Gamma}$. We denote the standard basis of $W(\Gamma^m)$ by $\{\chi^m_k(\cdot,t)\}_{k=1}^{K_\Gamma}$.

We also introduce $\pi^m : C(\Gamma^m) \to W(\Gamma^m)$, the standard interpolation operator at the nodes $\{\vec{q}_k^m\}_{k=1}^{K_\Gamma}$, and similarly $\vec{\pi}^m : [C(\Gamma^m)]^d \to \underline{V}(\Gamma^m)$. Throughout this paper, we will parameterize the new closed surface Γ^{m+1} over Γ^m, with the help of a parameterization $\vec{X}^{m+1} \in \underline{V}(\Gamma^m)$, i.e. $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$. Moreover, let $W_{\leq 1}(\Gamma^m) := \{\chi \in W(\Gamma^m) : |\chi| \leq 1\}$.

Given Γ^m, we let Ω_+^m denote the exterior of Γ^m and let Ω_-^m denote the interior of Γ^m, so that $\Gamma^m = \partial\Omega_-^m = \overline{\Omega_-^m} \cap \overline{\Omega_+^m}$. In addition, we define the piecewise constant unit normal $\vec{\nu}^m$ to Γ^m such that $\vec{\nu}^m$ points into Ω_+^m. We then partition the elements of the bulk mesh $\mathcal{T}^m$ into interior, exterior and interfacial elements as before, and we introduce ρ^m, $\mu^m \in S_0^m(\Omega)$, for $m \geq 0$, as

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

We also introduce the L^2–inner product $\langle\cdot,\cdot\rangle_{\Gamma^m}$ over the current polyhedral surface Γ^m, as well as the mass lumped inner product $\langle\cdot,\cdot\rangle_{\Gamma^m}^h$. In addition, similarly to (4.9a,b), we define

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

and

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

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

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

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

for $m = 1,\ldots,M$, and set $\vec{\Pi}_{-1}^0 := \vec{\pi}^0$. Analogously to (5.1) we also define $\Pi_{m-1}^m : C(\Gamma^{m-1}) \to W(\Gamma^m)$ and $\underline{\underline{\Pi}}_{m-1}^m : [C(\Gamma^{m-1})]^{d\times d} \to \underline{\underline{V}}(\Gamma^m)$. For later use, we also introduce the short hand notations

$$\alpha^m = \pi^m\,[\alpha(\mathfrak{C}^m)]\,, \quad \overline{\varkappa}^m = \pi^m\,[\overline{\varkappa}(\mathfrak{C}^m)]\,, \quad \alpha^{G,m} = \pi^m\,[\alpha^G(\mathfrak{C}^m)]\,, \tag{5.2}$$

for $m = 0,\ldots,M-1$. We note, similarly to (4.10), that

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

where $\vec{\omega}^m := \sum_{k=1}^{K_\Gamma} \chi_k^m\,\vec{\omega}_k^m \in \underline{V}(\Gamma^m)$, and where for $k = 1,\ldots,K_\Gamma$ we let $\Theta_k^m := \{j : \vec{q}_k^m \in \overline{\sigma_j^m}\}$ and set $\Lambda_k^m := \cup_{j\in\Theta_k^m} \overline{\sigma_j^m}$ and $\vec{\omega}_k^m := \frac{1}{\mathcal{H}^{d-1}(\Lambda_k^m)} \sum_{j\in\Theta_k^m} \mathcal{H}^{d-1}(\sigma_j^m)\,\vec{\nu}_j^m$.

For the approximation to the velocity and pressure on $\mathcal{T}^m$ we use the finite element spaces $\mathbb{U}^m(\vec{g})$ and $\mathbb{P}^m$, which are the direct time discrete analogues of $\mathbb{U}^h(\vec{g})$ and $\mathbb{P}^h(t_m)$, as well as $\widehat{\mathbb{P}}^m \subset \widehat{\mathbb{P}}$.

Analogously to (3.33), we recall the following discrete LBB$_\Gamma$ inf-sup assumption from [7]. Let there exist a $C_0 \in \mathbb{R}_{>0}$, independent of $\mathcal{T}^m$ and $\{\sigma_j^m\}_{j=1}^{J_\Gamma}$, such that

$$\inf_{(\varphi,\lambda,\eta)\in\widehat{\mathbb{P}}^m\times\mathbb{R}\times W(\Gamma^m)}\ \sup_{\vec{\xi}\in\mathbb{U}^m(\vec{0})} \frac{(\varphi, \nabla\,.\,\vec{\xi}) + \lambda\left\langle\vec{\omega}^m, \vec{\xi}\right\rangle_{\Gamma^m}^h + \left\langle\eta, \nabla_s\,.\,(\vec{\pi}^m\,\vec{\xi}\,|_{\Gamma^m})\right\rangle_{\Gamma^m}}{(\|\varphi\|_0 + |\lambda| + \|\eta\|_{0,\Gamma^m})\,(\|\vec{\xi}\|_1 + \|\underline{\underline{\mathcal{P}}}_{\Gamma^m}\,(\vec{\pi}^m\,\vec{\xi}\,|_{\Gamma^m})\|_{1,\Gamma^m,h})} \geq C_0\,, \tag{5.3}$$

where $\|\eta\|_{0,\Gamma^m}^2 := \langle\eta,\eta\rangle_{\Gamma^m}$ and $\|\vec{\eta}\|_{1,\Gamma^m,h}^2 := \langle\vec{\eta},\vec{\eta}\rangle_{\Gamma^m} + \sum_{j=1}^{J_\Gamma} \int_{\sigma_j^m} |\nabla_s\,\vec{\eta}|^2 \,{\rm d}\mathcal{H}^{d-1}$. See [7, (5.2)] for more details.

We are now in a position to state our fully discrete approximation of (4.15a,b), (4.28a,b), (4.16c,d) and (4.17a–d). Here we stress that it does not appear possible to prove a stability result for a fully discrete approximation. This is in line with approximations for other evolution problems involving curvature energies, and is mainly due to the fact that it does not appear possible to mimic the differentiation steps in (4.19a,b). To increase the practicality of our fully discrete scheme, we will decouple the fully discrete variant of (4.15a,b) from the remaining equations. For the remaining equations we follow the strategy from [7], which leads to a linear set of equations that couple the bulk and surface Navier–Stokes equations to the evolution of the interface. This fully discrete approximation is given as follows. Let Γ^0, an approximation to $\Gamma(0)$, as well as $\vec\kappa^0 \in \underline{V}(\Gamma^0)$, $\mathfrak{C}^0 \in W(\Gamma^0)$ and $\vec U^0 \in \mathbb{U}^0(\vec g)$ be given. For $m = 0, \ldots, M-1$, find $\vec U^{m+1} \in \mathbb{U}^m(\vec g)$, $P^{m+1} \in \widehat{\mathbb{P}}^m$, $P_{\rm sing}^{m+1} \in \mathbb{R}$, $P_\Gamma^{m+1} \in W(\Gamma^m)$, $\vec X^{m+1} \in \underline{V}(\Gamma^m)$, $\vec\kappa^{m+1} \in \underline{V}(\Gamma^m)$, $\underline{\underline{W}}^{m+1} \in \underline{\underline{V}}(\Gamma^m)$ and $\vec Y^{m+1}$, $\vec F_\Gamma^{m+1} \in \underline{V}(\Gamma^m)$ such that

$$
\begin{aligned}
&\tfrac12 \left(\frac{\rho^m\,\vec U^{m+1} - (I_0^m\,\rho^{m-1})\,\vec I_2^m\,\vec U^m}{\tau} + (I_0^m\,\rho^{m-1})\,\frac{\vec U^{m+1} - \vec I_2^m\,\vec U^m}{\tau}, \vec\xi \right) + 2\left(\mu^m\,\underline{\underline{D}}(\vec U^{m+1}), \underline{\underline{D}}(\vec\xi)\right) \\
&\quad + \tfrac12 \left(\rho^m, [(\vec I_2^m\,\vec U^m\,.\,\nabla)\,\vec U^{m+1}]\,.\,\vec\xi - [(\vec I_2^m\,\vec U^m\,.\,\nabla)\,\vec\xi]\,.\,\vec U^{m+1}\right) - \left(P^{m+1}, \nabla\,.\,\vec\xi\right) - P_{\rm sing}^{m+1}\left\langle \vec\omega^m, \vec\xi \right\rangle_{\Gamma^m}^h \\
&\quad + \rho_\Gamma \left\langle \frac{\vec U^{m+1} - \vec\Pi_{m-1}^m\,(\vec I_2^m\,\vec U^m)\,|_{\Gamma^{m-1}}}{\tau}, \vec\xi \right\rangle_{\Gamma^m}^h + 2\,\mu_\Gamma \left\langle \underline{\underline{D}}_s^m(\vec\pi^m\,\vec U^{m+1}), \underline{\underline{D}}_s^m(\vec\pi^m\,\vec\xi) \right\rangle_{\Gamma^m} - \left\langle P_\Gamma^{m+1}, \nabla_s\,.\,(\vec\pi^m\,\vec\xi) \right\rangle_{\Gamma^m} \\
&\qquad = \left(\rho^m\,\vec f^{m+1}, \vec\xi\right) + \left\langle \vec F_\Gamma^{m+1}, \vec\xi \right\rangle_{\Gamma^m}^h - \tfrac12\,\rho_+ \left\langle \vec U^m\,.\,\mathrm{n}, \vec U^m\,.\,\vec\xi \right\rangle_{\partial_2\Omega} \qquad \forall\ \vec\xi \in \mathbb{U}^m(\vec 0)\,,
\end{aligned} \tag{5.4a}
$$

$$
\left(\nabla\,.\,\vec U^{m+1}, \varphi\right) = 0 \qquad \forall\ \varphi \in \widehat{\mathbb{P}}^m \qquad \text{and} \qquad \left\langle \vec U^{m+1}, \vec\omega^m \right\rangle_{\Gamma^m}^h = 0\,, \tag{5.4b}
$$

$$
\left\langle \nabla_s\,.\,(\vec\pi^m\,\vec U^{m+1}), \eta \right\rangle_{\Gamma^m} = 0 \qquad \forall\ \eta \in W(\Gamma^m)\,, \tag{5.4c}
$$

$$
\left\langle \frac{\vec X^{m+1} - \vec{\rm id}}{\tau}, \vec\chi \right\rangle_{\Gamma^m}^h = \left\langle \vec U^{m+1}, \vec\chi \right\rangle_{\Gamma^m}^h \qquad \forall\ \vec\chi \in \underline{V}(\Gamma^m)\,, \tag{5.4d}
$$

and

$$
\left\langle \vec\kappa^{m+1}, \vec\eta \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s\,\vec X^{m+1}, \nabla_s\,\vec\eta \right\rangle_{\Gamma^m} = 0 \qquad \forall\ \vec\eta \in \underline{V}(\Gamma^m)\,, \tag{5.5a}
$$

$$
\left\langle \underline{\underline{W}}^{m+1}, \underline{\underline{\zeta}} \right\rangle_{\Gamma^m}^h + \tfrac12 \left\langle \vec\nu^m, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\,\vec\kappa^{m+1} + \nabla_s\,.\,[\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \right\rangle_{\Gamma^m}^h = 0 \qquad \forall\ \underline{\underline{\zeta}} \in \underline{\underline{V}}(\Gamma^m)\,, \tag{5.5b}
$$

$$
\left\langle \vec Y^{m+1}, \vec\xi \right\rangle_{\Gamma^m}^h - \left\langle \alpha^m\,(\vec\kappa^{m+1} - \overline{\varkappa}^m\,\vec\nu^m), \vec\xi \right\rangle_{\Gamma^m}^h - \left\langle \alpha^{G,m}\,(\vec\Pi_{m-1}^m\,\vec\kappa^m + \underline{\underline{\Pi}}_{m-1}^m\,\underline{\underline{W}}^m\,\vec\nu^m), \vec\xi \right\rangle_{\Gamma^m}^h = 0 \quad \forall\ \vec\xi \in \underline{V}(\Gamma^m)\,, \tag{5.5c}
$$

$$
\begin{aligned}
\left\langle \vec F_\Gamma^{m+1}, \vec\chi \right\rangle_{\Gamma^m}^h &= \left\langle \nabla_s\,\vec Y^{m+1}, \nabla_s\,\vec\chi \right\rangle_{\Gamma^m} + \left\langle \nabla_s\,.\,(\vec\Pi_{m-1}^m\,\vec Y^m), \nabla_s\,.\,\vec\chi \right\rangle_{\Gamma^m} - 2\left\langle [\nabla_s\,(\vec\Pi_{m-1}^m\,\vec Y^m)]^T, \underline{\underline{D}}_s^m(\vec\chi)\,(\nabla_s\,\vec{\rm id})^T \right\rangle_{\Gamma^m} \\
&\quad - \tfrac12 \left\langle \alpha^m\,|\vec\Pi_{m-1}^m\,\vec\kappa^m - \overline{\varkappa}^m\,\vec\nu^m|^2 - 2\,\vec\Pi_{m-1}^m\,\vec Y^m\,.\,\vec\Pi_{m-1}^m\,\vec\kappa^m, \nabla_s\,.\,\vec\chi \right\rangle_{\Gamma^m}^h - \left\langle \alpha^m\,\overline{\varkappa}^m\,\vec\Pi_{m-1}^m\,\vec\kappa^m, [\nabla_s\,\vec\chi]^T\,\vec\nu^m \right\rangle_{\Gamma^m}^h \\
&\quad - \beta\,\langle b_{GL}(\mathfrak{C}^m), \nabla_s\,.\,\vec\chi \rangle_{\Gamma^m}^h + \beta\,\gamma\,\langle (\nabla_s\,\mathfrak{C}^m) \otimes (\nabla_s\,\mathfrak{C}^m), \nabla_s\,\vec\chi \rangle_{\Gamma^m} \\
&\quad - \tfrac12 \left\langle \alpha^{G,m}\,(|\vec\Pi_{m-1}^m\,\vec\kappa^m|^2 + |\underline{\underline{\Pi}}_{m-1}^m\,\underline{\underline{W}}^m|^2), \nabla_s\,.\,\vec\chi \right\rangle_{\Gamma^m}^h + \left\langle \vec\nu^m\,.\,(\underline{\underline{Z}}^m\,\vec\Pi_{m-1}^m\,\vec\kappa^m + \nabla_s\,.\,\underline{\underline{Z}}^m), \nabla_s\,.\,\vec\chi \right\rangle_{\Gamma^m}^h \\
&\quad + \sum_{i=1}^d \left\langle \nu_i^m\,\nabla_s\,\vec Z_i^m, \nabla_s\,\vec\chi - 2\,\underline{\underline{D}}_s^m(\vec\chi) \right\rangle_{\Gamma^m} - \langle \underline{\underline{Z}}^m\,\vec\kappa^m + \nabla_s\,.\,\underline{\underline{Z}}^m, [\nabla_s\,\vec\chi]^T\,\vec\nu^m \rangle_{\Gamma^m}^h \quad \forall\ \vec\chi \in \underline{V}(\Gamma^m)\,,
\end{aligned} \tag{5.5d}
$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$. Hence $\vec{X}^{m+1}$ represents the positions of the vertices of the new discrete membrane. In the above we have defined $\vec{f}^{m+1} := \vec{I}^m_2\,\vec{f}(\cdot, t_{m+1})$, $\underline{\underline{Z}}^m = \underline{\underline{\pi}}^m[-\alpha^G(\mathfrak{C}^m)\,\underline{\underline{\Pi}}^m_{m-1}\,\underline{\underline{W}}^m]$ and $\vec{Z}^m_i = \underline{\underline{Z}}^m\,\vec{e}_i$, $i = 1 \to d$. We note that (5.5b) decouples from (5.4a–d) and (5.5a,c,d). In addition, we note that in the special case of uniform α and $\overline{\varkappa}$, and if $\alpha^G = \beta = 0$, the scheme (5.4a–d), (5.5a,c,d) collapses to the scheme (5.4a–f) and (5.5) with $\beta = 0$, from [7].

For the fully discrete approximation of (4.15a,b) for the case of the obstacle potential (2.11b) we consider a semi-implicit (surface) finite element approximation in the spirit of [12] in the planar case. Hence, having computed Γ^{m+1}, we find $\mathfrak{C}^{m+1} \in W_{\leq 1}(\Gamma^{m+1})$ and $\mathfrak{M}^{m+1} \in W(\Gamma^{m+1})$ such that

$$\frac{\vartheta}{\tau}\left\langle \mathfrak{C}^{m+1}, \chi^{m+1}_k\right\rangle^h_{\Gamma^{m+1}} + \left\langle \nabla_s\,\mathfrak{M}^{m+1}, \nabla_s\,\chi^{m+1}_k\right\rangle_{\Gamma^{m+1}} = \frac{\vartheta}{\tau}\left\langle \mathfrak{C}^m, \chi^m_k\right\rangle^h_{\Gamma^m} \quad \forall\, k \in \{1, \ldots, K_\Gamma\}\,. \tag{5.6a}$$

$$\begin{aligned}
\beta\,\gamma\left\langle \nabla_s\,\mathfrak{C}^{m+1}, \nabla_s\,[\chi - \mathfrak{C}^{m+1}]\right\rangle_{\Gamma^{m+1}} &\geq \left\langle \mathfrak{M}^{m+1} + \beta\,\gamma^{-1}\,\Pi^{m+1}_m\,\mathfrak{C}^m, \chi - \mathfrak{C}^{m+1}\right\rangle^h_{\Gamma^{m+1}} \\
&- \tfrac{1}{2}\left\langle \alpha'(\Pi^{m+1}_m\,\mathfrak{C}^m)\,|\vec{\Pi}^{m+1}_m\,\vec{\kappa}^{m+1} - \overline{\varkappa}(\Pi^{m+1}_m\,\mathfrak{C}^m)\,\vec{\nu}^{m+1}|^2, \chi - \mathfrak{C}^{m+1}\right\rangle^h_{\Gamma^{m+1}} \\
&+ \left\langle \overline{\varkappa}'(\Pi^{m+1}_m\,\mathfrak{C}^m)\,\alpha(\Pi^{m+1}_m\,\mathfrak{C}^m)\,(\vec{\Pi}^{m+1}_m\,\vec{\kappa}^{m+1} - \overline{\varkappa}(\Pi^{m+1}_m\,\mathfrak{C}^m)\,\vec{\nu}^{m+1})\,.\,\vec{\nu}^{m+1}, \chi - \mathfrak{C}^{m+1}\right\rangle^h_{\Gamma^{m+1}} \\
&- \tfrac{1}{2}\left\langle (\alpha^G)'(\Pi^{m+1}_m\,\mathfrak{C}^m)\,(|\vec{\Pi}^{m+1}_m\vec{\kappa}^{m+1}|^2 - |\underline{\underline{\Pi}}^{m+1}_m\,\underline{\underline{W}}^{m+1}|^2), \chi - \mathfrak{C}^{m+1}\right\rangle^h_{\Gamma^{m+1}} \quad \forall\,\chi \in W_{\leq 1}(\Gamma^{m+1})\,.
\end{aligned} \tag{5.6b}$$

In the absence of the LBB$_\Gamma$ condition (5.3) we need to consider the reduced system (5.4a,d), (5.5a–d), where $\mathbb{U}^m(\vec{0})$ in (5.4a) is replaced by $\mathbb{U}^m_0(\vec{0})$. Here we define

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

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

In order to prove the existence of a unique solution to (5.4a–d), (5.5a–d) we make the following very mild well-posedness assumption.

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

Theorem 5.1. *Let the assumption* ($\mathcal{A}$) *hold. If the LBB$_\Gamma$ condition* (5.3) *holds, then there exists a unique solution* $(\vec{U}^{m+1}, P^{m+1}, P^{m+1}_{\rm sing}, P^{m+1}_\Gamma, \vec{X}^{m+1}, \vec{\kappa}^{m+1}, \vec{Y}^{m+1}, \vec{F}^{m+1}_\Gamma, \underline{\underline{W}}^{m+1}) \in \mathbb{U}^m(\vec{g}) \times \widehat{\mathbb{P}}^m \times \mathbb{R} \times W(\Gamma^m) \times [\underline{V}(\Gamma^m)]^4 \times \underline{\underline{V}}(\Gamma^m)$ *to* (5.4a–d), (5.5a–d). *In all other cases, on assuming that* $\mathbb{U}^m_0(\vec{g})$ *is nonempty, there exists a unique solution* $(\vec{U}^{m+1}, \vec{X}^{m+1}, \vec{\kappa}^{m+1}, \vec{Y}^{m+1}, \vec{F}^{m+1}_\Gamma, \underline{\underline{W}}^{m+1}) \in \mathbb{U}^m_0(\vec{g}) \times [\underline{V}(\Gamma^m)]^4 \times \underline{\underline{V}}(\Gamma^m)$ *to the reduced system* (5.4a,d), (5.5a–d) *with* $\mathbb{U}^m(\vec{0})$ *replaced by* $\mathbb{U}^m_0(\vec{0})$. *Moreover, there exists a solution* $(\mathfrak{C}^{m+1}, \mathfrak{M}^{m+1}) \in W_{\leq 1}(\Gamma^{m+1}) \times W(\Gamma^{m+1})$ *to* (5.6a,b)*, with* $\mathfrak{C}^{m+1}$ *being unique.*

Proof. As the system (5.4a–d), (5.5a–d) is linear, existence follows from uniqueness. In order to establish the latter, we consider the homogeneous system. Find $(\vec{U}, P, P_{\rm sing}, P_\Gamma, \vec{X}, \vec{\kappa}, \vec{Y}, \vec{F}_\Gamma, \underline{\underline{W}}) \in \mathbb{U}^m(\vec{0}) \times \widehat{\mathbb{P}}^m \times \mathbb{R} \times W(\Gamma^m) \times [\underline{V}(\Gamma^m)]^4 \times \underline{\underline{V}}(\Gamma^m)$ such that

$$\begin{aligned}
&\tfrac{1}{2\tau}\left((\rho^m + I^m_0\,\rho^{m-1})\,\vec{U}, \vec{\xi}\right) + 2\left(\mu^m\,\underline{\underline{D}}(\vec{U}), \underline{\underline{D}}(\vec{\xi})\right) - \left(P, \nabla\,.\,\vec{\xi}\right) - P_{\rm sing}\left\langle \vec{\omega}^m, \vec{\xi}\right\rangle^h_{\Gamma^m} \\
&\quad + \tfrac{1}{2}\left(\rho^m, [(\vec{I}^m_2\,\vec{U}^m\,.\,\nabla)\,\vec{U}]\,.\,\vec{\xi} - [(\vec{I}^m_2\,\vec{U}^m\,.\,\nabla)\,\vec{\xi}]\,.\,\vec{U}\right) + \tfrac{1}{\tau}\,\rho_\Gamma\left\langle \vec{U}, \vec{\xi}\right\rangle^h_{\Gamma^m} + 2\,\mu_\Gamma\left\langle \underline{\underline{D}}^m_s(\vec{\pi}^m\,\vec{U}), \underline{\underline{D}}^m_s(\vec{\pi}^m\,\vec{\xi})\right\rangle_{\Gamma^m} \\
&\quad - \left\langle P_\Gamma, \nabla_s\,.\,(\vec{\pi}^m\,\vec{\xi})\right\rangle_{\Gamma^m} - \left\langle \vec{F}_\Gamma, \vec{\xi}\right\rangle^h_{\Gamma^m} = 0 \qquad \forall\,\vec{\xi} \in \mathbb{U}^m(\vec{0})\,,
\end{aligned} \tag{5.7a}$$

$$\left(\nabla\,.\,\vec{U},\varphi\right)=0\qquad\forall\,\varphi\in\widehat{\mathbb{P}}^m\qquad\text{and}\qquad\left\langle\vec{U},\vec{\varpi}^m\right\rangle_{\Gamma^m}^h=0\,,\tag{5.7b}$$

$$\left\langle\nabla_s\,.\,(\vec{\pi}^m\,\vec{U}),\eta\right\rangle_{\Gamma^m}=0\qquad\forall\,\eta\in W(\Gamma^m)\,,\tag{5.7c}$$

$$\tfrac{1}{\tau}\left\langle\vec{X},\vec{\chi}\right\rangle_{\Gamma^m}^h=\left\langle\vec{U},\vec{\chi}\right\rangle_{\Gamma^m}^h\qquad\forall\,\vec{\chi}\in\underline{V}(\Gamma^m)\,,\tag{5.7d}$$

$$\langle\vec{\kappa},\vec{\eta}\rangle_{\Gamma^m}^h+\left\langle\nabla_s\,\vec{X},\nabla_s\,\vec{\eta}\right\rangle_{\Gamma^m}=0\qquad\forall\,\vec{\eta}\in\underline{V}(\Gamma^m)\,,\tag{5.7e}$$

$$\left\langle\underline{\underline{W}},\underline{\underline{\zeta}}\right\rangle_{\Gamma^m}^h+\tfrac{1}{2}\left\langle\vec{\nu}^m,[\underline{\underline{\zeta}}+\underline{\underline{\zeta}}^T]\,\vec{\kappa}\right\rangle_{\Gamma^m}^h=0\qquad\forall\,\underline{\underline{\zeta}}\in\underline{\underline{V}}(\Gamma^m)\,,\tag{5.7f}$$

$$\left\langle\vec{Y},\vec{\eta}\right\rangle_{\Gamma^m}^h-\langle\alpha^m\,\vec{\kappa},\vec{\eta}\rangle_{\Gamma^m}^h=0\qquad\forall\,\vec{\eta}\in\underline{V}(\Gamma^m)\,,\tag{5.7g}$$

$$\left\langle\vec{F}_\Gamma,\vec{\chi}\right\rangle_{\Gamma^m}^h-\left\langle\nabla_s\,\vec{Y},\nabla_s\,\vec{\chi}\right\rangle_{\Gamma^m}=0\qquad\forall\,\vec{\chi}\in\underline{V}(\Gamma^m)\,.\tag{5.7h}$$

Choosing $\vec{\xi}=\vec{U}$ in (5.7a), $\varphi=P$ in (5.7b), $\eta=P_\Gamma$ in (5.7c), $\vec{\chi}=\vec{F}_\Gamma$ in (5.7d), $\vec{\chi}=\vec{X}$ in (5.7h), $\vec{\eta}=\vec{Y}$ in (5.7e) and $\vec{\eta}=\vec{\kappa}$ in (5.7g) yields that

$$\begin{aligned}&\tfrac{1}{2}\left((\rho^m+I_0^m\,\rho^{m-1})\,\vec{U},\vec{U}\right)+2\,\tau\left(\mu^m\,\underline{\underline{D}}(\vec{U}),\underline{\underline{D}}(\vec{U})\right)+\rho_\Gamma\left\langle\vec{U},\vec{U}\right\rangle_{\Gamma^m}^h+2\,\tau\,\mu_\Gamma\left\langle\underline{\underline{D}}_s^m(\vec{\pi}^m\,\vec{U}),\underline{\underline{D}}_s^m(\vec{\pi}^m\,\vec{U})\right\rangle_{\Gamma^m}\\&\quad=\tau\left\langle\vec{F}_\Gamma,\vec{U}\right\rangle_{\Gamma^m}^h=\left\langle\vec{F}_\Gamma,\vec{X}\right\rangle_{\Gamma^m}^h=\left\langle\nabla_s\,\vec{Y},\nabla_s\,\vec{X}\right\rangle_{\Gamma^m}=-\left\langle\vec{\kappa},\vec{Y}\right\rangle_{\Gamma^m}^h=-\,\langle\alpha^m\,\vec{\kappa},\vec{\kappa}\rangle_{\Gamma^m}^h\,.\end{aligned}\tag{5.8}$$

It immediately follows from (5.8), Korn's inequality and $\alpha^m>0$, that $\vec{U}=\vec{0}\in\mathbb{U}^m(\vec{0})$ and $\vec{\kappa}=\vec{0}$. (For the application of Korn's inequality we recall that $\mathcal{H}^{d-1}(\partial_1\Omega)>0$.) Hence (5.7d,f,g,h) yield that $\vec{X}=\vec{0}$, $\underline{\underline{W}}=\underline{\underline{0}}$, $\vec{Y}=\vec{0}$ and $\vec{F}_\Gamma=\vec{0}$, respectively. Finally, if (5.3) holds then (5.7a) with $\vec{U}=\vec{0}$ and $\vec{F}_\Gamma=\vec{0}$ implies that $P=0\in\widehat{\mathbb{P}}^m$, $P_{\rm sing}=0$ and $P_\Gamma=0\in W(\Gamma^m)$. This shows existence and uniqueness of $(\vec{U}^{m+1},P^{m+1},P_{\rm sing}^{m+1},P_\Gamma^{m+1},\vec{X}^{m+1},\vec{\kappa}^{m+1},\vec{Y}^{m+1},\vec{F}_\Gamma^{m+1},\underline{\underline{W}}^{m+1})\in\mathbb{U}^m(\vec{g})\times\widehat{\mathbb{P}}^m\times\mathbb{R}\times W(\Gamma^m)\times[\underline{V}(\Gamma^m)]^4\times\underline{\underline{V}}(\Gamma^m)$ to (5.4a–d), (5.5a–d). The proof for the reduced system is very similar. The homogeneous system to consider is (5.7a,d–h) with $\mathbb{U}^m(\vec{0})$ replaced by $\mathbb{U}_0^m(\vec{0})$. As before, we infer that (5.8) holds, which yields that $\vec{U}=\vec{0}\in\mathbb{U}_0^m(\vec{0})$, $\vec{\kappa}=\vec{0}$, and hence $\vec{X}=\vec{F}_\Gamma=\vec{Y}=\vec{0}$.

In order to prove the existence of a unique solution to (5.6a,b), we adapt the argument in [12] for the Cahn–Hilliard equation with obstacle potential on a bounded fixed domain in $\mathbb{R}^d$. We introduce the discrete inverse surface Laplacian $\mathcal{G}^{m+1}:W_{\!\int}(\Gamma^{m+1})\to W_{\!\int}(\Gamma^{m+1})$ defined by

$$\langle\nabla_s\,\mathcal{G}^{m+1}\,v,\nabla_s\,\xi\rangle_{\Gamma^{m+1}}=\langle v,\xi\rangle_{\Gamma^{m+1}}^h\qquad\forall\,\xi\in W_{\!\int}(\Gamma^{m+1})\,,\tag{5.9}$$

where $W_{\!\int}(\Gamma^{m+1}):=\{\xi\in W(\Gamma^{m+1}):\langle\xi,1\rangle_{\Gamma^{m+1}}=0\}$. It immediately follows from $\langle\nabla_s\,v,\nabla_s\,v\rangle_{\Gamma^{m+1}}=0\Rightarrow v=0$ for all $v\in W_{\!\int}(\Gamma^{m+1})$ that $\mathcal{G}^{m+1}$ is well-posed. Next we rewrite (5.6a,b) as

$$\frac{\vartheta}{\tau}\left\langle\mathfrak{C}^{m+1}-\widehat{\mathfrak{C}}^m,\chi_k^{m+1}\right\rangle_{\Gamma^{m+1}}^h+\langle\nabla_s\,\mathfrak{M}^{m+1},\nabla_s\,\chi_k^{m+1}\rangle_{\Gamma^{m+1}}=0\quad\forall\,k\in\{1,\ldots,K_\Gamma\}\,.\tag{5.10a}$$

$$\beta\,\gamma\,\langle\nabla_s\,\mathfrak{C}^{m+1},\nabla_s\,[\chi-\mathfrak{C}^{m+1}]\rangle_{\Gamma^{m+1}}\geq\langle\mathfrak{M}^{m+1}+g,\chi-\mathfrak{C}^{m+1}\rangle_{\Gamma^{m+1}}^h\quad\forall\,\chi\in W_{\leq1}(\Gamma^{m+1})\,,\tag{5.10b}$$

where $\widehat{\mathfrak{C}}^m\in W(\Gamma^{m+1})$ is such that $\langle\widehat{\mathfrak{C}}^m,\chi_k^{m+1}\rangle_{\Gamma^{m+1}}^h=\langle\mathfrak{C}^m,\chi_k^m\rangle_{\Gamma^m}^h$ for $k\in\{1,\ldots,K_\Gamma\}$. We note that

$$\langle\mathfrak{C}^{m+1},1\rangle_{\Gamma^{m+1}}=\left\langle\widehat{\mathfrak{C}}^m,1\right\rangle_{\Gamma^{m+1}}=\langle\mathfrak{C}^m,1\rangle_{\Gamma^m}\;.\tag{5.11}$$

It follows from (5.11), (5.10a) and (5.9) that

$$\mathfrak{M}^{m+1} = -\frac{\vartheta}{\tau}\,\mathcal{G}^{m+1}\,(\mathfrak{C}^{m+1} - \widehat{\mathfrak{C}}^m) + \lambda^{m+1}\,, \tag{5.12}$$

where $\lambda^{m+1} \in \mathbb{R}$ is a Lagrange multiplier associated with the constraint (5.11). Hence $\mathfrak{C}^{m+1} \in W_{\leq 1}(\Gamma^{m+1})$ is such that $\langle \mathfrak{C}^{m+1}, 1\rangle_{\Gamma^{m+1}} = \langle \mathfrak{C}^m, 1\rangle_{\Gamma^m}$ and

$$\beta\,\gamma\,\langle \nabla_s\,\mathfrak{C}^{m+1}, \nabla_s\,[\chi - \mathfrak{C}^{m+1}]\rangle_{\Gamma^{m+1}} + \frac{\vartheta}{\tau}\left\langle \mathcal{G}^{m+1}\,(\mathfrak{C}^{m+1} - \widehat{\mathfrak{C}}^m) - \lambda^{m+1} - g, \chi - \mathfrak{C}^{m+1}\right\rangle^h_{\Gamma^{m+1}} \geq 0 \qquad \forall\ \chi \in W_{\leq 1}(\Gamma^{m+1})\,. \tag{5.13}$$

Clearly, (5.13) is the Euler–Lagrange variational inequality for the strictly convex minimization problem

$$\min_{\substack{\chi \in W_{\leq 1}(\Gamma^{m+1})\\ \langle \chi, 1\rangle_{\Gamma^{m+1}} = \langle \mathfrak{C}^m, 1\rangle_{\Gamma^m}}} \left[\frac{\beta\,\gamma}{2}\,\langle \nabla_s\,\chi, \nabla_s\,\chi\rangle_{\Gamma^{m+1}} + \frac{\vartheta}{2\,\tau}\left\langle \nabla_s\,\mathcal{G}^{m+1}\,(\chi - \widehat{\mathfrak{C}}^m), \nabla_s\,\mathcal{G}^{m+1}\,(\chi - \widehat{\mathfrak{C}}^m)\right\rangle_{\Gamma^{m+1}} - \frac{\vartheta}{\tau}\,\langle g, \chi\rangle^h_{\Gamma^{m+1}}\right]. \tag{5.14}$$

Hence there exists a unique $\mathfrak{C}^{m+1} \in W_{\leq 1}(\Gamma^{m+1})$ with $\langle \mathfrak{C}^{m+1}, 1\rangle_{\Gamma^{m+1}} = \langle \mathfrak{C}^m, 1\rangle_{\Gamma^m}$ and solving (5.13). Existence of the Lagrange multiplier λ^{m+1} in (5.12) then follows from a fixed point argument, see [12, p. 151]. □

6. Solution methods

In this section we briefly describe possible solution methods for the linear system (5.4a–d), (5.5a–d), where we note that (5.5b) decouples from the remaining equations, and for the nonlinear system (5.6a,b).

In order to derive the linear system of equations for the coefficient vectors of the finite element functions $(\vec{U}^{m+1}, P^{m+1}, P^{m+1}_{\rm sing}, P^{m+1}_\Gamma, \delta\vec{X}^{m+1}, \vec\kappa^{m+1}, \vec{Y}^{m+1}, \vec{F}^{m+1}_\Gamma)$ corresponding to (5.4a–d), (5.5a,c,d), where $\delta\vec{X}^{m+1} = \vec{X}^{m+1} - \vec{\rm id}\,|_{\Gamma^m}$, we begin by introducing the following matrices and vectors, where we closely follow our previous work in [6]. The new ingredients needed here are the treatment of the terms depending on $\mathfrak{C}^m$, the terms involving $\underline{\underline{W}}^m$ and $\vec{Z}^m$, as well as an adapted Schur complement approach due to the presence of the variable $\vec{Y}^{m+1}$. For the benefit of the reader, and to aid reproducibility of the numerical results, we present the full linear system in detail. Let $i,\,j = 1,\ldots,K^m_{\mathbb{U}}$, $n,q = 1,\ldots,K^m_{\mathbb{P}}$ and $k,l = 1,\ldots,K_\Gamma$. Then

$$\begin{aligned}
[\vec{B}_\Omega]_{ij} :=\ & \left(\tfrac{\rho^m + I^m_0\,\rho^{m-1}}{2\,\tau}\,\phi^{\mathbb{U}^m}_j, \phi^{\mathbb{U}^m}_i\right) \underline{\underline{\rm Id}} + 2\left(\left(\mu^m\,\underline{\underline{D}}(\phi^{\mathbb{U}^m}_j\,\vec{e}_r), \underline{\underline{D}}(\phi^{\mathbb{U}^m}_i\,\vec{e}_s)\right)\right)_{r,s=1}^d \\
& + \tfrac12\left(\rho^m, [(\vec{I}^m_2\,\vec{U}^m\,.\,\nabla)\,\phi^{\mathbb{U}^m}_j]\,\phi^{\mathbb{U}^m}_i - [(\vec{I}^m_2\,\vec{U}^m\,.\,\nabla)\,\phi^{\mathbb{U}^m}_i]\,\phi^{\mathbb{U}^m}_j\right) \underline{\underline{\rm Id}}\,, \\
& + \frac{\rho_\Gamma}{\tau}\left\langle \varphi^{\mathbb{U}^m}_j, \varphi^{\mathbb{U}^m}_i\right\rangle^h_{\Gamma^m} \underline{\underline{\rm Id}} + 2\mu_\Gamma\left(\left\langle \underline{\underline{D}}^m_s(\pi^m\,\phi^{\mathbb{U}^m}_j\,\vec{e}_r), \underline{\underline{D}}^m_s(\pi^m\,\phi^{\mathbb{U}^m}_i\,\vec{e}_s)\right\rangle_{\Gamma^m}\right)_{r,s=1}^d \\
[\vec{C}_\Omega]_{iq} :=\ & -\left(\phi^{\mathbb{P}^m}_q, \left(\nabla\,.\,(\phi^{\mathbb{U}^m}_i\,\vec{e}_r)\right)\right)_{r=1}^d, \qquad [\vec{S}_{\Gamma,\Omega}]_{il} := -\left(\left\langle \chi^m_l, \nabla_s\,.\,(\pi^m\,\phi^{\mathbb{U}^m}_i\,\vec{e}_r)\right\rangle_{\Gamma^m}\right)_{r=1}^d, \\
\vec{b}_i =\ & \left(\tfrac{I^m_0\,\rho^{m-1}}{\tau}\,\vec{I}^m_2\,\vec{U}^m + \rho^m\,\vec{f}^{m+1}, \phi^{\mathbb{U}^m}_i\right) + \frac{\rho_\Gamma}{\tau}\left\langle \vec\Pi^m_{m-1}\,\vec{U}^m\,|_{\Gamma^{m-1}}, \varphi^{\mathbb{U}^m}_i\right\rangle^h_{\Gamma^m} - \tfrac12\,\rho_+\left\langle (\vec{U}^m\,.\,\vec{\rm n})\,\vec{U}^m, \phi^{\mathbb{U}^m}_i\right\rangle_{\partial_2\Omega};
\end{aligned} \tag{6.1}$$

where $\{\vec{e}_r\}_{r=1}^d$ denotes the standard basis in $\mathbb{R}^d$, and where we have used the convention that the subscripts in the matrix notations refer to the test and trial domains, respectively. A single subscript is used where the two domains are the same. The entries of $\vec{D}_\Omega$, for $i = 1,\ldots,K^m_{\mathbb{U}}$, are given by $[\vec{D}_\Omega]_{i,1} := -\langle \phi^{\mathbb{U}^m}_i, \vec\omega^m\rangle^h_{\Gamma^m}$.

In order to provide a matrix-vector formulation for the full system (5.4a–d), (5.5a,c,d), and in particular in view of (5.5c), we recall from [20, p. 64] that

$$
\begin{aligned}
&2\left\langle (\nabla_s\,\vec\xi)^T, \underline{\underline{D}}^m_s(\vec\chi)\,(\nabla_s\,\vec{\mathrm{id}})^T\right\rangle_{\Gamma^m}\\
&= \sum_{i,j=1}^d \left\langle (\nabla_s)_j\,(\vec\xi)_i, (\nabla_s)_i\,(\vec\chi)_j\right\rangle_{\Gamma^m} - \sum_{i,j=1}^d \left\langle (\vec\nu^m)_i\,(\vec\nu^m)_j\,\nabla_s\,(\vec\xi)_j, \nabla_s\,(\vec\chi)_i\right\rangle_{\Gamma^m} + \left\langle \nabla_s\,\vec\xi, \nabla_s\,\vec\chi\right\rangle_{\Gamma^m}\\
&= \sum_{i,j=1}^d \left\langle (\nabla_s)_j\,(\vec\xi)_i, (\nabla_s)_i\,(\vec\chi)_j\right\rangle_{\Gamma^m} + \sum_{i,j=1}^d \left\langle (\delta_{ij} - (\vec\nu^m)_i\,(\vec\nu^m)_j)\,\nabla_s\,(\vec\xi)_j, \nabla_s\,(\vec\chi)_i\right\rangle_{\Gamma^m}.
\end{aligned}
$$

Moreover, we observe that $\langle \nabla_s\,.\,\vec\xi, \nabla_s\,.\,\vec\chi\rangle_{\Gamma^m} = \sum_{i,j=1}^d \langle (\nabla_s)_j\,(\vec\xi)_j, (\nabla_s)_i\,(\vec\chi)_i\rangle_{\Gamma^m}$. Hence, in addition to (6.1), we introduce the following matrices and vectors, where $q = 1,\ldots,K^m_{\mathbb{U}}$, and $k,l = 1,\ldots,K_\Gamma$

$$
\begin{aligned}
&[\vec{\mathcal{B}}_\Gamma]_{kl} := \left(\langle [\nabla_s]_j\,\chi^m_l, [\nabla_s]_i\,\chi^m_k\rangle_{\Gamma^m}\right)_{i,j=1}^d, \qquad [\vec{\mathcal{R}}_\Gamma]_{kl} := \left\langle \nabla_s\,\chi^m_l\,.\,\nabla_s\,\chi^m_k, \underline{\underline{\mathrm{Id}}} - \vec\nu^m\otimes\vec\nu^m\right\rangle_{\Gamma^m},\\
&[\vec M_{\Gamma,\Omega}]_{ql} := \left\langle \chi^m_l, \phi^{\mathbb{U}^m}_q\right\rangle_{\Gamma^m}\underline{\underline{\mathrm{Id}}}, \qquad [\vec M_\Gamma]_{kl} := \langle \chi^m_l, \chi^m_k\rangle^h_{\Gamma^m}\,\underline{\underline{\mathrm{Id}}},\\
&[\vec M_{\Gamma,\alpha}]_{kl} := \langle \alpha^m\,\chi^m_l, \chi^m_k\rangle^h_{\Gamma^m}\,\underline{\underline{\mathrm{Id}}}, \qquad [A_\Gamma]_{kl} := \langle \nabla_s\,\chi^m_l, \nabla_s\,\chi^m_k\rangle_{\Gamma^m}, \qquad [\vec A_\Gamma]_{kl} := [A_\Gamma]_{kl}\,\underline{\underline{\mathrm{Id}}},\\
&\vec c_k := -\langle \alpha^m\,\overline{\varkappa}^m\,\vec\nu^m, \chi^m_k\rangle^h_{\Gamma^m} + \left\langle \alpha^{G,m}\,(\vec\Pi^m_{m-1}\,\vec\kappa^m + \underline{\underline{\Pi}}^m_{m-1}\,\underline{\underline{W}}^m\,\vec\nu^m), \chi^m_k\right\rangle^h_{\Gamma^m},\\
&[\vec d_\alpha]_k := \left\langle \alpha^m\,\overline{\varkappa}^m, (\vec\Pi^m_{m-1}\,\vec\kappa^m\,.\,\nabla_s\,\chi^m_k)\,\vec\nu^m\right\rangle^h_{\Gamma^m},\\
&[\vec d_\kappa]_k := \tfrac12\left\langle \alpha^m\,|\vec\Pi^m_{m-1}\,\vec\kappa^m - \overline{\varkappa}^m\,\vec\nu^m|^2 - 2\,\vec\Pi^m_{m-1}\,\vec Y^m\,.\,\vec\Pi^m_{m-1}\,\vec\kappa^m, \nabla_s\,\chi^m_k\right\rangle^h_{\Gamma^m},\\
&[\vec d_\beta]_k := \beta\,\langle b_{GL}(\mathfrak{C}^m), \nabla_s\,\chi^m_k\rangle^h_{\Gamma^m} - \beta\,\gamma\left(\langle(\nabla_s\,\mathfrak{C}^m)\otimes(\nabla_s\,\mathfrak{C}^m), \vec e_r\otimes\nabla_s\,\chi^m_k\rangle_{\Gamma^m}\right)_{r=1}^d\\
&\qquad = \beta\,\langle b_{GL}(\mathfrak{C}^m), \nabla_s\,\chi^m_k\rangle^h_{\Gamma^m} - \beta\,\gamma\,\langle \nabla_s\,\mathfrak{C}^m\,.\,\nabla_s\,\chi^m_k, \nabla_s\,\mathfrak{C}^m\rangle_{\Gamma^m},\\
&[\vec d_G]_k := \tfrac12\left\langle \alpha^{G,m}\,(|\vec\Pi^m_{m-1}\,\vec\kappa^m|^2 + |\underline{\underline{\Pi}}^m_{m-1}\,\underline{\underline{W}}^m|^2), \nabla_s\,\chi^m_k\right\rangle^h_{\Gamma^m},\\
&[\vec d_Z]_k := \left\langle (\underline{\underline{Z}}^m\,\vec\Pi^m_{m-1}\,\vec\kappa^m + \nabla_s\,.\,\underline{\underline{Z}}^m)\,.\,\nabla_s\,\chi^m_k, \vec\nu^m\right\rangle^h_{\Gamma^m} - \left\langle (\underline{\underline{Z}}^m\,\vec\Pi^m_{m-1}\,\vec\kappa^m + \nabla_s\,.\,\underline{\underline{Z}}^m)\,.\,\vec\nu^m, \nabla_s\,\chi^m_k\right\rangle^h_{\Gamma^m}\\
&\qquad - \sum_{i=1}^d \left(\left\langle \nu^m_i\,\nabla_s\,\vec Z^m_i, \nu^m_r\,[\vec\nu^m\otimes\nabla_s\,\chi^m_k] - \nabla_s\,\chi^m_k\otimes\vec e_r\right\rangle_{\Gamma^m}\right)_{r=1}^d.
\end{aligned}
$$

Here we have made use of the facts that

$$
\begin{aligned}
[\vec{\mathcal{B}}_\Gamma]_{kl} &= \left(\langle \nabla_s\,.\,(\chi^m_l\,\vec e_j), \nabla_s\,.\,(\chi^m_k\,\vec e_i)\rangle_{\Gamma^m}\right)_{i,j=1}^d = \left(\langle (\nabla_s\,\chi^m_l)\,.\,\vec e_j, (\nabla_s\,\chi^m_k)\,.\,\vec e_i\rangle_{\Gamma^m}\right)_{i,j=1}^d\\
&= \left(\langle [\nabla_s]_j\,\chi^m_l, [\nabla_s]_i\,\chi^m_k\rangle_{\Gamma^m}\right)_{i,j=1}^d
\end{aligned}
$$

and that

$$
\begin{aligned}
&\left(\left\langle \nu^m_i\,\nabla_s\,\vec Z^m_i, \vec e_r\otimes\nabla_s\,\chi^m_k - \underline{\underline{\mathcal{P}}}_{\Gamma^m}\,[\vec e_r\otimes\nabla_s\,\chi^m_k] - [\nabla_s\,\chi^m_k\otimes\vec e_r]\,\underline{\underline{\mathcal{P}}}_{\Gamma^m}\right\rangle_{\Gamma^m}\right)_{r=1}^d\\
&\qquad = \left(\left\langle \nu^m_i\,\nabla_s\,\vec Z^m_i, [\vec\nu^m\otimes\vec\nu^m]\,[\vec e_r\otimes\nabla_s\,\chi^m_k] - \nabla_s\,\chi^m_k\otimes\vec e_r + [\nabla_s\,\chi^m_k\otimes\vec e_r]\,[\vec\nu^m\otimes\vec\nu^m]\right\rangle_{\Gamma^m}\right)_{r=1}^d\\
&\qquad = \left(\left\langle \nu^m_i\,\nabla_s\,\vec Z^m_i, \nu^m_r\,[\vec\nu^m\otimes\nabla_s\,\chi^m_k] - \nabla_s\,\chi^m_k\otimes\vec e_r + \nu^m_r\,[\nabla_s\,\chi^m_k\otimes\vec\nu^m]\right\rangle_{\Gamma^m}\right)_{r=1}^d
\end{aligned}
$$

$$= \left(\left\langle \nu_i^m \, \nabla_s \, \vec{Z}_i^m , \nu_r^m \, [\vec{\nu}^m \otimes \nabla_s \, \chi_k^m] - \nabla_s \, \chi_k^m \otimes \vec{e}_r \right\rangle_{\Gamma^m} \right)_{r=1}^{d}$$

for $i = 1, \ldots, d$, on noting that $\nabla_s \, \vec{Z}_i^m : [\nabla_s \, \chi_k^m \otimes \vec{\nu}^m] = [(\nabla_s \, \vec{Z}_i^m) \, \vec{\nu}^m] \, . \, \nabla_s \, \chi_k^m = \vec{0} \, . \, \nabla_s \, \chi_k^m = 0$. Moreover, it clearly holds that $([\vec{\mathcal{B}}_\Gamma]_{kl})^T = [\vec{\mathcal{B}}_\Gamma]_{lk} =: [\vec{\mathcal{B}}^\star_\Gamma]_{kl}$.

Denoting the system matrix

$$\begin{pmatrix} \vec{B}_\Omega & \vec{C}_\Omega & \vec{D}_\Omega & \vec{S}_{\Gamma,\Omega} \\ \vec{C}_\Omega^T & 0 & 0 & 0 \\ \vec{D}_\Omega^T & 0 & 0 & 0 \\ \vec{S}_{\Gamma,\Omega}^T & 0 & 0 & 0 \end{pmatrix}$$

as $\begin{pmatrix} \vec{B}_\Omega & \vec{\mathcal{C}} \\ \vec{\mathcal{C}}^T & 0 \end{pmatrix}$, and letting $\widetilde{P}^{m+1} = (P^{m+1}, P^{m+1}_{\text{sing}}, \, P^{m+1}_\Gamma)^T$, then the linear system (5.4a–d), (5.5a,c,d) can be written as

$$\begin{pmatrix} \vec{B}_\Omega & \vec{\mathcal{C}} & 0 & 0 & 0 & -\vec{M}_{\Gamma,\Omega} \\ \vec{\mathcal{C}}^T & 0 & 0 & 0 & 0 & 0 \\ (\vec{M}_{\Gamma,\Omega})^T & 0 & 0 & -\frac{1}{\tau}\vec{M}_\Gamma & 0 & 0 \\ 0 & 0 & \vec{M}_\Gamma & \vec{A}_\Gamma & 0 & 0 \\ 0 & 0 & -\vec{M}_{\Gamma,\alpha} & 0 & \vec{M}_\Gamma & 0 \\ 0 & 0 & 0 & 0 & -\vec{A}_\Gamma & \vec{M}_\Gamma \end{pmatrix} \begin{pmatrix} \vec{U}^{m+1} \\ \widetilde{P}^{m+1} \\ \vec{\kappa}^{m+1} \\ \delta\vec{X}^{m+1} \\ \vec{Y}^{m+1} \\ \vec{F}_\Gamma^{m+1} \end{pmatrix} = \begin{pmatrix} \vec{b} \\ 0 \\ 0 \\ -\vec{A}_\Gamma \, \vec{X}^m \\ \vec{c} \\ \vec{\mathcal{Z}}_\Gamma \, \vec{Y}^m - \vec{d} \end{pmatrix}, \tag{6.2}$$

where $\vec{\mathcal{Z}}_\Gamma := \vec{\mathcal{B}}_\Gamma - \vec{\mathcal{B}}^\star_\Gamma - \vec{\mathcal{R}}_\Gamma$ and $\vec{d} = \vec{d}_\kappa + \vec{d}_\alpha + \vec{d}_\beta + \vec{d}_G + \vec{d}_Z$. For the solution of (6.2) a Schur complement approach similar to [6] can be used. In particular, the Schur approach for eliminating $(\vec{\kappa}^{m+1}, \delta\vec{X}^{m+1}, \vec{Y}^{m+1}, \vec{F}_\Gamma^{m+1})$ from (6.2) can be obtained as follows. Let

$$\Theta_\Gamma := \begin{pmatrix} 0 & -\frac{1}{\tau}\vec{M}_\Gamma & 0 & 0 \\ \vec{M}_\Gamma & \vec{A}_\Gamma & 0 & 0 \\ -\vec{M}_{\Gamma,\alpha} & 0 & \vec{M}_\Gamma & 0 \\ 0 & 0 & -\vec{A}_\Gamma & \vec{M}_\Gamma \end{pmatrix}.$$

Then (6.2) can be reduced to

$$\begin{pmatrix} \vec{B}_\Omega + \alpha \, \vec{T}_\Omega & \vec{\mathcal{C}} \\ \vec{\mathcal{C}}^T & 0 \end{pmatrix} \begin{pmatrix} \vec{U}^{m+1} \\ \widetilde{P}^{m+1} \end{pmatrix} = \begin{pmatrix} \vec{b} + \alpha \, \vec{g} \\ 0 \end{pmatrix} \tag{6.3a}$$

and

$$\begin{pmatrix} \vec{\kappa}^{m+1} \\ \delta\vec{X}^{m+1} \\ \vec{Y}^{m+1} \\ \vec{F}_\Gamma^{m+1} \end{pmatrix} = \Theta_\Gamma^{-1} \begin{pmatrix} -(\vec{M}_{\Gamma,\Omega})^T \, \vec{U}^{m+1} \\ -\vec{A}_\Gamma \, \vec{X}^m \\ \vec{c} \\ \vec{\mathcal{Z}}_\Gamma \, \vec{Y}^m - \vec{d} \end{pmatrix}. \tag{6.3b}$$

In (6.3a) we have used the definitions

$$\vec{T}_\Omega = (0 \; 0 \; 0 \; \vec{M}_{\Gamma,\Omega}) \, \Theta_\Gamma^{-1} \begin{pmatrix} (\vec{M}_{\Gamma,\Omega})^T \\ 0 \\ 0 \\ 0 \end{pmatrix} = \tau \, \vec{M}_{\Gamma,\Omega} \, \vec{M}_\Gamma^{-1} \, \vec{A}_\Gamma \, \vec{M}_\Gamma^{-1} \, \vec{M}_{\Gamma,\alpha} \, \vec{M}_\Gamma^{-1} \, \vec{A}_\Gamma \, \vec{M}_\Gamma^{-1} \, (\vec{M}_{\Gamma,\Omega})^T$$

and

$$\vec{g} = (0 \; 0 \; 0 \; \vec{M}_{\Gamma,\Omega}) \, \Theta_\Gamma^{-1} \begin{pmatrix} 0 \\ -\vec{A}_\Gamma \, \vec{X}^m \\ \vec{c} \\ \vec{\mathcal{Z}}_\Gamma \, \vec{Y}^m - \vec{d} \end{pmatrix}.$$

For the linear system (6.3a) well-known solution methods for finite element discretizations for the standard Navier–Stokes equations may be employed. We refer to [4, §5], where we describe such solution methods in detail for a very similar situation.

The nonlinear system of algebraic equations arising from the discrete surface Cahn–Hilliard equation (5.6a,b) can be solved in the same way that such variational inequalities for standard Cahn–Hilliard equations are solved. In practice we employ the projection Gauss–Seidel method from [9], or the Uzawa-type iteration from [3].

7. Numerical results

We implemented the scheme (5.4a–d), (5.5a–d), (5.6a,b) with the help of the finite element toolbox ALBERTA, see [40]. For the bulk mesh adaptation in our numerical computations we use the strategy from [4], which results in a fine mesh around Γ^m and a coarse mesh further away from it.

Given the initial triangulation Γ^0 and $\mathfrak{C}^0 \in W(\Gamma^0)$, with $\mathfrak{C}^0 \in [-1,1]$, the initial data $\vec{Y}^0 \in \underline{V}(\Gamma^0)$, $\vec{\kappa}^0 \in \underline{V}(\Gamma^0)$ and $\underline{\underline{W}}^0 \in \underline{\underline{V}}(\Gamma^0)$ are always computed as

$$\left\langle \vec{Y}^0, \vec{\eta} \right\rangle_{\Gamma^0}^h = \left\langle \alpha(\mathfrak{C}^0)\,(\vec{\kappa}^0 - \overline{\varkappa}(\mathfrak{C}^0)\,\vec{\nu}^0) - \alpha^G(\mathfrak{C}^0)\,(\vec{\kappa}^0 + \underline{\underline{W}}^0\,\vec{\nu}^0), \vec{\eta} \right\rangle_{\Gamma^0}^h \qquad \forall\, \vec{\eta} \in \underline{V}(\Gamma^0)\,,$$

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

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

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

$$\left\langle \underline{\underline{W}}^0, \underline{\underline{\zeta}} \right\rangle_{\Gamma^0}^h + \tfrac{1}{2} \left\langle \vec{\nu}^0, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]\,\vec{\kappa}^0 + \nabla_s \,.\, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \right\rangle_{\Gamma^0}^h = 0 \qquad \forall\, \underline{\underline{\zeta}} \in \underline{\underline{V}}(\Gamma^0)\,.$$

Throughout this section we set

$$\alpha(s) = \alpha_L(s) := \tfrac{1}{2}\,(\alpha_+ + \alpha_-) + \tfrac{1}{2}\,(\alpha_+ - \alpha_-)\,s\,, \tag{7.1a}$$

$$\overline{\varkappa}(s) = \tfrac{1}{2}\,(\overline{\varkappa}_+ + \overline{\varkappa}_-) + \tfrac{1}{2}\,(\overline{\varkappa}_+ - \overline{\varkappa}_-)\,s\,, \tag{7.1b}$$

$$\alpha^G(s) = \tfrac{1}{2}\,(\alpha^G_+ + \alpha^G_-) + \tfrac{1}{2}\,(\alpha^G_+ - \alpha^G_-)\,s\,. \tag{7.1c}$$

We recall from the discussion around (1.3) that it follows from (7.1c), (1.2a) and (1.3) that only the difference $(\alpha^G_+ - \alpha^G_-)$ plays a role in the evolutions with Gaussian curvature. Moreover, for the choices (7.1a,c) the constraint (1.4) reduces to

$$\min\{\alpha_-, \alpha_+\} \geq \tfrac{1}{2}\,|\alpha^G_+ - \alpha^G_-|\,. \tag{7.2}$$

Unless otherwise stated, we use $\rho_\pm = 0$, $\mu_\pm = 1$, $\mu_\Gamma = 1$, $\rho_\Gamma = 0$, $\alpha_\pm = 1$, $\overline{\varkappa}_\pm = 0$ and $\alpha^G_\pm = 0$. Moreover, we normally use $\vartheta = \beta = 1$.

At times we will discuss the discrete energy of the numerical solutions. On recalling Theorem 4.2 and (5.2), the discrete energy is defined by

$$\mathcal{E}^h_{total} = \mathcal{E}^h_{kin} + \mathcal{E}^h_\kappa + \mathcal{E}^h_{GL}\,,$$

where

$$\begin{aligned}
\mathcal{E}^h_{kin} &= \tfrac{1}{2}\,\|[\rho^m]^{\frac{1}{2}}\,\vec{U}^{m+1}\|_0^2 + \tfrac{1}{2}\,\rho_\Gamma \left\langle \vec{U}^{m+1}, \vec{U}^{m+1} \right\rangle_{\Gamma^m}^h,\\
\mathcal{E}^h_\kappa &= \tfrac{1}{2}\left\langle \alpha^m, |\vec{\kappa}^{m+1} - \overline{\varkappa}^m\,\vec{\nu}^m|^2 \right\rangle_{\Gamma^m}^h + \tfrac{1}{2}\left\langle \alpha^{G,m}, |\vec{\kappa}^{m+1}|^2 - |\underline{\underline{W}}^{m+1}|^2 \right\rangle_{\Gamma^m}^h,\\
\mathcal{E}^h_{GL} &= \beta\,\left\langle b_{GL}(\mathfrak{C}^m), 1 \right\rangle_{\Gamma^m}^h,
\end{aligned}$$

represent the kinetic, curvature and Cahn–Hilliard parts of the discrete energy.

In plots where we show the concentration $\mathfrak{C}^m$ in grey scales, the shade scales linearly with $\mathfrak{C}^m$ ranging from -1 (white) to 1 (black).

7.1. Numerical simulations in 2D

We start with an initial shape in the form of a smooth letter "U". The curve has length 2.823 and we use 257 elements on it. For our choice of $\gamma = 0.02$ this yields on average about 6 elements across the interface, which asymptotically has thickness $\gamma\,\pi$. The time step size is $\tau = 5 \times 10^{-4}$. For the computational domain we choose $\Omega = (-1,1)^2$, and we choose a random distribution for $\mathfrak{C}^0$ with mean value -0.4. An experiment for $\overline{\varkappa}_- = -\frac{1}{2}$ and $\overline{\varkappa}_+ = -2$ is shown in Figures 2. We observe that due to the choice of $\overline{\varkappa}_\pm$, the phase $+1$ occupies the regions with smaller principal radius, while the phase -1 can be found where the membrane is rather flat. We show some more detail of the initial spinodal decomposition in Figure 3.

We conducted the following shearing experiments on the domain $\Omega = (-2,2)^2$ for an initial interface in the form of an ellipse, centred at the origin, with axis lengths 1 and 2.5. The length of the polygonal interface is 5.75, and it has 257 elements. For our choice of $\gamma = 0.05$ this yields on average about 7 elements across the interface. The time step size is $\tau = 5 \times 10^{-4}$. Once again we choose a random distribution for $\mathfrak{C}^0$ with mean value -0.4. In particular, we prescribe the inhomogeneous Dirichlet boundary condition $\vec{g}(\vec{z}) = (z_2, 0)^T$ on $\partial_1\Omega = [-2,2] \times \{\pm 2\}$. The remaining parameters are given by $\rho = \rho_\Gamma = 1$, $\alpha_- = 0.05$, $\alpha_+ = 0.2$ and either

$$\text{(a)} \quad \mu_+ = 1, \quad \mu_- = 1\,, \quad \text{or} \quad \text{(b)} \quad \mu_+ = 1, \quad \mu_- = 10\,. \tag{7.3}$$

The results can be seen in Figures 4 and 5, and they should be compared to the corresponding computations in the absence of any species effect, i.e. for $\mathfrak{C}^0 = -1$ constant, which can be seen in Figures 2 and 3 in [6]. As there, we observe tank treading when there is no viscosity contrast between inner and outer phase, and we observe tumbling when there is a viscosity contrast. The main difference to the computations in [6], though, is that here the regions occupied by the $+1$ phase on the vesicle remain relatively straight throughout. This means that the tank treading motion in Figure 4 leads to concave shapes at times. Similarly, the phase distributions on the tumbling vesicle in Figure 5 have a notable effect on the vesicle shape, when compared with Figure 3 in [6].

Next we show a computation that highlights the Marangoni-type effects due to the tangential terms in (2.9). To this end, we start off with an initial interface that has an elliptic shape, on which the two phases are already well separated. The values of $\overline{\varkappa}_\pm$ are then chosen such that a tangential movement of the phases leads to a decrease in energy. In particular, we let $\overline{\varkappa}_- = 0.5$, $\overline{\varkappa}_+ = 2$ and $\beta = 10$. The length of the polygonal interface is 5.75, and it has 257 elements. For our choice of $\gamma = 0.05$ this yields on average about 7 elements across the interface. The computational domain is $\Omega = (-2,2)^2$, and the chosen time step size is $\tau = 5 \times 10^{-4}$. The results of the simulation are shown in Figure 6. It can be seen that due to the choice of $\overline{\varkappa}_\pm$, the $+1$ phase moves away from an area of large convex bending to an area that is at first almost flat, and then settles on an area with a small concave bending. In Figure 7 we visualize the flow field for this computation, and compare it with a computation when $\mathfrak{C}^0 = 1$ constant, so that there are no tangential forces in (2.9). One clearly sees the effect of the tangential force which induces flow close to the interface also at later times.

On replacing the definition in (7.1a) with

$$\alpha(s) = s^2\,\alpha_L(s) = \tfrac{1}{2}\,(\alpha_+ + \alpha_-)\,s^2 + \tfrac{1}{2}\,(\alpha_+ - \alpha_-)\,s^3\,, \tag{7.4a}$$

$$\text{or} \quad \alpha(s) = (s^2 + \delta)\,\alpha_L(s)\,, \qquad \delta > 0\,, \tag{7.4b}$$

we can simulate C^0–junctions, see also [29], as long as $\delta \to 0$ for $\gamma \to 0$. We obtain interesting results starting from an ellipse, on which the two phases are already well separated, and using $\overline{\varkappa}_- = -0.2$, $\overline{\varkappa}_+ = -2$ and $\beta = 10$. The length of the polygonal interface is 5.75, and it has 257 elements. For our choice of $\gamma = 0.05$ this yields on average about 7 elements across the interface. The computational domain is $\Omega = (-2,2)^2$, and the chosen

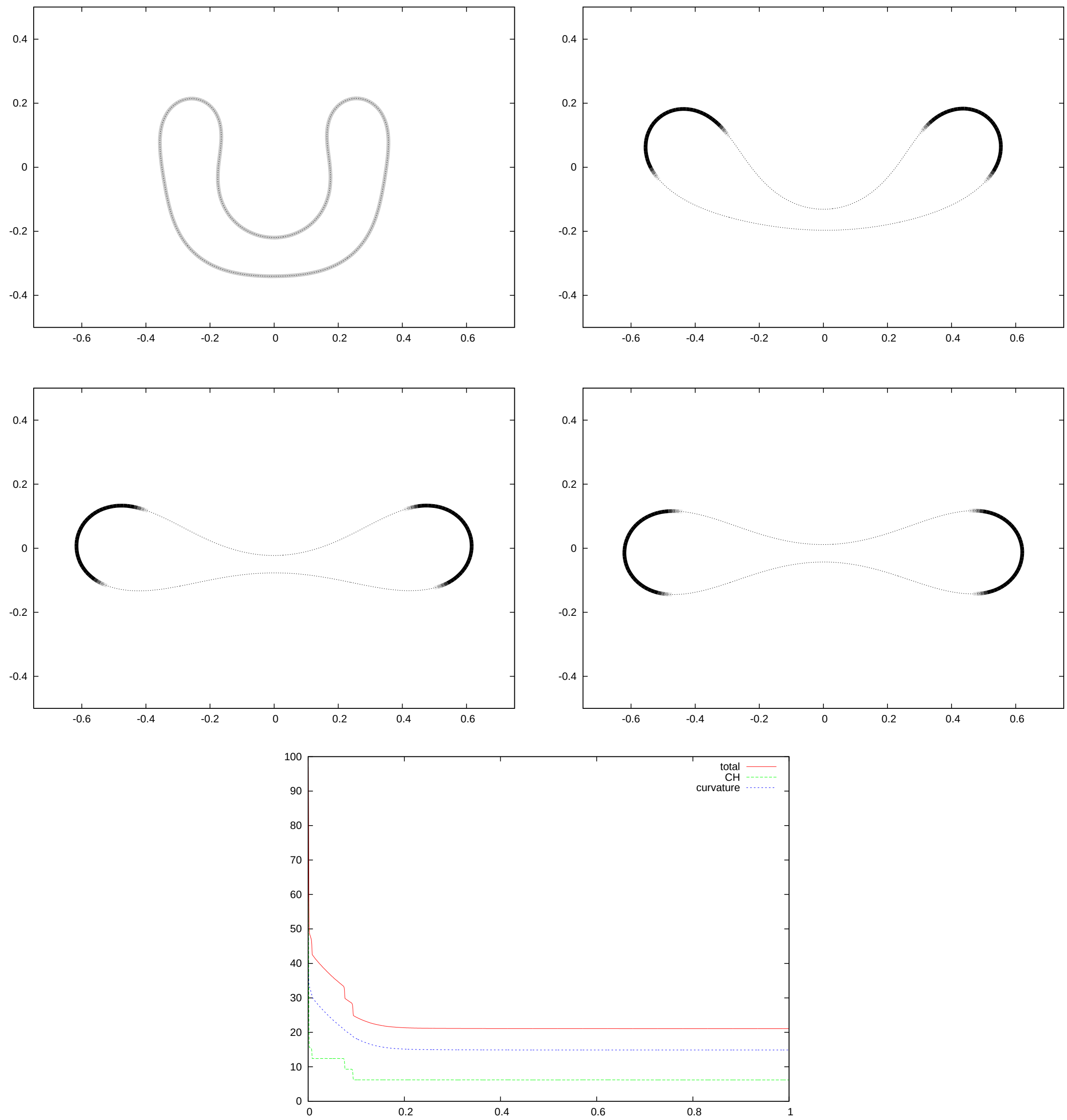

FIGURE 2. ($\alpha_\pm = 1$, $\overline{\varkappa}_- = -\frac{1}{2}$, $\overline{\varkappa}_+ = -2$, $\beta = 1$) Flow for a smooth letter "U". We show $\mathfrak{C}^m$ on Γ^m at times $t = 0,\ 0.1,\ 0.2,\ 1$. Below a superimposed plot of the total discrete energy $\mathcal{E}^h_{total}$, the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 1]$.

time step size is $\tau = 5 \times 10^{-4}$. In Figure 8 we show the numerical steady states for the two different evolutions, where for the C^0–case we employ the definition (7.4a). The nature of the C^0–junction can clearly be seen, which allows for tangent discontinuities at the interface. This allows the $+1$ phase to reduce its contribution to the overall curvature energy. As a result, the total energy for the C^0–steady state is 33.52, which is smaller than the value 33.97 for the C^1–case. For the curvature energy contributions the comparison is 2.32 versus 2.83, again in favour of the C^0–junction.

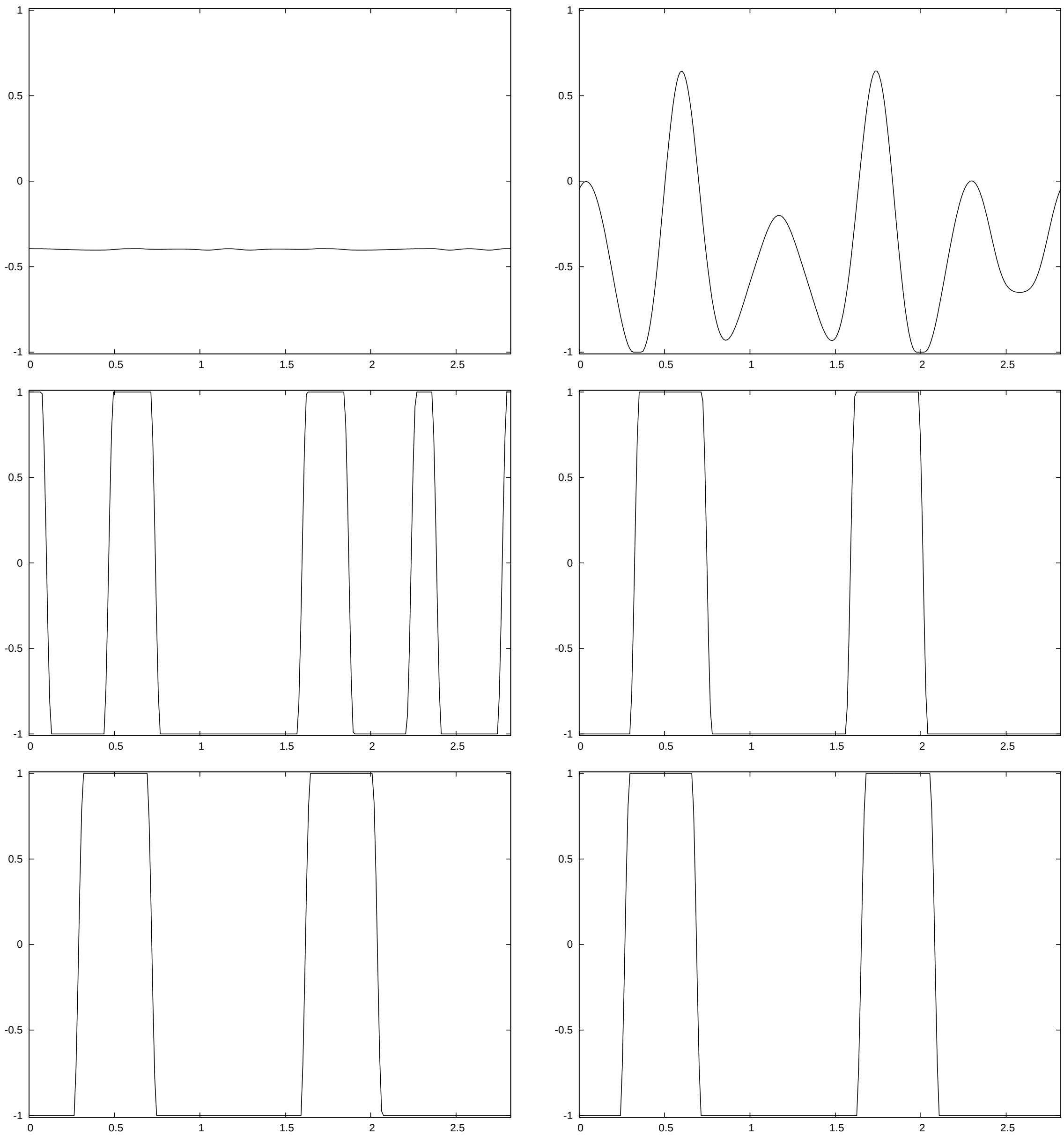

FIGURE 3. ($\alpha_\pm = 1$, $\overline{\varkappa}_- = -\frac{1}{2}$, $\overline{\varkappa}_+ = -2$, $\beta = 1$) Flow for a smooth letter "U". We show arclength plots of $\mathfrak{C}^m$ at times $t = 0$, 0.001, 0.01, 0.1, 0.2, 1.

7.2. **Numerical simulations in 3D**

As a first example for a three-dimensional simulation, we consider the evolution for an initially flat plate of total dimension $4 \times 4 \times 1$, similarly to [6, Fig. 8]. The triangulations Γ^m satisfy $(K_\Gamma, J_\Gamma) = (1538, 3072)$, and the polygonal surfaces have a surface area of 35.7. This means that for our chosen value of $\gamma = 0.2$, there are on average about 5 elements across the interfacial region on Γ^m. As the computational domain we choose $\Omega = (-2.5, 2.5)^3$, and we use the time step size $\tau = 10^{-3}$. First we set $\alpha_\pm = 1$, $\overline{\varkappa}_\pm = 0$ and $\beta = 1$, so that

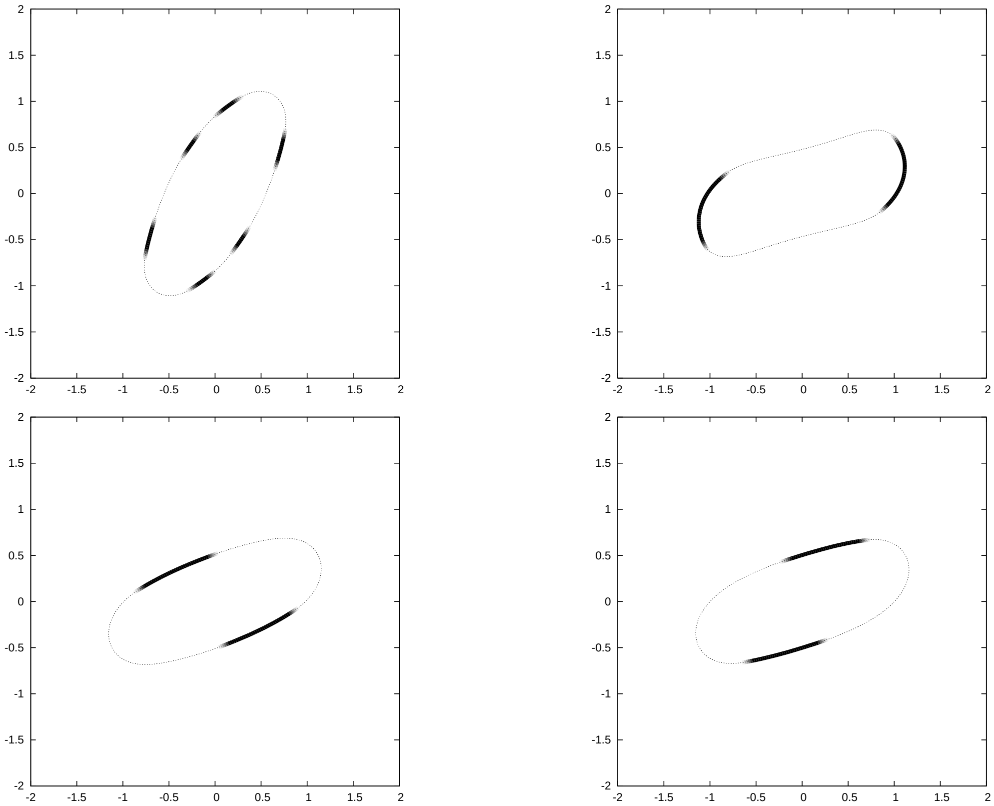

FIGURE 4. ($\alpha_- = 0.05$, $\alpha_+ = 0.2$, $\overline{\varkappa}_\pm = 0$, $\beta = 1$) Shear flow with parameters as in (7.3a), leading to tank treading. The plots show the interface Γ^m, together with the concentration $\mathfrak{C}^m$ at times $t = 1,\ 11,\ 13,\ 15$ (top left to bottom right).

the only effect of the two phase aspect is given by the line energy contributions in the free energy. The initial distribution for $\mathfrak{C}^0$ is random with mean value -0.4. See Figure 9 for the evolution in this case. Repeating the same experiment for $\alpha_- = \frac{1}{2}$, $\alpha_+ = 2$ gives the results in Figure 10. We note that the final shape is now a bit flatter, since the $+1$ phase does not allow the inner part of the membrane to become very concave.

In order to investigate budding, we start from a four-armed shape with well-developed interfaces between the two surface phases. As we use a finer mesh with $(K_\Gamma, J_\Gamma) = (3074, 6144)$, we now choose $\gamma = 0.1$. Moreover, we have set $\alpha_\pm = 1$, $\overline{\varkappa}_- = -\frac{1}{2}$, $\overline{\varkappa}_+ = -2$ to encourage the forming of the buds. In the first experiment we set $\beta = 1$ and observe the results shown in Figure 11. The same experiment with $\beta = 5$ is shown in Figure 12, where we observe budding behaviour now. In particular, the $+1$ phase would like to pinch off the membrane at the four corners.

The numerical simulation of a vesicle flowing through a constriction can be seen in Figure 13. This is a two-phase analogue of the simulation shown in [6, Figure 9]. Here we choose the initial shape of the interface to be a biconcave surface resembling a human red blood cell. The shape has surface area 2.23, and the triangulations Γ^m satisfy $(K_\Gamma, J_\Gamma) = (3074, 6144)$. This means that for our chosen value of $\gamma = 0.05$, there are on average about 6 elements across the interfacial region on Γ^m. As the computational domain we choose $\Omega = (-2,-1)\times(-1,1)^2 \cup [-1,1]\times(-0.5,0.5)^2 \cup (1,2)\times(-1,1)^2$. We define $\partial_2\Omega = \{2\}\times(-1,1)^2$ and on $\partial_1\Omega$ we set no-slip conditions, except on the left hand part $\{-2\}\times[-1,1]^2$, where we prescribe the inhomogeneous boundary conditions $\vec{g}(\vec{z}) = ([1 - z_2^2 - z_3^2]_+, 0, 0)^T$ in order to model a Poiseuille-type flow. For the remaining parameters we set $\alpha_- = 0.05$, $\alpha_+ = 0.1$ and $\vartheta = 100$. We notice that during the evolution the membrane in

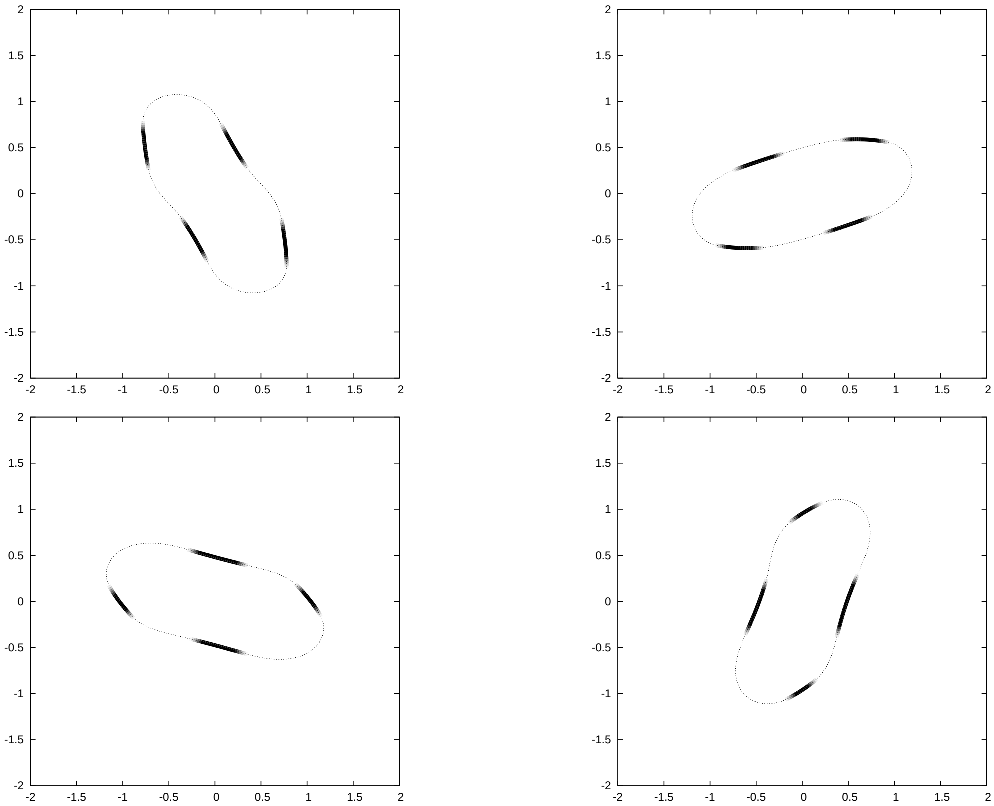

FIGURE 5. ($\alpha_- = 0.05$, $\alpha_+ = 0.2$, $\overline{\varkappa}_\pm = 0$, $\beta = 1$) Shear flow with parameters as in (7.3b), leading to tumbling. The plots show the interface Γ^m, together with the concentration $\mathfrak{C}^m$ at times $t = 8,\ 11,\ 14,\ 17$ (top left to bottom right).

Figure 13 deforms more than in the corresponding simulation with only a single phase $\mathfrak{C}^0 = 1$, see [6, Figure 9]. In particular, we observe that the $+1$ phase, which prefers a relatively flat surface, forces the surface to remain deformed also long after it has left the constriction.

In Figure 14 we show a numerical experiment for spinodal decomposition on a membrane, starting from a random distribution of phases with mean value -0.4. The shape has surface area 35.7, and the triangulations Γ^m satisfy $(K_\Gamma, J_\Gamma) = (6146, 12288)$. This means that for our chosen value of $\gamma = 0.1$, there are on average about 6 elements across the interfacial region on Γ^m. Similarly, in Figure 15 we show the evolution for spinodal decomposition on a seven-arm surface, where the initial phase variable is $\mathfrak{C}^0 = -0.4$ constant. The shape has surface area 10.5, and the triangulations Γ^m satisfy $(K_\Gamma, J_\Gamma) = (2314, 4624)$. This means that for our chosen value of $\gamma = 0.2$, there are on average about 9 elements across the interfacial region on Γ^m. For the phase parameters we choose $\overline{\varkappa}_- = -0.5$ and $\overline{\varkappa}_+ = -2$. The spontaneous curvature of the $+1$ phase leads to a preference of the $+1$ phase to be curved away from the outer normal. In accordance with this remark we observe that the $+1$ phase appears after the phase separation at the more highly curved tips of the fingers.

In the following, we present some computations for $\alpha^G_\pm \neq 0$. When we repeat the experiment in Figure 9 for the choices $\alpha^G_- = 0.5$, $\alpha^G_+ = 0$ and $\alpha^G_- = 0$, $\alpha^G_+ = 0.5$, we obtain the results in Figures 16 and 17, respectively. We note that for this choice of parameters, the bound (7.2) holds. Comparing the results in Figure 9 with the ones in Figures 16 and 17 clearly shows the influence of the Gaussian energy terms. In Figure 16 the region of the largest Gaussian curvature is in the $+1$ phase and the region of the smallest Gaussian curvature is in the -1 phase. This is in accordance with the fact that the energy penalizes Gaussian curvature only in the -1

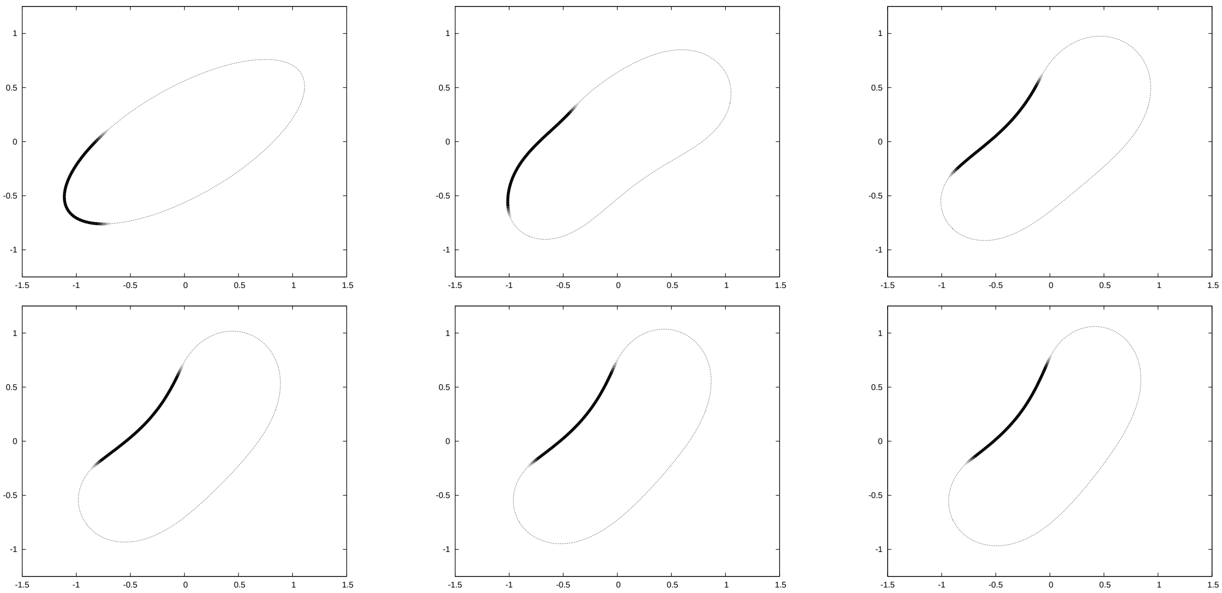

Figure 6. ($\alpha_\pm = 1$, $\overline{\varkappa}_- = 0.5$, $\overline{\varkappa}_+ = 2$, $\beta = 10$) Flow for an ellipse. We show $\mathfrak{C}^m$ on Γ^m at times $t = 0,\ 1,\ 2,\ 3,\ 4,\ 10$.

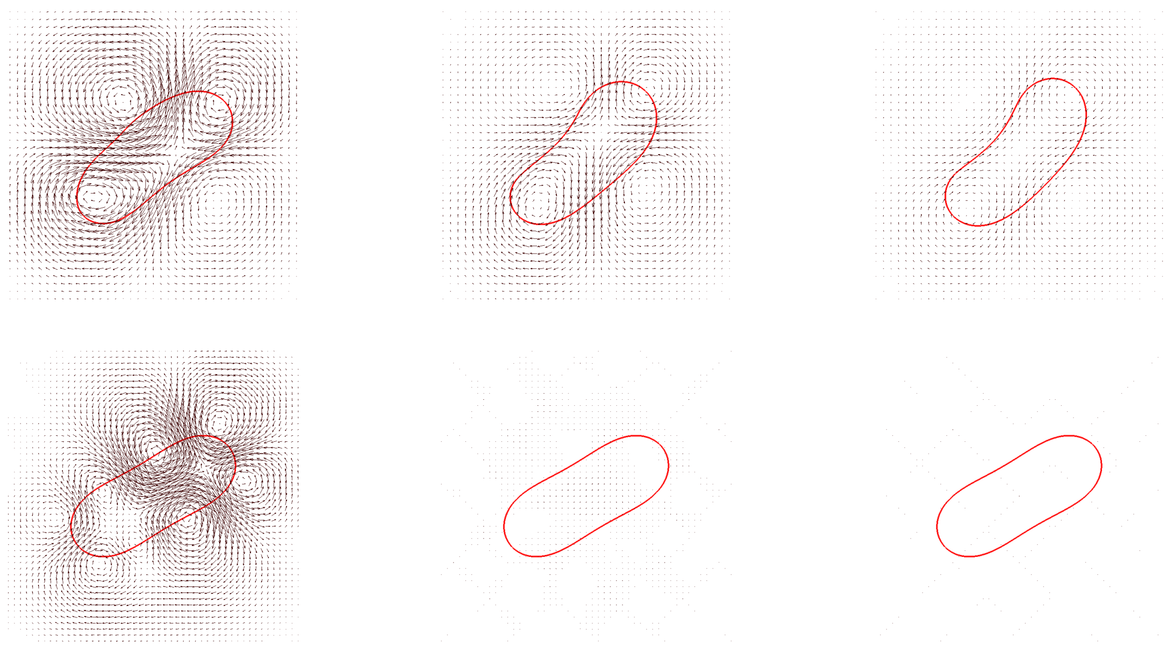

Figure 7. ($\alpha_\pm = 1$, $\overline{\varkappa}_- = 0.5$, $\overline{\varkappa}_+ = 2$, $\beta = 10$) Visualization of the flow field $\vec{U}^m$ at times $t = 1,\ 2, 3$ for the computation in Figure 6 (top), compared to the same computation with $\mathfrak{C}^m = 1$ constant throughout (bottom).

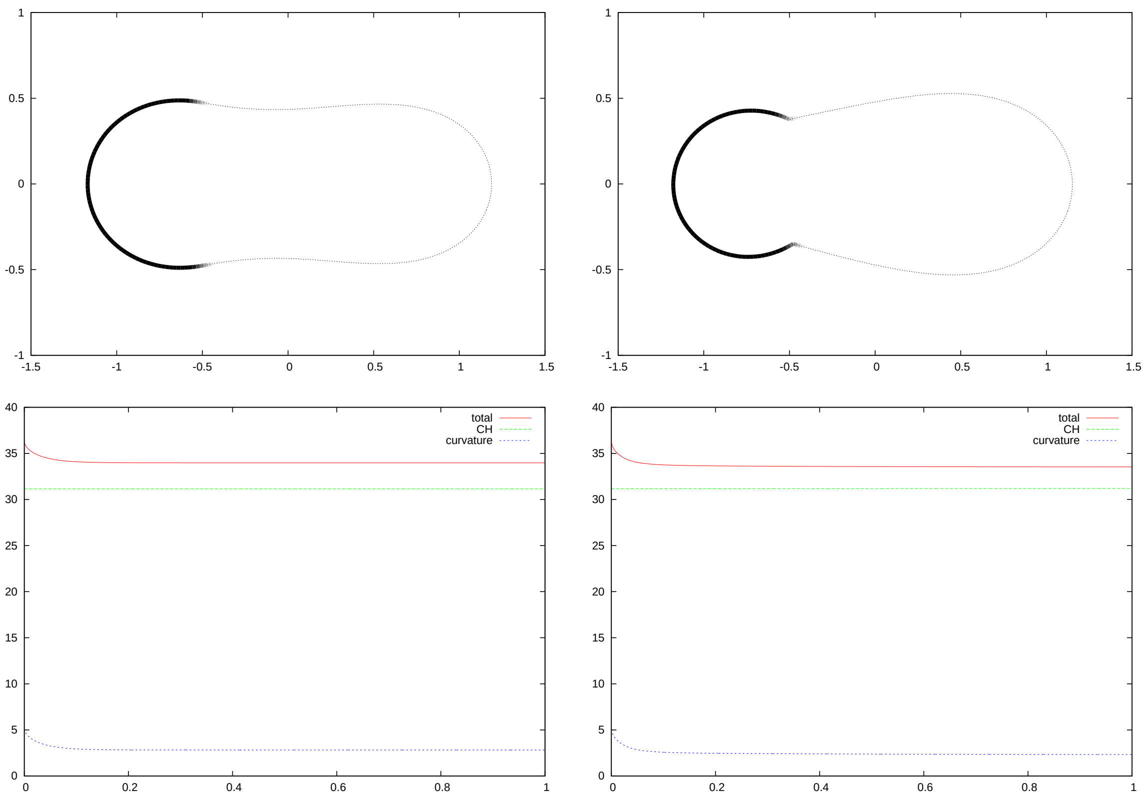

FIGURE 8. ($\alpha_\pm = 1$, $\overline{\varkappa}_- = -0.2$, $\overline{\varkappa}_+ = -2$, $\beta = 10$) Solution at time $t = 1$ for the C^1–case (left) and the C^0–case (right). Below a superimposed plot of the total discrete energy $\mathcal{E}^h_{total}$, the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 1]$.

phase. On the other hand, in Figure 17 the region with the largest Gaussian curvature is the -1 phase and the $+1$ phase has a smaller Gaussian curvature when compared to Figure 16.

Appendix A. Strong and weak formulations

The goal of this Appendix is to relate the weak formulation, (3.30a–e), (3.31b), of the first variations with respect to the geometry and $\mathfrak{c}$ of the energy in (1.2a), to the strong formulations (2.9) and (1.5b), respectively. As we allow for tangential motion, it is necessary to take into account variations which are not necessarily normal. This is in contrast to [25], where only normal variations were considered.

We recall that $\nabla_s = (\partial_{s_1}, \ldots, \partial_{s_d})^T$, and note from [21, Lemma 2.6] that for sufficiently smooth ϕ it holds that

$$\partial_{s_k} \partial_{s_i} \phi - \partial_{s_i} \partial_{s_k} \phi = [(\nabla_s \vec\nu) \nabla_s \phi]_i \, \nu_k - [(\nabla_s \vec\nu) \nabla_s \phi]_k \, \nu_i \qquad \forall\, i, k \in \{1, \ldots, d\} \quad \text{on } \Gamma(t)\,. \tag{A.1}$$

It follows from (2.13), (A.1) and (2.14) that

$$\Delta_s \vec\nu = \nabla_s (\nabla_s \,.\, \vec\nu) - |\nabla_s \vec\nu|^2 \, \vec\nu = -|\nabla_s \vec\nu|^2 \, \vec\nu - \nabla_s \varkappa\,. \tag{A.2}$$

Moreover, we have from (2.14), (3.22), (3.19), (2.13), (3.21a) and (A.2) that

$$\partial_\varepsilon^0 \varkappa = -\partial_\varepsilon^0 (\nabla_s \,.\, \vec\nu) = -[\nabla_s \vec\chi - 2\, \underline{\underline{D}}_s(\vec\chi)] : \nabla_s \vec\nu - \nabla_s \,.\, (\partial_\varepsilon^0 \vec\nu)$$

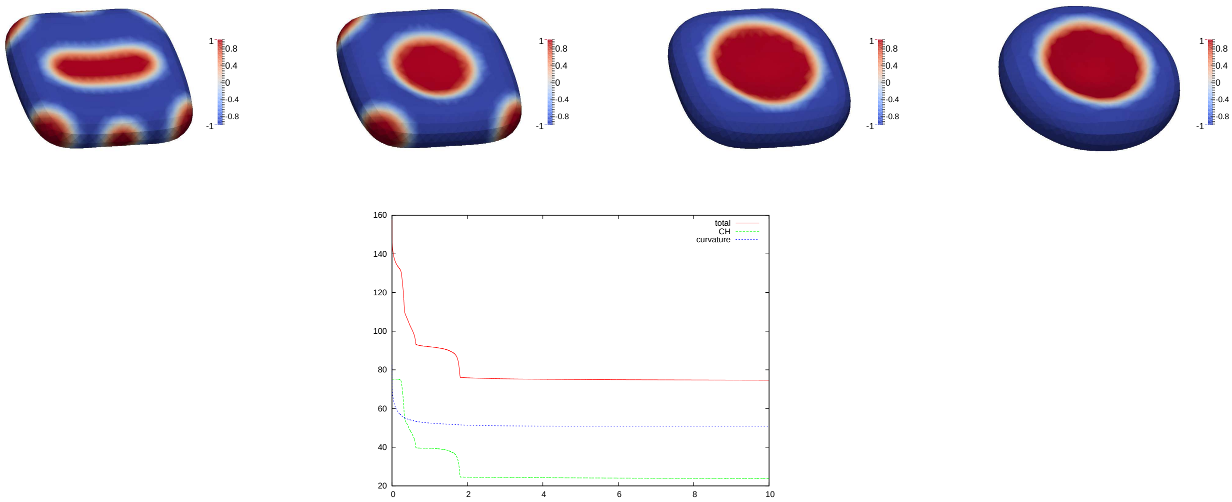

FIGURE 9. ($\alpha_\pm = 1$, $\overline{\varkappa}_\pm = 0$, $\beta = 1$) Plots of $\mathfrak{C}^m$ on Γ^m at times $t = 0.5,\ 1,\ 2,\ 10$. Below a superimposed plot of the total discrete energy $\mathcal{E}^h_{total}$, the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 10]$.

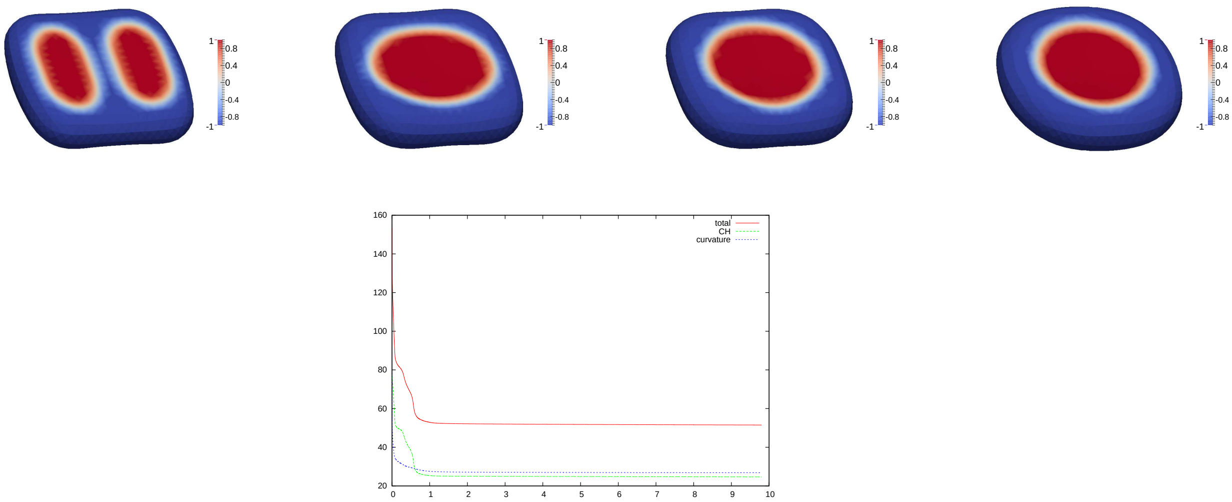

FIGURE 10. ($\alpha_- = \frac{1}{2}$, $\alpha_+ = 2$, $\overline{\varkappa}_\pm = 0$, $\beta = 1$) Plots of $\mathfrak{C}^m$ on Γ^m at times $t = 0.5,\ 1,\ 2,\ 10$. Compared to Figure 9, the final plot is less concave. Below a superimposed plot of the total discrete energy $\mathcal{E}^h_{total}$, the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 10]$.

$$
\begin{aligned}
&= \nabla_s \vec\chi : \nabla_s \vec\nu + \nabla_s \,.\, ([\nabla_s \vec\chi]^T \vec\nu) = 2\,\nabla_s \vec\chi : \nabla_s \vec\nu + (\Delta_s \vec\chi)\,\vec\nu = \Delta_s\,(\vec\chi \,.\, \vec\nu) - \vec\chi \,.\, \Delta_s \vec\nu \\
&= \Delta_s\,(\vec\chi \,.\vec\nu) + |\nabla_s \vec\nu|^2\,(\vec\chi \,.\, \vec\nu) + \vec\chi \,.\, \nabla_s \varkappa \,. \qquad \text{(A.3)}
\end{aligned}
$$

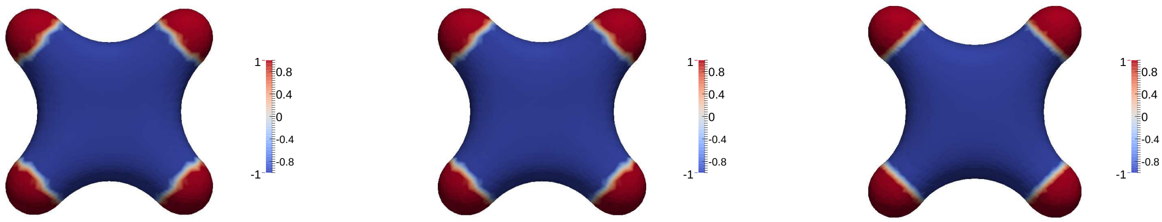

FIGURE 11. ($\alpha_\pm = 1$, $\overline{\varkappa}_- = -\frac{1}{2}$, $\overline{\varkappa}_+ = -2$, $\beta = 1$) Plots of $\mathfrak{C}^m$ on Γ^m at times $t = 0.5,\ 1,\ 5$.

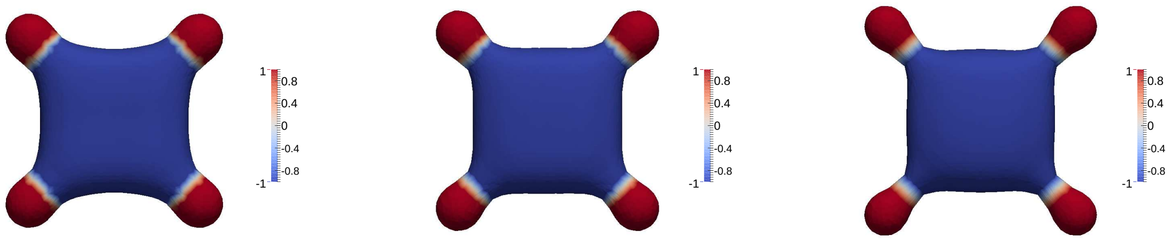

FIGURE 12. ($\alpha_\pm = 1$, $\overline{\varkappa}_- = -\frac{1}{2}$, $\overline{\varkappa}_+ = -2$, $\beta = 5$) Plots of $\mathfrak{C}^m$ on Γ^m at times $t = 0.5,\ 1,\ 5$.

A.1. **Derivation of the strong formulation**

We admit general variations $\vec\chi = \chi\,\vec\nu + \vec\chi_{\rm tan}$, where $\vec\chi_{\rm tan} \,.\, \vec\nu = 0$, of (1.2a) with respect to Γ, whereas in [25] only normal variations $\vec\chi = \chi\,\vec\nu$ of the geometry are considered.

We consider first the bending energy in (1.2a) and have from (3.17), on recalling (1.2b), that

$$\left[\frac{\delta}{\delta\Gamma}\,\langle b(\varkappa,\mathfrak{c}),1\rangle_{\Gamma(t)}\right](\vec\chi) = \left\langle \alpha(\mathfrak{c})\,(\varkappa - \overline{\varkappa}(\mathfrak{c})), \partial_\varepsilon^0\,\varkappa\right\rangle_{\Gamma(t)} + \langle b(\varkappa,\mathfrak{c}), \nabla_s\,.\,\vec\chi\rangle_{\Gamma(t)}\,. \tag{A.4}$$

We obtain from (A.4) and (A.3), on recalling (3.11), that

$$\begin{aligned}\left[\frac{\delta}{\delta\Gamma}\,\langle b(\varkappa,\mathfrak{c}),1\rangle_{\Gamma(t)}\right](\vec\chi) &= \left\langle \Delta_s\,[\alpha(\mathfrak{c})\,(\varkappa-\overline{\varkappa}(\mathfrak{c}))] + \alpha(\mathfrak{c})\,[(\varkappa-\overline{\varkappa}(\mathfrak{c}))\,|\nabla_s\,\vec\nu|^2 - \tfrac12\,(\varkappa-\overline{\varkappa}(\mathfrak{c}))^2\,\varkappa], \vec\chi\,.\,\vec\nu\right\rangle_{\Gamma(t)} \\ &\qquad - \langle \nabla_s\, b(\varkappa,\mathfrak{c}), \vec\chi\rangle_{\Gamma(t)} + \langle \alpha(\mathfrak{c})\,(\varkappa-\overline{\varkappa}(\mathfrak{c}))\,\nabla_s\,\varkappa, \vec\chi\rangle_{\Gamma(t)} \\ &= \left\langle \Delta_s\,[\alpha(\mathfrak{c})\,(\varkappa-\overline{\varkappa}(\mathfrak{c}))] + \alpha(\mathfrak{c})\,[(\varkappa-\overline{\varkappa}(\mathfrak{c}))\,|\nabla_s\,\vec\nu|^2 - \tfrac12\,(\varkappa-\overline{\varkappa}(\mathfrak{c}))^2\,\varkappa], \vec\chi\,.\,\vec\nu\right\rangle_{\Gamma(t)} \\ &\qquad - \langle b_{,\mathfrak{c}}(\varkappa,\mathfrak{c}), \vec\chi\,.\,\nabla_s\,\mathfrak{c}\rangle_{\Gamma(t)}\,. \end{aligned} \tag{A.5a}$$

In addition, it holds that

$$\left[\frac{\delta}{\delta\mathfrak{c}}\,\langle b(\varkappa,\mathfrak{c}),1\rangle_{\Gamma(t)}\right](\eta) = \langle b_{,\mathfrak{c}}(\varkappa,\mathfrak{c}),\eta\rangle_{\Gamma(t)}\,. \tag{A.5b}$$

Choosing just a normal variation, $\vec\chi = \chi\,\vec\nu$, means that (A.5a,b) collapses to the result in [25, (4.5)], on noting (2.10).

Next, we consider the interfacial energy in (1.2a). We have from (3.17), (3.24) and (3.11) that

$$\left[\frac{\delta}{\delta\Gamma}\,\langle b_{GL}(\mathfrak{c}),1\rangle_{\Gamma(t)}\right](\vec\chi) = -\gamma\,\langle \nabla_s\,\mathfrak{c}, (\nabla_s\,\vec\chi)\,\nabla_s\,\mathfrak{c}\rangle_{\Gamma(t)} + \left\langle \tfrac12\,\gamma\,|\nabla_s\,\mathfrak{c}|^2 + \gamma^{-1}\,\Psi(\mathfrak{c}), \nabla_s\,.\,\vec\chi\right\rangle_{\Gamma(t)}$$

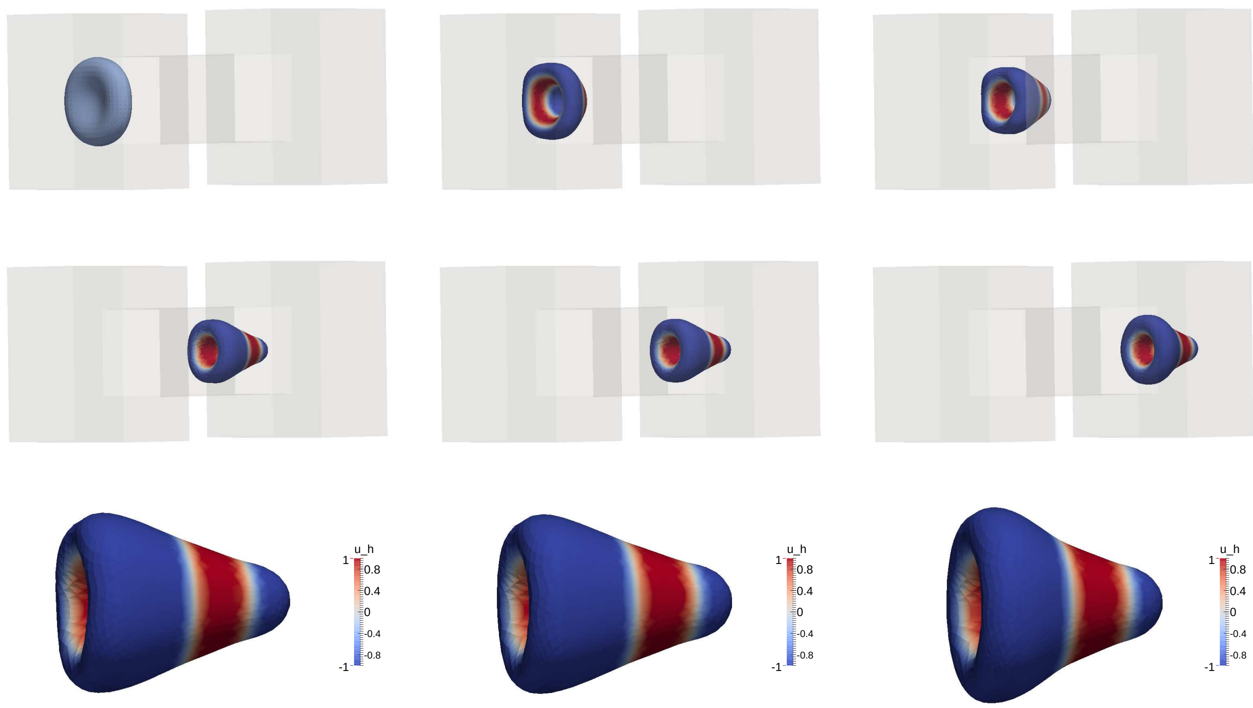

FIGURE 13. ($\alpha_- = 0.05$, $\alpha_+ = 0.1$, $\overline{\varkappa}_\pm = 0$, $\beta = 1$, $\vartheta = 100$) Flow through a constriction. Plots of $\mathfrak{C}^m$ on Γ^m at times $t = 0,\ 0.3,\ 0.5,\ 1,\ 1.2,\ 1.5$. Below we show enlarged plots of $\mathfrak{C}^m$ on Γ^m at times $t = 1,\ 1.2,\ 1.5$.

$$= -\left\langle (\tfrac{1}{2}\,\gamma\,|\nabla_s\,\mathfrak{c}|^2 + \gamma^{-1}\,\Psi(\mathfrak{c}))\,\varkappa, \vec\chi\,.\,\vec\nu\right\rangle_{\Gamma(t)} - \left\langle \nabla_s\,(\tfrac{1}{2}\,\gamma\,|\nabla_s\,\mathfrak{c}|^2 + \gamma^{-1}\,\Psi(\mathfrak{c})), \vec\chi\right\rangle_{\Gamma(t)} + \gamma\,\langle \nabla_s\,.\,[(\nabla_s\,\mathfrak{c})\otimes(\nabla_s\,\mathfrak{c})], \vec\chi\rangle_{\Gamma(t)}\,, \tag{A.6a}$$

where we have noted from (3.11) that

$$\langle \nabla_s\,\mathfrak{c}, (\nabla_s\,\vec\chi)\,\nabla_s\,\mathfrak{c}\rangle_{\Gamma(t)} = -\,\langle \nabla_s\,.\,[(\nabla_s\,\mathfrak{c})\otimes(\nabla_s\,\mathfrak{c})], \vec\chi\rangle_{\Gamma(t)}\,.$$

In addition, it holds that

$$\left[\frac{\delta}{\delta\mathfrak{c}}\,\langle b_{GL}(\mathfrak{c}), 1\rangle_{\Gamma(t)}\right](\eta) = \left\langle -\gamma\,\Delta_s\,\mathfrak{c} + \gamma^{-1}\,\Psi'(\mathfrak{c}), \eta\right\rangle_{\Gamma(t)}\,. \tag{A.6b}$$

Once again, choosing a normal variation, $\vec\chi = \chi\,\vec\nu$, means that (A.6a,b) collapses to [25, (4.8)], on noting that

$$\vec\nu\,.\,(\nabla_s\,.\,[(\nabla_s\,\mathfrak{c})\otimes(\nabla_s\,\mathfrak{c})]) = -\nabla_s\,\vec\nu : [(\nabla_s\,\mathfrak{c})\otimes(\nabla_s\,\mathfrak{c})]\,.$$

For $d = 3$ only, we compute the first variation of the Gaussian curvature bending energy in (1.2a). We start by deriving an expression for $\partial_\varepsilon^0\,\mathcal{K}$. On recalling (2.15), we first compute

$$\tfrac{1}{2}\,\partial_\varepsilon^0\,|\nabla_s\,\vec\nu|^2 = \nabla_s\,\vec\nu : \partial_\varepsilon^0\,(\nabla_s\,\vec\nu)\,. \tag{A.7}$$

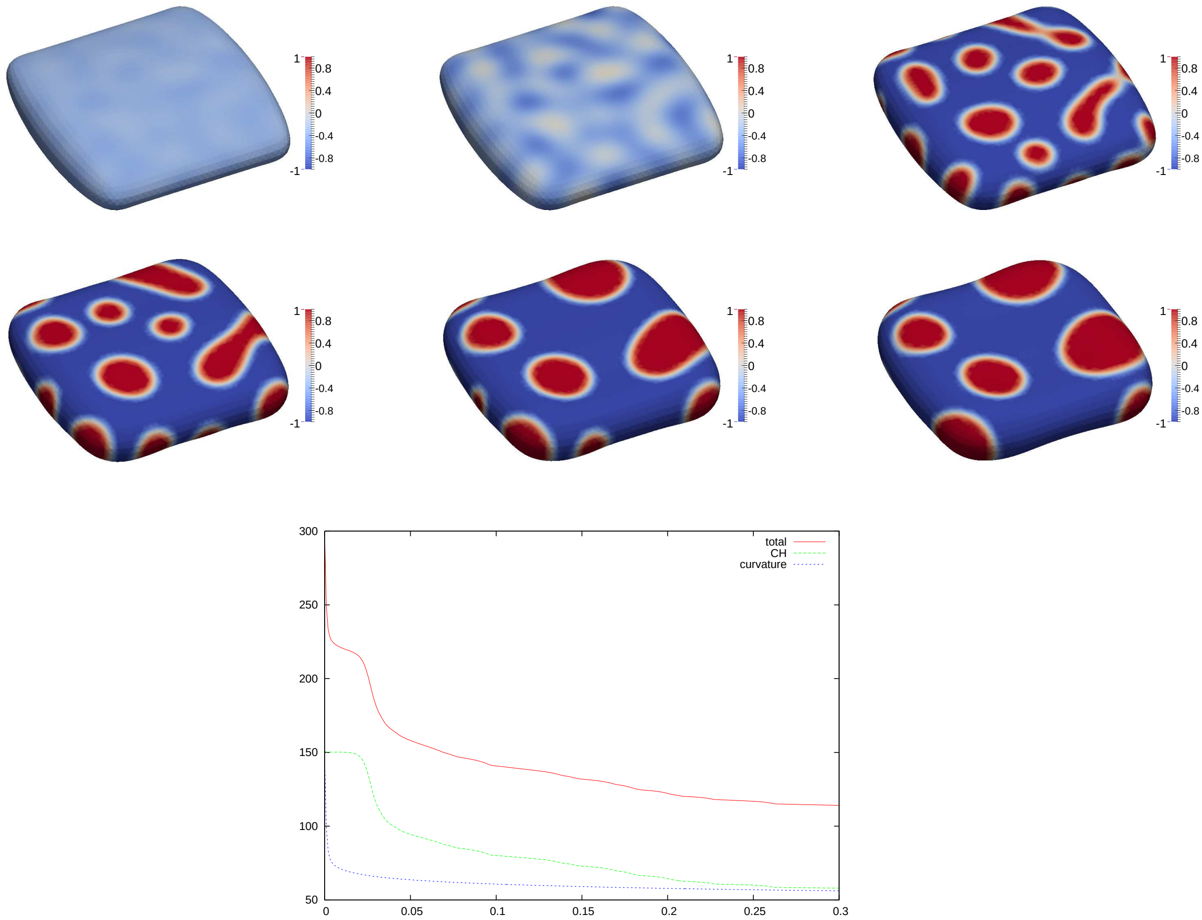

FIGURE 14. ($\alpha_\pm = 1$, $\overline{\varkappa}_\pm = 0$, $\beta = 1$) Spinodal decomposition on a membrane. Plots of $\mathfrak{C}^m$ on Γ^m at times $t = 0.01,\ 0.02,\ 0.05,\ 0.1,\ 0.2,\ 0.3$. Below a superimposed plot of the total discrete energy $\mathcal{E}^h_{total}$, the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 0.3]$.

From (3.23) we have that

$$\partial_\varepsilon^0 \, (\nabla_s \, \nu_i) = [\nabla_s \, \vec\chi - 2 \, \underline{\underline{D}}_s(\vec\chi)] \, \nabla_s \, \nu_i + \nabla_s \, (\partial_\varepsilon^0 \, \nu_i) \qquad i \in \{1, 2, 3\} \,,$$

yielding, on noting (2.13) and (3.19), that

$$\partial_\varepsilon^0 \, (\nabla_s \, \vec\nu) = \partial_\varepsilon^0 \, (\nabla_s \, \vec\nu)^T = [\nabla_s \, \vec\chi - 2 \, \underline{\underline{D}}_s(\vec\chi)] \, (\nabla_s \, \vec\nu)^T + [\nabla_s \, (\partial_\varepsilon^0 \, \vec\nu)]^T = [\nabla_s \, \vec\chi - 2 \, \underline{\underline{D}}_s(\vec\chi)] \, \nabla_s \, \vec\nu + [\nabla_s \, ([\nabla_s \, \vec\chi]^T \, \vec\nu)]^T \,. \tag{A.8}$$

We deduce from (A.7), (A.8), (2.13), (2.7b) and (3.21a) that

$$\tfrac{1}{2} \, \partial_\varepsilon^0 \, |\nabla_s \, \vec\nu|^2 = -\nabla_s \, \vec\nu : (\nabla_s \, \vec\chi)^T \, \nabla_s \, \vec\nu - \nabla_s \, \vec\nu : \nabla_s \, ([\nabla_s \vec\chi]^T \, \vec\nu) = T_1 + T_2 \,. \tag{A.9}$$

Adopting the standard summation convention, we have that

$$= -(\partial_{s_j} \, \nu_i) \, (\partial_{s_k} \, \chi_i) \, \partial_{s_j} \, \nu_k = -(\partial_{s_i} \, \nu_k) \, (\partial_{s_j} \, \chi_k) \, \partial_{s_i} \, \nu_j = -(\partial_{s_k} \, \nu_i) \, (\partial_{s_j} \, \chi_k) \, \partial_{s_j} \, \nu_i \tag{A.10}$$

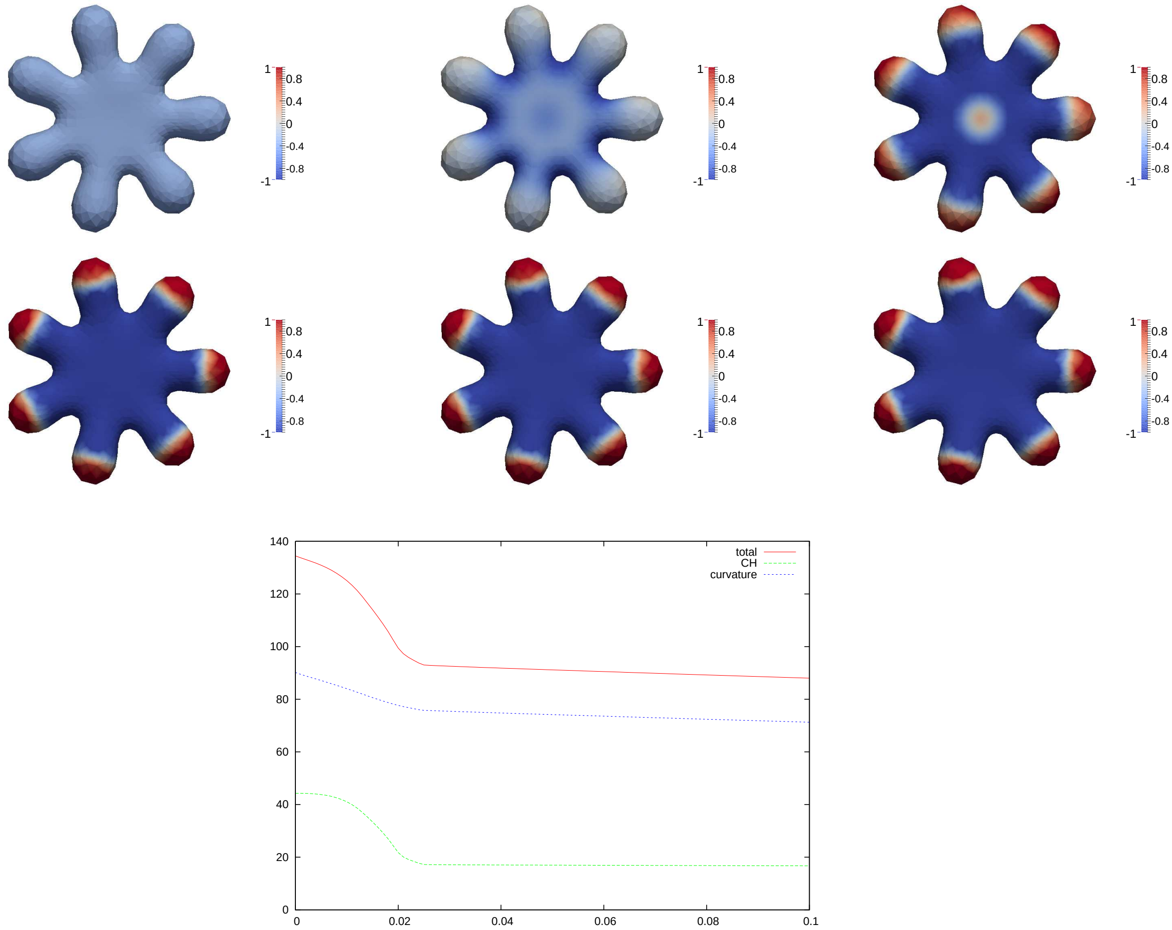

FIGURE 15. ($\alpha_\pm = 1$, $\overline{\varkappa}_- = -0.5$, $\overline{\varkappa}_+ = -2$, $\beta = 1$) Spinodal decomposition on a seven-arm membrane. Plots of $\mathfrak{C}^m$ on Γ^m at times $t = 0,\ 0.01,\ 0.02,\ 0.03,\ 0.05,\ 0.1$. Below a superimposed plot of the total discrete energy $\mathcal{E}^h_{total}$, the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 0.1]$.

and, on noting (2.13), that

$$\begin{aligned} T_2 &= -(\partial_{s_j}\,\nu_i)\,\partial_{s_j}\,((\partial_{s_i}\,\chi_k)\,\nu_k) = -(\partial_{s_j}\,\nu_i)\,\partial_{s_j}\,(\partial_{s_i}\,(\chi_k\,\nu_k) - \chi_k\,\partial_{s_i}\,\nu_k) \\ &= -\partial_{s_j}\,((\partial_{s_j}\,\nu_i)\,\partial_{s_i}\,(\chi_k\,\nu_k)) + (\partial_{s_j}\,\partial_{s_j}\,\nu_i)\,\partial_{s_i}\,(\chi_k\,\nu_k) + (\partial_{s_j}\,\nu_i)\,\partial_{s_j}\,(\chi_k\,\partial_{s_k}\,\nu_i) \\ &= -\partial_{s_j}\,((\partial_{s_j}\,\nu_i)\,\partial_{s_i}\,(\chi_k\,\nu_k)) + (\partial_{s_j}\,\partial_{s_j}\,\nu_i)\,\partial_{s_i}\,(\chi_k\,\nu_k) + (\partial_{s_j}\,\nu_i)\,\big[(\partial_{s_j}\,\partial_{s_k}\,\nu_i)\,\chi_k + (\partial_{s_j}\,\chi_k)\,\partial_{s_k}\,\nu_i\big] \\ &= -\nabla_s\,.\,((\nabla_s\,\vec\nu)\,\nabla_s\,(\vec\chi\,.\,\vec\nu)) + (\Delta_s\,\vec\nu)\,.\,\nabla_s\,(\vec\chi\,.\,\vec\nu) + (\partial_{s_j}\,\nu_i)\,\big[(\partial_{s_j}\,\partial_{s_k}\,\nu_i)\,\chi_k + (\partial_{s_j}\,\chi_k)\,\partial_{s_k}\,\nu_i\big]\,. \end{aligned} \tag{A.11}$$

Next, we note from (A.7) and (2.13) that

$$\chi_k\,(\partial_{s_j}\,\nu_i)\,(\partial_{s_j}\,\partial_{s_k}\,\nu_i) = \chi_k\,(\partial_{s_j}\,\nu_i)\,\big[\partial_{s_k}\,\partial_{s_j}\,\nu_i - [(\nabla_s\,\vec\nu)\,\nabla_s\,\nu_i]_j\,\nu_k\big] = \tfrac12\,\vec\chi\,.\,\nabla_s\,|\nabla_s\,\vec\nu|^2 - ((\nabla_s\,\vec\nu)^2 : \nabla_s\,\vec\nu)\,\vec\chi\,.\,\vec\nu\,. \tag{A.12}$$

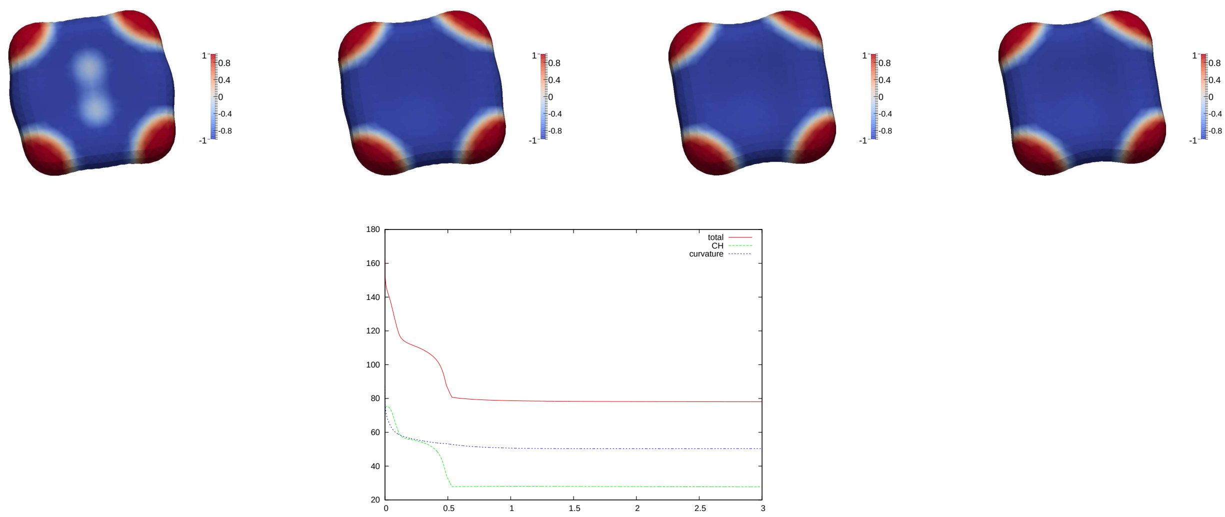

Figure 16. ($\alpha_\pm = 1$, $\overline{\varkappa}_\pm = 0$, $\alpha^G_- = 0.5$, $\alpha^G_+ = 0$, $\beta = 1$) Plots of $\mathfrak{C}^m$ on Γ^m at times $t = 0.5,\ 1,\ 2,\ 3$. Below a superimposed plot of the total discrete energy $\mathcal{E}^h_{total}$, the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 3]$.

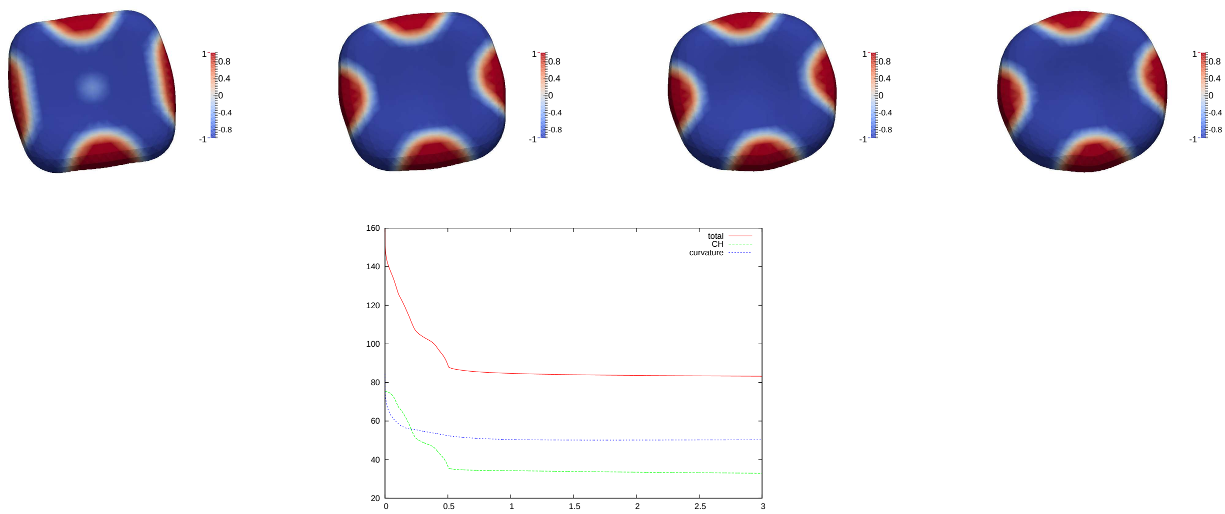

Figure 17. ($\alpha_\pm = 1$, $\overline{\varkappa}_\pm = 0$, $\alpha^G_- = 0$, $\alpha^G_+ = 0.5$, $\beta = 1$) Plots of $\mathfrak{C}^m$ on Γ^m at times $t = 0.5,\ 1,\ 2,\ 3$. Below a superimposed plot of the total discrete energy $\mathcal{E}^h_{total}$, the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 3]$.

Combining (A.9)–(A.12) and noting (2.13) yields that

$$\tfrac{1}{2}\,\partial^0_\varepsilon\,|\nabla_s\,\vec{\nu}|^2 = -\nabla_s\,.\,((\nabla_s\,\vec{\nu})\,\nabla_s\,(\vec{\chi}\,.\,\vec{\nu})) + (\Delta_s\,\vec{\nu})\,.\,\nabla_s\,(\vec{\chi}\,.\,\vec{\nu}) + \tfrac{1}{2}\,\vec{\chi}\,.\,\nabla_s\,|\nabla_s\,\vec{\nu}|^2 - \operatorname{tr}((\nabla_s\,\vec{\nu})^3)\,\vec{\chi}\,.\,\vec{\nu}\,. \tag{A.13}$$

As the eigenvalues of $-\nabla_s\vec{\nu}$ are 0, $\varkappa_1$ and $\varkappa_2$, we have from (2.13) and (2.14) that

$$(\nabla_s\,\vec{\nu})^2 : (\nabla_s\,\vec{\nu}) = \operatorname{tr}((\nabla_s\,\vec{\nu})^3) = -(\varkappa_1^3 + \varkappa_2^3) = -(\varkappa_1^2 + \varkappa_2^2 - \varkappa_1\,\varkappa_2)\,(\varkappa_1 + \varkappa_2) = (\mathcal{K} - |\nabla_s\,\vec{\nu}|^2)\,\varkappa\,. \tag{A.14}$$

Combining (A.13) and (A.14), on noting (A.2), yields that

$$\tfrac{1}{2}\,\partial_\varepsilon^0\,|\nabla_s\,\vec\nu|^2 = -\nabla_s\,.\,((\nabla_s\,\vec\nu)\,\nabla_s\,(\vec\chi\,.\,\vec\nu)) - (\nabla_s\,\varkappa)\,.\,\nabla_s\,(\vec\chi\,.\,\vec\nu) + \tfrac{1}{2}\,(\nabla_s\,|\nabla_s\,\vec\nu|^2)\,.\,\vec\chi + (|\nabla_s\,\vec\nu|^2 - \mathcal{K})\,\varkappa\,\vec\chi\,.\,\vec\nu\,. \tag{A.15}$$

On recalling (2.15) and (A.3), and combining with (A.15), we finally have that

$$\begin{aligned}
\partial_\varepsilon^0\,\mathcal{K} &= \tfrac{1}{2}\,\partial_\varepsilon^0\,(\varkappa^2 - |\nabla_s\,\vec\nu|^2) = \varkappa\,\partial_\varepsilon^0\,\varkappa - \tfrac{1}{2}\,\partial_\varepsilon^0\,|\nabla_s\,\vec\nu|^2 \\
&= \varkappa\left[\Delta_s\,(\vec\chi\,.\,\vec\nu) + |\nabla_s\,\vec\nu|^2\,\vec\chi\,.\,\vec\nu + \vec\chi\,.\,\nabla_s\,\varkappa\right] + \nabla_s\,.\,((\nabla_s\,\vec\nu)\,\nabla_s\,(\vec\chi\,.\,\vec\nu)) + (\nabla_s\,\varkappa)\,.\,\nabla_s\,(\vec\chi\,.\,\vec\nu) - \tfrac{1}{2}\,(\nabla_s\,|\nabla_s\,\vec\nu|^2)\,.\,\vec\chi \\
&\qquad - (|\nabla_s\,\vec\nu|^2 - \mathcal{K})\,\varkappa\,\vec\chi\,.\,\vec\nu \\
&= \varkappa\,\Delta_s\,(\vec\chi\,.\,\vec\nu) + \tfrac{1}{2}\,(\nabla_s\,\varkappa^2)\,.\,\vec\chi - \tfrac{1}{2}\,(\nabla_s\,|\nabla_s\,\vec\nu|^2)\,.\,\vec\chi + \nabla_s\,.\,((\nabla_s\,\vec\nu)\,\nabla_s\,(\vec\chi\,.\,\vec\nu)) + (\nabla_s\,\varkappa)\,.\,\nabla_s\,(\vec\chi\,.\,\vec\nu) + \mathcal{K}\,\varkappa\,\vec\chi\,.\,\vec\nu \\
&= \nabla_s\,.\,[(\varkappa\,\underline{\underline{\mathrm{Id}}} + \nabla_s\,\vec\nu)\,\nabla_s\,(\vec\chi\,.\,\vec\nu)] + \nabla_s\,\mathcal{K}\,.\,\vec\chi + \mathcal{K}\,\varkappa\,\vec\chi\,.\,\vec\nu\,.
\end{aligned} \tag{A.16}$$

On noting (3.17), (3.11) and (A.16), we have that

$$\begin{aligned}
\left[\frac{\delta}{\delta\Gamma}\,\left\langle\alpha^G(\mathfrak{c}),\mathcal{K}\right\rangle_{\Gamma(t)}\right](\vec\chi) &= \left\langle\alpha^G(\mathfrak{c}),\partial_\varepsilon^0\,\mathcal{K}\right\rangle_{\Gamma(t)} + \left\langle\alpha^G(\mathfrak{c})\,\mathcal{K},\nabla_s\,.\,\vec\chi\right\rangle_{\Gamma(t)} \\
&= -\left\langle\mathcal{K},\vec\chi\,.\,\nabla_s\,\alpha^G(\mathfrak{c})\right\rangle_{\Gamma(t)} + \left\langle\alpha^G(\mathfrak{c}),\partial_\varepsilon^0\,\mathcal{K} - \vec\chi\,.\,\nabla_s\,\mathcal{K} - \varkappa\,\mathcal{K}\,\vec\chi\,.\vec\nu\right\rangle_{\Gamma(t)} \\
&= -\left\langle\mathcal{K},\vec\chi\,.\,\nabla_s\,\alpha^G(\mathfrak{c})\right\rangle_{\Gamma(t)} + \left\langle\alpha^G(\mathfrak{c}),\nabla_s\,.\,[(\varkappa\,\underline{\underline{\mathrm{Id}}} + \nabla_s\,\vec\nu)\,\nabla_s\,(\vec\chi\,.\,\vec\nu)]\right\rangle_{\Gamma(t)} \\
&= -\left\langle\mathcal{K},\vec\chi\,.\,\nabla_s\,\alpha^G(\mathfrak{c})\right\rangle_{\Gamma(t)} + \left\langle\nabla_s\,.\,[(\varkappa\,\underline{\underline{\mathrm{Id}}} + \nabla_s\,\vec\nu)\,\nabla_s\,\alpha^G(\mathfrak{c})],\vec\chi\,.\,\vec\nu]\right\rangle_{\Gamma(t)}\,.
\end{aligned} \tag{A.17a}$$

In addition, it holds that

$$\left[\frac{\delta}{\delta\mathfrak{c}}\,\left\langle\alpha^G(\mathfrak{c}),\mathcal{K}\right\rangle_{\Gamma(t)}\right](\eta) = \left\langle(\alpha^G)'(\mathfrak{c})\,\eta,\mathcal{K}\right\rangle_{\Gamma(t)}\,. \tag{A.17b}$$

Once again, (A.17a,b) collapses to [25, (4.6)] if $\vec\chi = \chi\,\vec\nu$. Finally, the Cayley–Hamilton theorem applied to $-\nabla_s\,\vec\nu$ yields, on recalling (2.13), that

$$(\nabla_s\,\vec\nu)^3 + \varkappa\,(\nabla_s\,\vec\nu)^2 + \mathcal{K}\,\nabla_s\,\vec\nu = \underline{\underline{0}} \quad\Rightarrow\quad (\nabla_s\,\vec\nu + \varkappa\,\underline{\underline{\mathrm{Id}}})\,\underline{\underline{\mathcal{P}_\Gamma}} = \mathcal{K}\,(-\nabla_s\,\vec\nu)^{-1}\,\underline{\underline{\mathcal{P}_\Gamma}}\,,$$

where we note that $(\nabla_s\,\vec\nu)^{-1}$ is well-defined on the tangent space. With this identity it is possible to show that $\nabla_s\,.\,([\varkappa\,\underline{\underline{\mathrm{Id}}} + \nabla_s\,\vec\nu]\,\nabla_s\,\alpha^G(\mathfrak{c})) = \widehat\Delta_s\,\alpha^G(\mathfrak{c})$, where $\widehat\Delta_s$ is the second surface Laplacian used in the paper [36] to derive the first variation of the Gaussian curvature bending energy. However, comparing our (2.9) and e.g. Lemma 5.1 in [36], there appears to be a sign discrepancy in the latter.

It follows from (A.5a,b), (A.6a,b), (A.17a,b) and (1.2a,b) that

$$\left[\frac{\delta}{\delta\Gamma}\,E(\Gamma(t),\mathfrak{c}(t))\right](\vec\chi) = -\left\langle\vec f_\Gamma,\vec\chi\right\rangle_{\Gamma(t)} \tag{A.18a}$$

and

$$\left[\frac{\delta}{\delta\mathfrak{c}}\,E(\Gamma(t),\mathfrak{c}(t))\right](\eta) = \langle\mathfrak{m},\eta\rangle_{\Gamma(t)}\,, \tag{A.18b}$$

where $\vec f_\Gamma$ and $\mathfrak{m}$ are defined in (2.9) and (1.5b), respectively.

A.2. **Weak formulation equals strong formulation**

Here we show that the weak formulation (3.30a–e), (3.31b) equals the strong formulation (2.9), (1.5b).

Recall from (3.29a) and (3.30a) that minus the first variation of the Lagrangian (3.28) with respect to the geometry is given by

$$
\begin{aligned}
\vec f_\Gamma &= - \left[\frac{\delta}{\delta \Gamma} L\right](\vec\chi) \\
&= \langle \nabla_s \vec y, \nabla_s \vec\chi\rangle_{\Gamma(t)} + \langle \nabla_s \,.\, \vec y, \nabla_s \,.\, \vec\chi\rangle_{\Gamma(t)} - 2\left\langle (\nabla_s \vec y)^T, \underline{\underline{D}}_s(\vec\chi)\,(\nabla_s \vec{\rm id})^T\right\rangle_{\Gamma(t)} \\
&\quad - \tfrac12 \left\langle [\alpha(\mathfrak{c})\,|\vec\varkappa - \overline\varkappa(\mathfrak{c})\,\vec\nu|^2 - 2\,(\vec y\,.\,\vec\varkappa)]\,\nabla_s \vec{\rm id}, \nabla_s \vec\chi\right\rangle_{\Gamma(t)} - \left\langle \alpha(\mathfrak{c})\,(\vec\varkappa - \overline\varkappa(\mathfrak{c})\,\vec\nu)\,\overline\varkappa(\mathfrak{c}), [\nabla_s \vec\chi]^T\,\vec\nu\right\rangle_{\Gamma(t)} \\
&\quad - \beta\left\langle \tfrac12\,\gamma\,|\nabla_s \mathfrak{c}|^2 + \gamma^{-1}\,\Psi(\mathfrak{c}), \nabla_s \,.\, \vec\chi\right\rangle_{\Gamma(t)} + \beta\,\gamma\,\langle (\nabla_s \mathfrak{c}) \otimes (\nabla_s \mathfrak{c}), \nabla_s \vec\chi\rangle_{\Gamma(t)} \\
&\quad - \tfrac12\left\langle \alpha^G(\mathfrak{c})\,(|\vec\varkappa|^2 - |\underline{\underline{w}}|^2), \nabla_s \,.\, \vec\chi\right\rangle_{\Gamma(t)} + \left\langle \underline{\underline{w}} : \underline{\underline{z}}, \nabla_s \,.\, \vec\chi\right\rangle_{\Gamma(t)} + \left\langle \vec\nu\,.\,(\nabla_s \,.\, \underline{\underline{z}}), \nabla_s \,.\, \vec\chi\right\rangle_{\Gamma(t)} + \left\langle \vec\nu\,.\,(\underline{\underline{z}}\,\vec\varkappa), \nabla_s \,.\, \vec\chi\right\rangle_{\Gamma(t)} \\
&\quad + \sum_{i=1}^d \left[\langle \nu_i\,\nabla_s \vec z_i, \nabla_s \vec\chi\rangle_{\Gamma(t)} - 2\left\langle \nu_i\,(\nabla_s \vec z_i)^T, \underline{\underline{D}}_s(\vec\chi)\,(\nabla_s \vec{\rm id})^T\right\rangle_{\Gamma(t)}\right] \\
&\quad - \left\langle \underline{\underline{z}}\,\vec\varkappa, [\nabla_s \vec\chi]^T\,\vec\nu\right\rangle_{\Gamma(t)} - \left\langle \nabla_s \,.\, \underline{\underline{z}}, [\nabla_s \vec\chi]^T\,\vec\nu\right\rangle_{\Gamma(t)} = \sum_{\ell=1}^{14} T_\ell
\end{aligned} \tag{A.19}
$$

for $\vec\chi \in [H^1(\Gamma(t))]^d$.

On recalling Remark 3.2 and $\vec\varkappa = \varkappa\,\vec\nu$, we have that

$$
\underline{\underline{z}} = -\alpha^G(\mathfrak{c})\,\underline{\underline{w}} = -\alpha^G(\mathfrak{c})\,\nabla_s \vec\nu \quad\Rightarrow\quad \vec z_i = \underline{\underline{z}}\,\vec e_i = -\alpha^G(\mathfrak{c})\,\nabla_s \nu_i = -\alpha^G(\mathfrak{c})\,\partial_{s_i} \vec\nu\,, \tag{A.20}
$$

and so it follows that $\underline{\underline{z}}\,\vec\varkappa = \vec 0$. Hence $T_{11} = T_{13} = 0$. Moreover, $\vec\nu\,.\,[\nabla_s \vec\chi]^T\,\vec\nu = 0$, which implies that $T_5 = 0$. In addition, we recall from (3.30b) and $\underline{\underline{w}}^T\,\vec\nu = \underline{\underline{w}}\,\vec\nu = \vec 0$ that

$$
\vec y = y\,\vec\nu \quad \text{with} \quad y = \alpha(\mathfrak{c})\,(\varkappa - \overline\varkappa(\mathfrak{c})) + \alpha^G(\mathfrak{c})\,\varkappa\,, \tag{A.21}
$$

and so as $\nabla_s \,.\, \vec\nu = -\varkappa$ it holds, on recalling (1.2b), (3.9) and (3.11), that

$$
\begin{aligned}
\sum_{\ell \in \{2,4,8\}} T_\ell &= -\langle y\,\varkappa, \nabla_s \,.\, \vec\chi\rangle_{\Gamma(t)} + T_4 + T_8 = -\left\langle b(\varkappa,\mathfrak{c}) + \alpha^G(\mathfrak{c})\,\mathcal{K}, \nabla_s \,.\, \vec\chi\right\rangle_{\Gamma(t)} \\
&= \left\langle \nabla_s\left[b(\varkappa,\mathfrak{c}) + \alpha^G(\mathfrak{c})\,\mathcal{K}\right], \vec\chi\right\rangle_{\Gamma(t)} + \left\langle \left[b(\varkappa,\mathfrak{c}) + \alpha^G(\mathfrak{c})\,\mathcal{K}\right]\varkappa, \vec\chi\,.\,\vec\nu\right\rangle_{\Gamma(t)}\,.
\end{aligned} \tag{A.22}
$$

It also holds, on noting [8, (A.22), (A.19)] and (3.21b), where we stress that the notation $\underline{\underline{D}}(\vec\chi)$ there differs from $\underline{\underline{D}}_s(\vec\chi)$ here by a factor 2 and by the absence of the projections $\underline{\underline{\mathcal{P}}}_\Gamma$, that

$$
\begin{aligned}
\sum_{\ell \in \{1,3\}} T_\ell &= \langle \nabla_s\,(y\,\vec\nu), \nabla_s \vec\chi\rangle_{\Gamma(t)} - 2\left\langle [\nabla_s\,(y\,\vec\nu)]^T, \underline{\underline{D}}_s(\vec\chi)\,(\nabla_s \vec{\rm id})^T\right\rangle_{\Gamma(t)} \\
&= \langle \nabla_s\,(y\,\vec\nu), \nabla_s \vec\chi\rangle_{\Gamma(t)} - \left\langle [\nabla_s\,(y\,\vec\nu)]^T, (\nabla_s \vec\chi + (\nabla_s \vec\chi)^T)\,\underline{\underline{\mathcal{P}}}_\Gamma\right\rangle_{\Gamma(t)} \\
&= \langle \nabla_s\,(y\,\vec\nu), (\vec\nu \otimes \vec\nu)\,\nabla_s \vec\chi\rangle_{\Gamma(t)} - \langle y\,\nabla_s \vec\nu, \nabla_s \vec\chi\rangle_{\Gamma(t)} \\
&= \langle \nabla_s\, y, \nabla_s\,(\vec\chi\,.\,\vec\nu)\rangle_{\Gamma(t)} - \left\langle \nabla_s \,.\, [y\,(\nabla_s \vec\nu)^T\,\vec\chi], 1\right\rangle_{\Gamma(t)} - \left\langle y\,(|\nabla_s \vec\nu|^2\,\vec\nu + \nabla_s\,\varkappa), \vec\chi\right\rangle_{\Gamma(t)} \\
&= \langle \nabla_s\, y, \nabla_s\,(\vec\chi\,.\,\vec\nu)\rangle_{\Gamma(t)} - \left\langle y\,(|\nabla_s \vec\nu|^2\,\vec\nu + \nabla_s\,\varkappa), \vec\chi\right\rangle_{\Gamma(t)}\,,
\end{aligned} \tag{A.23}
$$

where in the last equality we have noted that $\Gamma(t)$ is a closed surface. Moreover, we note from (A.21) and (1.2b) that

$$\begin{aligned} y\,\nabla_s\,\varkappa &= [\alpha(\mathfrak{c})\,(\varkappa - \overline{\varkappa}(\mathfrak{c})) + \alpha^G(\mathfrak{c})\,\varkappa]\,\nabla_s\,\varkappa \\ &= \nabla_s\,(b(\varkappa,\mathfrak{c}) + \tfrac12\,\alpha^G(\mathfrak{c})\,\varkappa^2) - [b_{,\mathfrak{c}}(\varkappa,\mathfrak{c}) + \tfrac12\,(\alpha^G)'(\mathfrak{c})\,\varkappa^2]\,\nabla_s\,\mathfrak{c}\,. \end{aligned} \tag{A.24}$$

Combining (A.22), (A.23) and (A.24) yields, on noting (3.11), (A.21) and (3.9), that

$$\begin{aligned} \sum_{\ell\in\{1,\ldots,4,8\}} T_\ell &= -\left\langle \Delta_s\,[\alpha(\mathfrak{c})\,(\varkappa - \overline{\varkappa}(\mathfrak{c})) + \alpha^G(\mathfrak{c})\,\varkappa], \vec\chi\,.\,\vec\nu\right\rangle_{\Gamma(t)} + \left\langle [b(\varkappa,\mathfrak{c}) + \alpha^G(\mathfrak{c})\,\mathcal{K}]\,\varkappa, \vec\chi\,.\,\vec\nu\right\rangle_{\Gamma(t)} \\ &\quad + \left\langle [b_{,\mathfrak{c}}(\varkappa,\mathfrak{c}) + \tfrac12\,(\alpha^G)'(\mathfrak{c})\,\varkappa^2]\,\nabla_s\,\mathfrak{c}, \vec\chi\right\rangle_{\Gamma(t)} - \left\langle (\alpha(\mathfrak{c})\,(\varkappa - \overline{\varkappa}(\mathfrak{c})) + \alpha^G(\mathfrak{c})\,\varkappa)\,|\nabla_s\,\vec\nu|^2, \vec\chi\,.\,\vec\nu\right\rangle_{\Gamma(t)} \\ &\quad - \tfrac12\left\langle \nabla_s\,(\alpha^G(\mathfrak{c})\,|\nabla_s\,\vec\nu|^2), \vec\chi\right\rangle_{\Gamma(t)}\,. \end{aligned} \tag{A.25}$$

It holds on noting (3.11) that

$$\begin{aligned} \sum_{\ell\in\{6,7\}} T_\ell &= \beta\left\langle \nabla_s\,[\tfrac12\,\gamma\,|\nabla_s\,\mathfrak{c}|^2 + \gamma^{-1}\,\Psi(\mathfrak{c})], \vec\chi\right\rangle_{\Gamma(t)} + \beta\left\langle [\tfrac12\,\gamma\,|\nabla_s\,\mathfrak{c}|^2 + \gamma^{-1}\,\Psi(\mathfrak{c})]\,\varkappa, \vec\chi\,.\,\vec\nu\right\rangle_{\Gamma(t)} \\ &\quad - \beta\,\gamma\,\langle \nabla_s\,.\,((\nabla_s\,\mathfrak{c})\otimes(\nabla_s\,\mathfrak{c})), \vec\chi\rangle_{\Gamma(t)}\,. \end{aligned} \tag{A.26}$$

In addition, we have from (A.20) that

$$\sum_{\ell\in\{9,10\}} T_\ell = \left\langle \underline{\underline{w}} : \underline{\underline{z}} + \vec\nu\,.\,(\nabla_s\,.\,\underline{\underline{z}}), \nabla_s\,.\,\vec\chi\right\rangle_{\Gamma(t)} = -\left\langle \alpha^G(\mathfrak{c})\,|\nabla_s\,\vec\nu|^2 + \vec\nu\,.\,[\nabla_s\,.\,(\alpha^G(\mathfrak{c})\,\nabla_s\,\vec\nu)], \nabla_s\,.\,\vec\chi\right\rangle_{\Gamma(t)} = 0\,,$$

where we have observed from (A.2) that

$$\begin{aligned} \vec\nu\,.\,[\nabla_s\,.\,(\alpha^G(\mathfrak{c})\,\nabla_s\,\vec\nu)] &= \vec\nu\,.\,[\alpha^G(\mathfrak{c})\,\Delta_s\,\vec\nu + (\nabla_s\,\vec\nu)\,\nabla_s\,\alpha^G(\mathfrak{c})] = \alpha^G(\mathfrak{c})\,\vec\nu\,.\,\Delta_s\,\vec\nu \\ &= \alpha^G(\mathfrak{c})\,\vec\nu\,.\,[-|\nabla_s\,\vec\nu|^2\,\vec\nu - \nabla_s\,\varkappa] = -\alpha^G(\mathfrak{c})\,|\nabla_s\,\vec\nu|^2\,. \end{aligned}$$

It follows from (3.21b) and $\underline{\underline{\mathcal{P}}}_\Gamma = \nabla_s\,\vec{\mathrm{id}}$ that

$$T_{12} = \sum_{i=1}^d \left[\langle \nu_i\,\nabla_s\,\vec z_i, \nabla_s\,\vec\chi\rangle_{\Gamma(t)} - 2\left\langle \nu_i\,(\nabla_s\,\vec z_i)^T, \underline{\underline{D}}_s(\vec\chi)\,(\nabla_s\,\vec{\mathrm{id}})^T\right\rangle_{\Gamma(t)}\right] = -\sum_{i=1}^d \left\langle \nu_i\,(\nabla_s\,\vec z_i)^T, \nabla_s\,\vec\chi\right\rangle_{\Gamma(t)}\,, \tag{A.27}$$

provided that we can show that

$$\sum_{i=1}^d \left[\langle \nu_i\,\nabla_s\,\vec z_i, \nabla_s\,\vec\chi\rangle_{\Gamma(t)} - \left\langle \nu_i\,(\nabla_s\,\vec z_i)^T, (\nabla_s\,\vec\chi)^T\,\underline{\underline{\mathcal{P}}}_\Gamma\right\rangle_{\Gamma(t)}\right] = 0\,. \tag{A.28}$$

In order to establish (A.28), we note, on recalling (A.20) and (A.1), that

$$\begin{aligned} \nu_i\,\nabla_s\,\vec z_i : \nabla_s\,\vec\chi - \nu_i\,(\nabla_s\,\vec z_i)^T : [(\nabla_s\,\vec\chi)^T\,\underline{\underline{\mathcal{P}}}_\Gamma] &= \nu_i\,(\nabla_s\,\vec z_i)_{kj}\left[\partial_{s_j}\,\chi_k - (\partial_{s_j}\,\chi_l)\,(\delta_{lk} - \nu_l\,\nu_k)\right] \\ &= \nu_i\,(\nabla_s\,\vec z_i)_{kj}\,(\partial_{s_j}\,\chi_l)\,\nu_l\,\nu_k = -\nu_i\,[\partial_{s_j}\,(\alpha^G(\mathfrak{c})\,\partial_{s_k}\nu_i)]\,(\partial_{s_j}\,\chi_l)\,\nu_l\,\nu_k \\ &= -\nu_i\,\nu_l\,\nu_k\,\alpha^G(\mathfrak{c})\,(\partial_{s_j}\,\partial_{s_k}\,\nu_i)\,\partial_{s_j}\,\chi_l = \nu_i\,\nu_l\,\nu_k\,\alpha^G(\mathfrak{c})\,[(\nabla_s\,\vec\nu)\,\nabla_s\,\nu_i]_j\,\nu_k\,\partial_{s_j}\,\chi_l \\ &= \nu_i\,\nu_l\,\alpha^G(\mathfrak{c})\,[(\nabla_s\,\vec\nu)\,\nabla_s\,\nu_i]_j\,\partial_{s_j}\,\chi_l = \nu_i\,\nu_l\,\alpha^G(\mathfrak{c})\,(\partial_{s_k}\,\nu_j)\,(\partial_{s_k}\,\nu_i)\,\partial_{s_j}\,\chi_l = 0\,, \end{aligned}$$

since $\nu_i\,\partial_{s_k}\,\nu_i = \frac{1}{2}\,\partial_{s_k}\,|\vec\nu|^2 = 0$.

Returning to (A.27), we have on noting (A.20), (3.11), (A.1) and (A.2) that

$$\begin{aligned}
T_{12} &= -\sum_{i=1}^{d} \left\langle \nu_i\,\nabla_s\,\vec z_i, (\nabla_s\,\vec\chi)^T \right\rangle_{\Gamma(t)} = \left\langle \nu_i\,\partial_{s_l}\,(\alpha^G(\mathfrak{c})\,\partial_{s_k}\,\nu_i), \partial_{s_k}\,\chi_l \right\rangle_{\Gamma(t)} \\
&= \left\langle \alpha^G(\mathfrak{c})\,\nu_i\,\partial_{s_l}\,\partial_{s_k}\,\nu_i, \partial_{s_k}\,\chi_l \right\rangle_{\Gamma(t)} = -\left\langle \alpha^G(\mathfrak{c})\,(\partial_{s_l}\,\nu_i)\,\partial_{s_k}\,\nu_i, \partial_{s_k}\,\chi_l \right\rangle_{\Gamma(t)} \\
&= \left\langle \alpha^G(\mathfrak{c})\,[(\partial_{s_k}\,\partial_{s_l}\,\nu_i)\,\partial_{s_k}\,\nu_i + (\partial_{s_l}\,\nu_i)\,\partial_{s_k}\,\partial_{s_k}\,\nu_i] + (\partial_{s_k}\,\alpha^G(\mathfrak{c}))\,(\partial_{s_l}\,\nu_i)\,\partial_{s_k}\,\nu_i, \chi_l \right\rangle_{\Gamma(t)} \\
&= \left\langle \alpha^G(\mathfrak{c})\,\partial_{s_k}\,\nu_i\,[\partial_{s_l}\,\partial_{s_k}\,\nu_i - [(\nabla_s\,\vec\nu)\,\nabla_s\,\nu_i]_k\,\nu_l]\,, \chi_l \right\rangle_{\Gamma(t)} - \left\langle \alpha^G(\mathfrak{c})\,(\partial_{s_l}\,\nu_i)\,\partial_{s_i}\,\varkappa, \chi_l \right\rangle_{\Gamma(t)} \\
&\qquad + \left\langle (\partial_{s_k}\,\alpha^G(\mathfrak{c}))\,(\partial_{s_l}\,\nu_i)\,\partial_{s_k}\,\nu_i, \chi_l \right\rangle_{\Gamma(t)} \\
&= \tfrac{1}{2}\left\langle \alpha^G(\mathfrak{c})\,\nabla_s\,|\nabla_s\,\vec\nu|^2, \vec\chi \right\rangle_{\Gamma(t)} - \left\langle \alpha^G(\mathfrak{c})\,(\nabla_s\,\vec\nu)^2, \nabla_s\,\vec\nu\,(\vec\chi\,.\,\vec\nu) \right\rangle_{\Gamma(t)} \\
&\qquad - \left\langle \alpha^G(\mathfrak{c})\,(\nabla_s\,\vec\nu)\,\nabla_s\,\varkappa, \vec\chi \right\rangle_{\Gamma(t)} + \left\langle (\nabla_s\,\vec\nu)^2\,\nabla_s\,\alpha^G(\mathfrak{c}), \vec\chi \right\rangle_{\Gamma(t)}\,.
\end{aligned} \tag{A.29}$$

The remaining term from (A.19) can be rewritten, on noting (A.20), (3.11), (A.2) and (2.13), as

$$\begin{aligned}
T_{14} &= -\sum_{i=1}^{d} \left\langle (\partial_{s_i}\,\vec z_i) \otimes \vec\nu, (\nabla_s\,\vec\chi)^T \right\rangle_{\Gamma(t)} = \left\langle \partial_{s_i}\,(\alpha^G(\mathfrak{c})\,\partial_{s_i}\,\nu_k), \nu_l\,\partial_{s_k}\,\chi_l \right\rangle_{\Gamma(t)} \\
&= \left\langle (\partial_{s_i}\,\alpha^G(\mathfrak{c}))\,\partial_{s_i}\,\nu_k + \alpha^G(\mathfrak{c})\,\partial_{s_i}\,\partial_{s_i}\,\nu_k, \nu_l\,\partial_{s_k}\,\chi_l \right\rangle_{\Gamma(t)} \\
&= \left\langle (\partial_{s_i}\,\alpha^G(\mathfrak{c}))\,\partial_{s_i}\,\nu_k - \alpha^G(\mathfrak{c})\,\partial_{s_k}\,\varkappa, \nu_l\,\partial_{s_k}\,\chi_l \right\rangle_{\Gamma(t)} \\
&= -\left\langle (\partial_{s_k}\,[(\partial_{s_i}\,\alpha^G(\mathfrak{c}))\,\partial_{s_i}\,\nu_k])\,\nu_l + (\partial_{s_i}\,\alpha^G(\mathfrak{c}))\,(\partial_{s_i}\,\nu_k)\,\partial_{s_k}\,\nu_l, \chi_l \right\rangle_{\Gamma(t)} - \left\langle (\partial_{s_i}\,\alpha^G(\mathfrak{c}))\,(\partial_{s_k}\,\nu_i)\,\varkappa\,\nu_k, \chi_l\,\nu_l \right\rangle_{\Gamma(t)} \\
&\qquad + \left\langle (\partial_{s_k}\,[\alpha^G(\mathfrak{c})\,\partial_{s_k}\,\varkappa])\,\nu_l + \alpha^G(\mathfrak{c})\,(\partial_{s_k}\,\varkappa)\,\partial_{s_k}\,\nu_l, \chi_l \right\rangle_{\Gamma(t)} \\
&= -\left\langle \nabla_s\,.\,[(\nabla_s\,\vec\nu)\,\nabla_s\,\alpha^G(\mathfrak{c})], \vec\chi\,.\,\vec\nu \right\rangle_{\Gamma(t)} - \left\langle (\nabla_s\,\vec\nu)^2\,\nabla_s\,\alpha^G(\mathfrak{c}), \vec\chi \right\rangle_{\Gamma(t)} \\
&\qquad + \left\langle \nabla_s\,.\,(\alpha^G(\mathfrak{c})\,\nabla_s\,\varkappa), \vec\chi\,.\,\vec\nu \right\rangle_{\Gamma(t)} + \left\langle \alpha^G(\mathfrak{c})\,(\nabla_s\,\vec\nu)\,\nabla_s\,\varkappa, \vec\chi \right\rangle_{\Gamma(t)}\,.
\end{aligned} \tag{A.30}$$

Hence we have from (A.29) and (A.30), on noting (A.14) for $d = 3$ and on recalling that $\alpha^G = 0$ for $d = 2$, that

$$\begin{aligned}
\sum_{\ell\in\{12,14\}} T_\ell &= \tfrac{1}{2}\left\langle \alpha^G(\mathfrak{c})\,\nabla_s\,|\nabla_s\,\vec\nu|^2, \vec\chi \right\rangle_{\Gamma(t)} + \left\langle \alpha^G(\mathfrak{c})\,[|\nabla_s\,\vec\nu|^2 - \mathcal{K}]\,\varkappa, \vec\chi\,.\,\vec\nu \right\rangle_{\Gamma(t)} \\
&\qquad - \left\langle \nabla_s\,.\,[(\nabla_s\,\vec\nu)\,\nabla_s\,\alpha^G(\mathfrak{c})], \vec\chi\,.\,\vec\nu \right\rangle_{\Gamma(t)} + \left\langle \nabla_s\,.\,[\alpha^G(\mathfrak{c})\,\nabla_s\,\varkappa], \vec\chi\,.\,\vec\nu \right\rangle_{\Gamma(t)}\,.
\end{aligned} \tag{A.31}$$

Combining (A.31) with (A.25) yields, on recalling (3.9), that

$$\begin{aligned}
\sum_{\ell\in\{1,\ldots 4,8,12,14\}} T_\ell &= -\left\langle \Delta_s\,[\alpha(\mathfrak{c})\,(\varkappa - \overline{\varkappa}(\mathfrak{c}))] + \alpha(\mathfrak{c})\,(\varkappa - \overline{\varkappa}(\mathfrak{c}))\,|\nabla_s\vec\nu|^2 - b(\varkappa,\mathfrak{c})\,\varkappa, \vec\chi\,.\,\vec\nu \right\rangle_{\Gamma(t)} \\
&\qquad - \left\langle \nabla_s\,.\,([\varkappa\,\underline{\underline{\mathrm{Id}}} + \nabla_s\,\vec\nu]\,\nabla_s\,\alpha^G(\mathfrak{c})), \vec\chi\,.\,\vec\nu \right\rangle_{\Gamma(t)} + \left\langle [b_{,\mathfrak{c}}(\varkappa,\mathfrak{c}) + (\alpha^G)'(\mathfrak{c})\,\mathcal{K}]\,\nabla_s\,\mathfrak{c}, \vec\chi \right\rangle_{\Gamma(t)}\,.
\end{aligned} \tag{A.32}$$

Summing (A.32) and (A.26) yields the strong form (2.9).

Finally, (3.31b), (2.10), (A.20), (2.15) and (3.11) immediately yield (1.5b).

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