Finite Element Discretization Error Analysis of a General Interfacial Stress Functional

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FINITE ELEMENT DISCRETIZATION ERROR ANALYSIS OF A GENERAL INTERFACIAL STRESS FUNCTIONAL

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Abstract. A stationary, incompressible two-phase flow problem with a variable interfacial stress tensor $\boldsymbol{\sigma}^\Gamma(x)$ is considered. Variable interfacial tension is included as a special case. In the weak formulation, the interfacial stress gives rise to a functional which is supported on the interface Γ. A new finite element discretization of this functional is presented and analyzed. The discretization admits almost independent meshes for the approximation of the interface and the approximation of the flow variables. The main result is an $\mathcal{O}(h^{k+1/2})$-error-bound in a natural norm, if the discrete interface is an $\mathcal{O}(h^{k+1})$-approximation of Γ. The bound is shown to be sharp in a numerical experiment.

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1. Introduction. Two immiscible, incompressible, Newtonian fluids are contained in the subdomains Ω^1, Ω^2 of a bounded domain $\Omega \subset \mathbb{R}^n$, $n \geq 2$. At the common boundary $\Gamma = \bar{\Omega}^1 \cap \bar{\Omega}^2$, the interaction of the fluids gives rise to the interfacial tension force, which yields a force term in the Navier-Stokes equations. If Γ meets $\partial\Omega$, additional force terms appear on $\Gamma \cap \partial\Omega$ which are not the subject of this paper. Therefore, it is assumed that the closure of Ω^1 is contained in Ω which implies that $\Gamma = \partial\Omega^1$ does not intersect $\partial\Omega$. A standard model is that the interfacial tension is a contact force which is described by an interfacial stress tensor $\boldsymbol{\sigma}^\Gamma$, [SSO07, Isr92]. The force exerted on a small patch $\gamma \subset \Gamma$ is

$$-\int_{\partial\gamma} \boldsymbol{\sigma}^\Gamma \boldsymbol{\nu}, \tag{1.1}$$

where $\boldsymbol{\nu}$ is the outer unit-length normal of $\partial\gamma$ which is tangential to Γ. A special feature of this term is that it is localized at the interface Γ, which is an embedded manifold of codimension 1 in Ω. The interfacial stress tensor depends only on the tangential components of the vectors on which it acts. If $\mathbf{P}(\xi)$ denotes the orthogonal projector on the tangent space of Γ at $\xi \in \Gamma$, this means

$$\mathbf{P}^T \boldsymbol{\sigma}^\Gamma \mathbf{P} = \boldsymbol{\sigma}^\Gamma \quad \text{on } \Gamma. \tag{1.2}$$

The formulation (1.1) comprises many classical models for interfacial tension: If Γ is modeled as a 'clean interface', that is an interface without a surface-active, dissolved species (surfactant) in its vicinity, one obtains

$$\boldsymbol{\sigma}^\Gamma = \tau \mathbf{P}$$

with the constant interfacial tension coefficient $\tau > 0$ as stiffness-parameter, cf. [SSO07]. If the phases contain a surfactant, classical models of Langmuir, von Szyszkowski, and Frumkin, [LH92, Lan18, VS08, Fru25], express τ as a function of the surfactant concentration s close to or on Γ. This turns τ into a scalar function on Γ.

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In the presence of complex surfactants, the interface may exhibit viscous behavior. A standard model in this case is the Boussinesq-Scriven model, [DADL95, Scr60, Bou13],

$$\boldsymbol{\sigma}^\Gamma = \tau \mathbf{P} + (\lambda_\Gamma - \mu_\Gamma)\operatorname{div}_\Gamma \mathbf{u}\,\mathbf{P} + \mu_\Gamma \mathbf{D}_\Gamma(\mathbf{u}), \quad \mathbf{D}_\Gamma(\mathbf{u}) = \mathbf{P}(D_\Gamma \mathbf{u} + (D_\Gamma \mathbf{u})^T)\mathbf{P},$$

where the constants $\lambda_\Gamma > \mu_\Gamma > 0$ are the interfacial dilatational viscosity and the interfacial shear viscosity; D_Γ is the tangential gradient, $\operatorname{div}_\Gamma$ is the interfacial divergence, and $\mathbf{D}_\Gamma(\mathbf{u})$ is the interfacial deformation tensor which depends on the velocity field $\mathbf{u}$ on Γ.

The weak formulation of (1.1) discussed in this paper is

$$f(\mathbf{v}) = -\int_\Gamma (\operatorname{div}_\Gamma \boldsymbol{\sigma}^\Gamma)^T \mathbf{v} \quad \text{for all } \mathbf{v} \in H^1(\Omega)^n,$$

which is obtained from (1.1) via Gauß' theorem. Let $(\Omega_h^1)_{h>0}$ be a family of approximations of Ω^1. The discrete interfaces Γ_h are defined as the boundaries $\Gamma_h := \partial\Omega_h^1$. The analysis uses two main quantitative assumptions on Γ_h. Let d be the signed distance to Γ which is negative in Ω^1, and let d_h be the signed distance to Γ_h which is negative in Ω_h^1. The first assumption is that d_h approximates d with order $\mathcal{O}(h^{k+1})$ for some integer $k \geq 1$ and that the gradient Dd_h approximates Dd with order $\mathcal{O}(h^k)$. A family $(\boldsymbol{\sigma}_h^\Gamma)_{h>0}$ of approximations to $\boldsymbol{\sigma}^\Gamma$ is required, in which the tensor $\boldsymbol{\sigma}_h^\Gamma$ is defined on Γ_h. The second assumption is that $\boldsymbol{\sigma}_h^\Gamma$ is an $\mathcal{O}(h^{k+1})$-approximation on Γ_h of a suitable extension of $\boldsymbol{\sigma}^\Gamma$.

Furthermore, improved approximations $\tilde{\mathbf{n}}$ of $\mathbf{n} := Dd$ are required, which are assumed to be a family of $\mathcal{O}(h^{k+1})$-approximations. All of the previous requirements are reasonable; some concrete settings in which they hold are given in Remark 6.1.

The analysis imposes almost no requirements on the finite element discretization of the Navier-Stokes equations. A shape regular family $(\mathcal{T}_H)_{H>0}$ of Ω is assumed with a mesh-width H which may be different from h. A weak requirement is that H should not be arbitrarily smaller than h in the vicinity of Γ_h. No further conditions are necessary. In particular, $\mathcal{T}_H$ does not have to be aligned to Γ_h, and the discrete interfaces Γ_h may be defined independently of $\mathcal{T}_H$. For the family of velocity spaces $(\mathbf{V}_H)_{H>0}$, only a standard inverse inequality is required.

Let $\tilde{\mathbf{Q}} = \mathbf{I} - \frac{1}{\tilde{\alpha}}\mathbf{n}_h\tilde{\mathbf{n}}^T$, $\tilde{\alpha} = \mathbf{n}_h^T\tilde{\mathbf{n}}$, $\mathbf{n}_h = Dd_h$, which is an oblique projector arising in the analysis. The discrete interfacial tension functional is defined as

$$f_h(\mathbf{v}) = \int_{\Gamma_h} \tilde{\mathbf{Q}}^T \boldsymbol{\sigma}_h^\Gamma : D\mathbf{v} \quad \text{for all } \mathbf{v} \in \mathbf{V}_H,$$

where $\mathbf{A} : \mathbf{B} = \operatorname{tr}(\mathbf{A}^T\mathbf{B})$ is the Frobenius-inner-product of matrices. The main result of this paper, Theorem 6.10, is the bound

$$\sup_{\mathbf{v}\in\mathbf{V}_H} \frac{f(\mathbf{v}) - f_h(\mathbf{v})}{\|\mathbf{v}\|_{H^1(\Omega)^n}} \leq c h^{k+\frac{1}{2}}$$

for f_h, which holds under the previously stated assumptions and some minor technical conditions. A numerical experiment for $k = 1$ confirms that the bound is sharp. A minor result is Theorem 6.9, an estimate of the form

$$\|D_{\Gamma,h}\mathbf{v}\|_{\Gamma_h\cap T} \leq c H_T^{-\frac{1}{2}} \|D\mathbf{v}\|_{L^2(T)} \quad \text{for all } \mathbf{v} \in \mathbf{V}_H, T \in \mathcal{T}_H, H > 0,$$

which generalizes [GR07, Thm. 4.6] to the interfaces considered here.

The literature on numerical methods for surfactants and variable interfacial tension mainly contains numerical studies of discretization errors, [JL04, Poz04, XLLZ06, MT08, RZ13]. The only other paper known to the author which contains rigorous error bounds for an interfacial tension functional is [GR07], where constant interfacial tension is assumed, and the error analysis yields an $\mathcal{O}(h)$-bound for the discretization error. This discretization is compared to f_h in a numerical experiment in Section 8 showing that it is an $\mathcal{O}(h^{3/2})$-approximation of f_h for constant interfacial tension.

The paper is organized as follows: In Section 2, basic concepts from differential geometry are introduced which are needed to state the weak formulation of f. Section 3 contains the weak formulation of the two-phase Navier-Stokes problem and of the interfacial tension. The discrete Navier-Stokes problem is stated in Section 3.2. The discretization of f is performed in Section 4. Section 5 contains some prerequisites for the analysis of the discretization error in Section 6. Some consequences of Theorem 6.10 for the implementation of f_h are discussed in Section 7. Two numerical experiments and their results are discussed in Section 8.

2. Geometry of the interfacial region. Let $\Gamma = \partial\Omega^1 \subset \Omega^\circ$ be a compact hypersurface which is at least of class C^2. This means that its signed distance function d is in $C^2(U)$ for some open neighborhood U of Γ. Reducing U if necessary, this implies that $U \subset \Omega$ is a tubular neighborhood of Γ which encompasses the following properties, cf. [Lee12]: The signed distance function d of Γ is in $C^2(U)$. Its gradient $Dd =: \mathbf{n}$ is a map $U \to S^n$ which agrees with the normal field of Γ when restricted to the latter. Finally, there is a retraction map $p\colon U \to \Gamma$ with the property

$$x = p(x) + d(x)\mathbf{n}(x) \quad \text{for all } x \in U,$$

and this decomposition is unique. Due to the compactness of Γ, there is a number $r_0 > 0$ such that $U_{r_0} := \{x \in \Omega \mid |d(x)| \le r_0\} \subset U$. We simply set $U := U_{r_0}$. Let $B(x, r_0)$ be an open ball with center x and radius r_0. There holds

$$B(x, r_0) \subset U \quad \text{for all } x \in \Gamma \tag{2.1}$$

because d is Lipschitz-continuous with Lipschitz-constant 1, and for any $y \in B(x, r_0)$ there holds $|d(y)| = |d(y) - d(x)| \le |x - y| \le r_0$. The notation $|\cdot|$ is used for the absolute value of scalars, the Euclidean norm of vectors, and the spectral norm of matrices.

The orthogonal projector on the tangent space of Γ can be written as

$$\mathbf{P} = \mathbf{I} - \mathbf{n}\mathbf{n}^T.$$

The symmetric matrix $\mathbf{H}(x) = D^2 d(x)$ is the Hessian of d. Differentiating $|\mathbf{n}| \equiv 1$, yields $\mathbf{H}\mathbf{n} = 0$ on U. For $\mathbf{P}$, this implies $\mathbf{HP} = \mathbf{H} = \mathbf{PH}$ on U. Furthermore, $\mathbf{n}^T D\mathbf{n} = \mathbf{n}^T\mathbf{H} = 0$ implies that the normal field $\mathbf{n}$ is constant along normals. An elementary computation yields

$$Dp = \mathbf{P} - d\mathbf{H} = (\mathbf{I} - d\mathbf{H})\mathbf{P} \quad \text{on } U.$$

A useful identity for $\mathbf{H}$ follows from differentiating $\mathbf{n}(x) = \mathbf{n}(p(x))$,

$$\mathbf{H}(x) = \mathbf{H}(\xi)\big(\mathbf{I} + d(x)\mathbf{H}(\xi)\big)^{-1} \quad \text{with } \xi = p(x) \quad \text{for all } x \in U. \tag{2.2}$$

The mean curvature of Γ is $\kappa = \operatorname{tr}\mathbf{H}$; the maximal curvature on Γ is denoted by

$$\kappa_\Gamma = \max\{|\mathbf{H}(\xi)| \mid \xi \in \Gamma\},$$

and the eigenvalues of $\mathbf{H}(x)$ are denoted $\kappa_i(x)$, $i \in \{1, \dots, n\}$, where $\kappa_n(x) = 0$. Possibly reducing r_0 to $r_0 \leq \frac{1}{2}\kappa_\Gamma^{-1}$, equation (2.2) yields

$$|\mathbf{H}| \leq 2\kappa_\Gamma \quad \text{on } U.$$

A fundamental connection between the tangential gradient D_Γ, which is intrinsic to Γ, and the gradient D on $\mathbb{R}^n$ is

$$D_\Gamma = \mathbf{P}D. \tag{2.3}$$

That is, the interfacial gradient is the orthogonal projection of the gradient in $\mathbb{R}^n$ to the tangent space. To apply (2.3), one uses an arbitrary (sufficiently smooth) extension of a function on Γ to compute the right-hand side. The restriction to Γ is the intrinsic quantity on the left-hand side. The interfacial divergence is defined as $\operatorname{div}_\Gamma \mathbf{v} = D_\Gamma \cdot \mathbf{v} = \mathbf{P} : D\mathbf{v}$ for vector valued functions, where the gradient $D\mathbf{v}$ is the transpose of the Jacobian matrix. The interfacial divergence for matrix-valued functions is $\operatorname{div}_\Gamma \mathbf{A} = (\operatorname{div}_\Gamma A^1, \dots, \operatorname{div}_\Gamma A^n)^T$ with the columns A^i of $\mathbf{A}$.

The pullback of a function on Γ along the fibers of p is defined and denoted as

$$f^e(x) := f(p(x)) \quad \text{for all } x \in U.$$

It is constant on the fibers of p. The name pullback comes from the fact that the domain of f is 'pulled back' from the image of p to its domain. The derivative of a pullback is given by the chain rule of differentiation, here

$$Df^e(x) = (\mathbf{I} - d(x)\mathbf{H}(x))\mathbf{P}(x)(Df)^e(x) \quad \text{for all } x \in U.$$

The pull-back of vector-valued and matrix-valued functions is given by the same formula.

The following elementary fact from differential geometry is required: There exists a positive constant c_m such that for any n-ball $B \subset U$ with radius r and for any set $S = \{x \in U \mid |d(x)| \leq s\} \subseteq U$ there hold

$$\operatorname{meas}(B \cap \Gamma) \leq c_m r^{n-1}, \quad \operatorname{meas}(B \cap S) \leq c_m r^{n-1} s. \tag{2.4}$$

3. The Navier-Stokes equations with interfacial tension. The incompressible Navier-Stokes equations relate the fluid velocity $\mathbf{u}\colon \Omega \to \mathbb{R}^n$ and the fluid pressure $p\colon \Omega \to \mathbb{R}$ to the forces acting on the fluid. Let μ be the viscosity and

$$\boldsymbol{\sigma} = \mu\mathbf{D}(\mathbf{u}) - p\mathbf{I}, \quad \mathbf{D}(\mathbf{u}) = \frac{1}{2}(D\mathbf{u} + (D\mathbf{u})^T) \tag{3.1}$$

be the stress and the deformation tensor. The viscosity is a assumed to be a piecewise constant function with a possible discontinuity at Γ. Let $\gamma \subset \Gamma$.

THEOREM 3.1 (Gauß). *For any vector-valued function $\mathbf{v} \in C^1(\gamma, \mathbb{R}^n)$ which is everywhere tangential to γ there holds*

$$\int_\gamma \operatorname{div}_\Gamma \mathbf{v} = \int_{\partial\gamma} \boldsymbol{\nu}^T \mathbf{v},$$

where $\boldsymbol{\nu}$ is the unit-length normal on $\partial\gamma$ which is also tangential to Γ.

Applying Theorem 3.1 to (1.1) on increasingly smaller patches γ yields the strong form of the interfacial tension,

$$f = -\operatorname{div}_\Gamma \boldsymbol{\sigma}^\Gamma \quad \text{on } \Gamma. \tag{3.2}$$

As an example, in the case of variable interfacial tension $\tau(x)$, (3.2) yields $-\operatorname{div}_\Gamma \boldsymbol{\sigma}^\Gamma = \tau\kappa\mathbf{n} - D_\Gamma\tau$. Throughout this paper, it is assumed that

$$\left\|\boldsymbol{\sigma}^\Gamma\right\|_{L^2(\Gamma)}^2 + \left\|\operatorname{div}_\Gamma \boldsymbol{\sigma}^\Gamma\right\|_{L^2(\Gamma)}^2 =: \left\|\boldsymbol{\sigma}^\Gamma\right\|_{div}^2 \tag{3.3}$$

is a finite constant. The standard way to include the interfacial tension into the Navier-Stokes equations is to let it balance the jump of the normal stress between Ω^1 and Ω^2,

$$[\![\boldsymbol{\sigma}\mathbf{n}]\!]_\Gamma = -\operatorname{div}_\Gamma \boldsymbol{\sigma}^\Gamma. \tag{3.4}$$

Under the assumption that $\mathbf{u}$ is continuous at Γ, the Navier-Stokes equations considered in this paper can be written formally as

$$\begin{aligned} \rho\mathbf{u}^T D\mathbf{u} - \operatorname{div}(\mu\mathbf{D}(\mathbf{u})) - Dp &= -\delta_\Gamma \operatorname{div}_\Gamma \boldsymbol{\sigma}^\Gamma && \text{on } \Omega, \\ \operatorname{div}\mathbf{u} &= 0 && \text{on } \Omega. \end{aligned} \tag{3.5}$$

Here, ρ is the piecewise constant density of the fluids and δ_Γ is the Dirac-δ-distribution of Γ. We refer to [Pes77, CHMO96] and the references in the latter for details. The time-dependence and additional force terms are omitted to simplify the presentation; they have no effect on the subsequent error analysis. Also for simplicity, homogeneous Dirichlet boundary conditions are assumed. A rigorous weak formulation formulation is obtained in the spaces

$$\mathbf{V} = H_0^1(\Omega)^n, \quad Q = \left\{ q \in L^2(\Omega) \;\middle|\; \int_\Omega q = 0 \right\}, \tag{3.6}$$

cf. [GR86]. The Sobolev-norm on $\mathbf{V}$ is denoted as $\|\cdot\|_{\mathbf{V}}$; the $L^2(\Omega)$-inner product is denoted by $(\cdot,\cdot)$. For matrix valued functions, one uses the inner product $(\mathbf{A}(x), \mathbf{B}(x)) = \int_\Omega \mathbf{A}(x) : \mathbf{B}(x)\,dx$. A standard weak formulation of (3.5) is

$$\begin{aligned} \left(\rho\mathbf{u}^T D\mathbf{u}, \mathbf{v}\right) + (\mu\mathbf{D}(\mathbf{u}), \mathbf{D}(\mathbf{v})) + (p, \operatorname{div}\mathbf{v}) &= f(\mathbf{v}) && \text{for all } \mathbf{v} \in \mathbf{V}, \\ (\operatorname{div}\mathbf{u}, q) &= 0 && \text{for all } q \in Q, \end{aligned} \tag{3.7}$$

with the interfacial tension functional

$$f(\mathbf{v}) = -\int_\Gamma (\operatorname{div}_\Gamma \boldsymbol{\sigma}^\Gamma)^T \mathbf{v}\,dx. \tag{3.8}$$

If Γ and τ are sufficiently smooth, there holds a standard trace theorem for $\mathbf{V}$, which implies

$$|f(\mathbf{v})| \le \left\|\operatorname{div}_\Gamma \boldsymbol{\sigma}^\Gamma\right\|_\Gamma \|\mathbf{v}\|_{L^2(\Gamma)} \le c(\Gamma) \left\|\boldsymbol{\sigma}^\Gamma\right\|_{div} \|\mathbf{v}\|_{\mathbf{V}} \quad \text{for all } \mathbf{v} \in \mathbf{V}. \tag{3.9}$$

Hence, f is a bounded, linear functional on $\mathbf{V}$, which makes (3.7) a well-posed problem, cf. [GR86].

3.1. Weak formulation of the interfacial tension. Let $\mathbf{v} \in C^1(U, \mathbb{R}^n)$ be an arbitrary function. By (1.2), $\boldsymbol{\sigma}^\Gamma\mathbf{v}$ is tangential to Γ everywhere, and, using (2.3), one computes $\operatorname{div}_\Gamma(\boldsymbol{\sigma}^\Gamma\mathbf{v}) = (\operatorname{div}_\Gamma \boldsymbol{\sigma}^\Gamma)^T\mathbf{v} + \boldsymbol{\sigma}^\Gamma : D\mathbf{v}$.

Gauß' theorem 3.1, equation (3.8), and $\partial\Gamma = \emptyset$ imply

$$0 = \int_\Gamma \operatorname{div}_\Gamma(\boldsymbol{\sigma}^\Gamma\mathbf{v}) = \int_\Gamma (\operatorname{div}_\Gamma(\boldsymbol{\sigma}^\Gamma)^T\mathbf{v} + \int_\Gamma \boldsymbol{\sigma}^\Gamma : D\mathbf{v}. \tag{3.10}$$

Due to (1.2), $\boldsymbol{\sigma}^\Gamma : D\mathbf{v} = \boldsymbol{\sigma}^\Gamma : \mathbf{P}D\mathbf{v}$ which shows that the expression depends only on quantities intrinsic to Γ. It follows that

$$f(\mathbf{v}) = \int_\Gamma \boldsymbol{\sigma}^\Gamma : \mathbf{P}D\mathbf{v} \quad \text{for all } \mathbf{v} \in C^1(U, \mathbb{R}^n). \tag{3.11}$$

By a standard density argument, (3.11) holds on conforming finite element spaces with piecewise smooth functions. This is the starting point for the discretization of (1.1), respectively (3.8). The above use of Gauß' theorem is known as the Laplace-Beltrami technique in the literature, cf. [Bän01, Hys06] for the case $\boldsymbol{\sigma}^\Gamma = \tau\mathbf{P}$.

3.2. Discretization of the Navier-Stokes equation. The weak formulation (3.7) is discretized with finite elements. Let $\mathcal{T}_H$, $H > 0$ be a family of triangulations of Ω. It is *not* assumed that the $\mathcal{T}_H$ are aligned to Γ. Generally, the triangulations are refined in the vicinity of Γ. It is only required that the family $(\mathcal{T}_H)_{H>0}$ is shape-regular, that is, there exists a positive constant c_S such that

$$H_T \le c_S \rho_T \quad \text{for all } T \in \mathcal{T}_H, H > 0, \tag{3.12}$$

where H_T is the diameter of the simplex T and ρ_T is the diameter of the largest ball $B \subset T$. As the diameter of the simplexes in $\mathcal{T}_H$ usually varies strongly across Ω, one avoids statements about the global mesh-width $\max\{H_T \mid T \in \mathcal{T}_H\}$. Instead, the mesh-width H is defined as a piecewise constant function on Ω,

$$H = H(x) = \max\{H_T \mid x \in T, T \in \mathcal{T}_H\}.$$

Let $\mathbf{V}_H \subset \mathbf{V}$, $H > 0$, be a family of $\mathbf{V}$-conforming finite element spaces for the velocity. Any such family is admissible that satisfies the standard inverse inequality

$$\|D\mathbf{v}\|_{L^\infty(T)} \le c_{inv} H_T^{-\frac{n}{2}} \|D\mathbf{v}\|_{L^2(T)} \quad \text{for all } \mathbf{v} \in \mathbf{V}_H, T \in \mathcal{T}_H \tag{3.13}$$

with a fixed positive constant c_{inv}. This estimate holds for all finite element spaces which are defined by smooth functions on the reference element, cf. [CL91]; for example, it holds for the velocity spaces of the Hood-Taylor-pairs. Let $Q_H \subset Q$, $H > 0$, be a family of finite element spaces on $(\mathcal{T}_H)_{H>0}$ for the pressure. The discrete Navier-Stokes problem is: Find $(\mathbf{u}_H, p_H) \in \mathbf{V}_H \times Q_H$ such that

$$\begin{aligned} \left(\rho \mathbf{u}_H^T D\mathbf{u}_H, \mathbf{v}\right) + (\mu \mathbf{D}(\mathbf{u}_H), \mathbf{D}(\mathbf{v})) + (p_H, \operatorname{div} \mathbf{v}) &= f(\mathbf{v}) \quad \text{for all } \mathbf{v} \in \mathbf{V}_H, \\ (\operatorname{div} \mathbf{u}_H, q) &= 0 \qquad\ \text{for all } q \in Q_H. \end{aligned} \tag{3.14}$$

There are well-known restrictions on the choice of $\mathbf{V}_H$ and $\mathbf{Q}_H$ to obtain a stable discrete problem; there are also well-known stabilization techniques for unstable pairs $\mathbf{V}_H$, $\mathbf{Q}_H$. For the purpose of analyzing the discretization error of f, these are not important, respectively, can be considered separately.

The evaluation of $f(\mathbf{v})$ in (3.14) is not feasible as the computationally unavailable interface Γ is needed. Thus, f is replaced by a family of approximations f_h, $h > 0$. The quality measure required in the finite element error analysis of (3.14) is the dual norm $\|f_h - f\|_{\mathbf{V}_H'}$. Writing out its definition, one obtains a typical term in a Strang-type lemma concerning a variational crime,

$$\|f_h - f\|_{\mathbf{V}_H'} = \sup_{\mathbf{v} \in \mathbf{V}_H} \frac{f(\mathbf{v}) - f_h(\mathbf{v})}{\|\mathbf{v}\|_{\mathbf{V}}}. \tag{3.15}$$

4. Discretization of the interfacial tension.

4.1. The discrete interfaces. Let $(\Omega_h^1)_{h>0}$ be a family of approximations of Ω^1 such that each Ω_h^1 is a Lipschitz domain, cf. [AF03]. Let $\Gamma_h = \partial\Omega_h^1$. A domain of integration in Γ_h is a relatively open, precompact subset set $A \subseteq \Gamma_h$ such that ∂A has $(n-1)$-dimensional measure 0 in Γ_h. A quasi-partition of Γ_h is a family $(\gamma_h^j)_{j\in J_h}$ of subsets $\gamma_h^j \subseteq \Gamma_h$, each J_h is a finite index set, such that

$$\gamma_h^j \cap \gamma_h^k = \emptyset \quad \text{for all } j,k \in J_h \text{ with } j \neq k \quad \text{and} \quad \Gamma_h = \cup \left\{ \overline{\gamma_h^j} \;\middle|\; j \in J_h \right\}.$$

It is assumed that each discrete interface Γ_h has a finite quasi-partition $(\gamma_h^j)_{j\in J_h}$ with the following properties: Each γ_h^j, $j \in J_h$, is a C^2-embedded submanifold of $\mathbb{R}^n$, and it is a domain of integration. The integral on Γ_h is

$$\int_{\Gamma_h} f = \sum_{j\in J_h} \int_{\gamma_h^j} f.$$

Let d_h be the signed distance function of Γ_h which is negative in Ω_h^1, and let $\mathbf{n}_h := Dd_h$. The almost everywhere defined unit-length vector-field $\mathbf{n}_h$ is the normal vector-field of Γ_h a. e. on Γ_h. The orthogonal projector on the tangential space of Γ_h is

$$\mathbf{P}_h = \mathbf{I} - \mathbf{n}_h\mathbf{n}_h^T.$$

It is assumed that Γ_h is the graph over Γ of a homeomorphism F which is piecewise smooth and which has the form $\xi \mapsto x_h = \xi + a(\xi)\mathbf{n}(\xi)$ for all $\xi \in \Gamma$. One can think of $a(\xi)$ as the altitude of x_h over Γ, equivalently, $a(\xi) = d(x_h)$. This assumption is reasonable, cf. Remark 6.1. Let

$$F(\xi) = \xi + a^e(\xi)\mathbf{n}(\xi) \quad \text{for all } \xi \in \Gamma.$$

The function F is actually defined a. e. on U, where it has the derivative

$$DF = \mathbf{I} + a^e\mathbf{H} + (\mathbf{I} - d\mathbf{H})\mathbf{P}(Da)^e\mathbf{n}^T \quad \text{a. e. on } U. \tag{4.1}$$

The pullback of a function f on Γ_h along F is the function

$$f^* = f \circ F \quad \text{on } \Gamma.$$

Let

$$\mathbf{Q} = \mathbf{I} - \frac{1}{\alpha}\mathbf{n}_h\mathbf{n}^T \quad \text{with } \alpha = \mathbf{n}_h^T\mathbf{n} \quad \text{a. e. on } U, \tag{4.2}$$

which is an oblique projector. By a direct computation, one finds

$$\mathbf{QP} = \mathbf{P}, \quad \mathbf{PQ} = \mathbf{Q}, \qquad \mathbf{P}_h\mathbf{Q} = \mathbf{P}_h, \quad \mathbf{QP}_h = \mathbf{Q}. \tag{4.3}$$

This characterizes the kernel and image of $\mathbf{Q}$ and $\mathbf{Q}^T$. There is a close connection between $\mathbf{P}Da$ and $\mathbf{n}_h$,

LEMMA 4.1. *There holds* $\mathbf{P}Da = -\frac{1}{\alpha^*}(\mathbf{I}+a\boldsymbol{H})\mathbf{P}\mathbf{n}_h^*$ *a. e. on* Γ *with* α *as in* (4.2).

Proof. At almost any point $\xi \in \Gamma$, the differential $(\mathbf{P}DF)^T$ maps the tangential space of Γ at ξ to the tangential space of Γ_h at $x_h = F(\xi)$. Thus, $\mathbf{n}_h(x_h)^T(\mathbf{P}DF(\xi))^T = 0$, which is inserted into (4.1) to obtain

$$(\mathbf{I} + a\mathbf{H})\mathbf{P}\mathbf{n}_h^* + \mathbf{P}Da\mathbf{n}^T\mathbf{n}_h^* = 0 \quad \text{a. e. on } \Gamma.$$

The conclusion follows from rearranging the terms of the equation. □

Lemma 4.1 and (4.1) yield

$$\mathbf{P}DF = (\mathbf{I} + a\mathbf{H})\mathbf{P}\mathbf{Q}^* \quad \text{a. e. on } \Gamma. \tag{4.4}$$

4.2. Transformation between Γ and Γ_h. Together with the chain rule, (4.4) leads to the transformation law for derivatives under the pullback with F, which plays a key role in the analysis below,

$$\mathbf{P}D(f\circ F)(x) = \mathbf{P}DF(x)Df(F(x)) \quad \text{a. e. on } \Gamma, \tag{4.5}$$

with DF as in (4.1). This formula looks, as if Df instead of $\mathbf{P}_h Df$ were required on the right-hand side, but because of (4.3) and (4.4), one has $\mathbf{P}DF = \mathbf{P}DF\mathbf{P}_{h*}$, so only the tangential derivatives are involved on either side.

Another basic formula required below is the transformation law induced by F for integrals on Γ and Γ_h,

$$\int_{\Gamma_h} f = \int_\Gamma \mu f^* \quad \text{with } \mu = \left(\alpha^* \prod_{i=1}^{n-1}(1+a\kappa_i)\right). \tag{4.6}$$

The factor μ is the $(n-1)$-dimensional Jacobian determinant of $(\mathbf{P}DF)^T$ for the surface measures which can be read off from (4.4) as $\mathbf{P}DF$ is the concatenation of linear maps. It can also be computed directly, cf. [Fed69].

The push forward of a function on Γ along F is the function $f\circ(F^{-1})$ on Γ_h, denoted as f_*. It is used below to shift F from the right-hand side to the left-hand side in (4.6), for example $\int_{\Gamma_h} f_*/\mu_* = \int_\Gamma f$.

4.3. The discrete interfacial tension functional. In (3.11), the integration over Γ is replaced by integration over Γ_h. Clearly, $\boldsymbol{\sigma}^\Gamma$ which is defined on Γ must be replaced by an approximation which is defined on Γ_h. This is $\boldsymbol{\sigma}_h^\Gamma$. Due to (4.5) and (4.4), the term $\mathbf{P}D\mathbf{v}$ in (3.11) transforms to $(\mathbf{I}+a\mathbf{H})\mathbf{P}\mathbf{Q}^*D\mathbf{v}$ which is approximated by $\mathbf{Q}D\mathbf{v}$ on Γ_h. This yields the tentative discretization

$$\int_{\Gamma_h} \mathbf{Q}^T\boldsymbol{\sigma}_h^\Gamma : D\mathbf{v} \quad \text{for all } \mathbf{v}\in\mathbf{V}_H$$

for f. By (4.3), there holds $\mathbf{Q} = \mathbf{Q}\mathbf{P}_h$, which shows that $\mathbf{Q}D\mathbf{v}$ is defined using only tangential derivatives with respect to Γ_h. As $\mathbf{Q}$ involves the computationally unavailable normal field $\mathbf{n}$, an approximation of $\mathbf{n}$ is required. The analysis makes clear that the $\mathcal{O}(h^k)$-approximation $\mathbf{n}_h$ is not sufficient, cf. Lemma 6.6 below. An $\mathcal{O}(h^{k+1})$-approximation $\tilde{\mathbf{n}}$ of $\mathbf{n}$ is required, which is used to define the oblique projector

$$\tilde{\mathbf{Q}} = \mathbf{I} - \frac{1}{\tilde\alpha}\mathbf{n}_h\tilde{\mathbf{n}}^T, \quad \tilde\alpha = \mathbf{n}_h^T\tilde{\mathbf{n}} \quad a.e. \text{ on } U.$$

The discretization of f in (3.11) becomes

$$f_h(\mathbf{v}) = \int_{\Gamma_h} \tilde{\mathbf{Q}}^T\boldsymbol{\sigma}_h^\Gamma : D\mathbf{v} \quad \text{for all } \mathbf{v}\in\mathbf{V}_H. \tag{4.7}$$

5. Preliminaries for the error analysis. The spectral norm $|\mathbf{Q}|$ is required in the analysis. It is computed with the help of the following elementary lemma which is proved in [Szy06].

LEMMA 5.1. *For any projector $\mathbf{Q}\notin\{\mathbf{I},\mathbf{0}\}$ there holds $|\mathbf{Q}| = |\mathbf{I}-\mathbf{Q}|$.*

A useful property of rank-1 matrices is

$$|\mathbf{u}\mathbf{v}^T| = |\mathbf{u}|\,|\mathbf{v}| \quad \text{for all } \mathbf{u},\mathbf{v}\in\mathbb{R}^n. \tag{5.1}$$

From Lemma 5.1 and (5.1), one obtains

$$|\mathbf{Q}| = \frac{1}{|\alpha|}\left|\mathbf{n}_h\mathbf{n}^T\right| = \frac{1}{|\alpha|}. \tag{5.2}$$

The bound $|\mathbf{A}|_F \le \sqrt{n}|\mathbf{A}|$ is used below. For example, in connection with the Cauchy-Schwarz inequality for the Frobenius inner product, one has

$$|\mathbf{A} : \mathbf{B}| \le n\,|\mathbf{A}|\,|\mathbf{B}| \quad \text{for all } \mathbf{A},\mathbf{B} \in \mathbb{R}^{n\times n}. \tag{5.3}$$

The notation $(f,g)_\Gamma$ is used for the $L^2(\Gamma)$-inner-product.

6. Approximation error analysis. The error analysis is based on the assumptions on the approximate interface Γ_h, the improved approximation $\tilde{\mathbf{n}}$ of $\mathbf{n}$, and the approximation $\boldsymbol{\sigma}_h^\Gamma$ of the the interfacial stress tensor $\boldsymbol{\sigma}^\Gamma$ which are collected here in one place. The approximate interface Γ_h is assumed to satisfy the following conditions,

$$|d| \le c_d h^{k+1} \quad \text{a. e. on } \Gamma_h, \tag{6.1}$$

$$|\mathbf{n}_h - \mathbf{n}| \le c_n h^k \quad \text{a. e. on } \Gamma_h, \tag{6.2}$$

$$h \le c_{\mathcal{T}} \min\{H_T \mid T \in \mathcal{T}\} \tag{6.3}$$

with some positive integer k. The inequalities quantify the asymptotic approximation properties of Γ_h with respect to Γ. Inequality (6.3) is the only combined constraint on the mesh-width of the finite element space $\mathbf{V}_H$ and the mesh width of the interface approximations Γ_h. The improved approximation of $\mathbf{n}$ is assumed to satisfy

$$|\mathbf{n} - \tilde{\mathbf{n}}| \le c_{\tilde{n}} h^{k+1} \quad \text{a. e. on } \Gamma_h. \tag{6.4}$$

The largest mesh width of Γ_h to which the subsequent analysis can be applied is denoted as h_0. The mesh-width is required to satisfy

$$0 < h \le h_0, \quad \max\left\{2\kappa_\Gamma c_d h_0^{k+1}, c_n h_0^k, 4c_{\tilde{n}} h_0^{k+1}\right\} \le 1. \tag{6.5}$$

Finally, an assumption on the interfacial stress tensor is required,

$$\left\|\boldsymbol{\sigma}_h^\Gamma - \boldsymbol{\sigma}_*^\Gamma\right\|_{\Gamma_h} \le c_\sigma h^{k+1}. \tag{6.6}$$

The bound (6.6) relates the value of $\boldsymbol{\sigma}_h^\Gamma$ at $x_h \in \Gamma_h$ to the value of $\boldsymbol{\sigma}^\Gamma$ at $p(x_h) \in \Gamma$. In the remainder of this section, (6.1) – (6.6) are tacitly assumed to hold.

REMARK 6.1. *All of the previous assumptions are reasonable. Let Γ be the zero level of the level set function φ which satisfies $\varphi \in C^{k+1}(U)$ and $\|D\varphi\|_{L^\infty(U)} > c > 0$ on some neighborhood U of Γ. Let I_h be the interpolation operators of a family of continuous, piecewise polynomial finite-element spaces of degree k on a shape-regular family of triangulations $(\mathcal{T}_h)_{h>0}$. The discrete family of interfaces Γ_h is given by the zero levels of the functions $I_h\varphi$. The covering $(\gamma_h^j)_{j\in J_h}$ is given by the intersections $\Gamma_h \cap T$ with the simplices of $\mathcal{T}_h$. In [EG13], it is shown that there is a piecewise smooth homeomorphism $\Gamma \to \Gamma_h$ of the form $\xi \mapsto \xi + a(\xi)\mathbf{n}(\xi)$. From [Reu13], it follows that* (6.1) *and* (6.2) *hold.*

The bound (6.6) *is derived in [ORG09] for $k = 1$ for the case in which $\boldsymbol{\sigma}^\Gamma = \tau\mathbf{P}$ is determined by a surface PDE on Γ which is discretized with an Eulerian finite element method. Some weak assumptions restrict the maximal admissible mesh width depending on the curvature of Γ.*

The improved normal field $\tilde{\mathbf{n}}$ *can be obtained from an approximation* $\tilde{d}$ *of* d *satisfying* (6.1) *and* (6.2) *with* k *replaced by* $k+1$*. An example with a piecewise quadratic level set function and its linear interpolant can be found in [GR07].*

An auxiliary interfacial tension functional $\tilde{f}$ is introduced. The transformation rules (4.6) and (4.5) yield

$$\tilde{f}(\mathbf{v}) := \big(\boldsymbol{\sigma}^\Gamma, \mathbf{P}D(\mathbf{v}\circ F)\big)_\Gamma = \big(\mu_*^{-1}\boldsymbol{\sigma}_*^\Gamma, \mathbf{P}DF_*D\mathbf{v}\big)_{\Gamma_h}. \tag{6.7}$$

The difference between the continuous and discrete interfacial tension in (3.11) and (4.7) is split into two terms,

$$\begin{aligned} f(\mathbf{v}) - f_h(\mathbf{v}) &= (f-\tilde{f})(\mathbf{v}) - (\tilde{f} - f_h)(\mathbf{v}) \\ &= \big(\boldsymbol{\sigma}^\Gamma, \mathbf{P}D(\mathbf{v} - \mathbf{v}\circ F)\big)_\Gamma + \big(\mu_*^{-1}(\mathbf{P}DF_*)^T\boldsymbol{\sigma}_*^\Gamma - \tilde{\mathbf{Q}}^T\boldsymbol{\sigma}_h^\Gamma, D\mathbf{v}\big)_{\Gamma_h} \\ &=: I + II. \end{aligned} \tag{6.8}$$

The analysis rests on the estimates of these terms in Lemma 6.2 and Lemma 6.8.

Lemma 6.2 (I). *With the positive constant* $c_I = 2^{n-1}c_d c_{inv} c_m^{1/2}$*, there holds*

$$\big|f(\mathbf{v}) - \tilde{f}(\mathbf{v})\big| \le c_I \left\|\operatorname{div}_\Gamma \boldsymbol{\sigma}^\Gamma\right\|_\Gamma \left\|H^{-\frac{1}{2}}D\mathbf{v}\right\|_U h^{k+1} \quad \text{for all } \mathbf{v}\in\mathbf{V}_H.$$

Proof. Applying (3.10) to I yields

$$\big|f(\mathbf{v}) - \tilde{f}(\mathbf{v})\big| = \left|-\int_\Gamma (\operatorname{div}_\Gamma \boldsymbol{\sigma}^\Gamma)^T(\mathbf{v}\circ F - \mathbf{v})\right| \le \left\|\operatorname{div}_\Gamma \boldsymbol{\sigma}^\Gamma\right\|_\Gamma \left\|\mathbf{v}\circ F - \mathbf{v}\right\|_\Gamma.$$

For any $x\in\Gamma$, the interval $(0,|a(x)|)$ is denoted as J and $l(s) = x + \operatorname{sgn}(a(x))\mathbf{n}(x)s$ parameterizes the fiber of p over x. The difference $\mathbf{v}(F(x)) - \mathbf{v}(x)$ can be written as

$$\mathbf{v}(F(x)) - \mathbf{v}(x) = \int_J D\mathbf{v}(l(s))^T\mathbf{n}\, ds.$$

The Cauchy-Schwarz inequality gives $|\mathbf{v}(F(x)) - \mathbf{v}(x)| \le |a(x)|^{1/2}\|D\mathbf{v}\circ l\|_J$. Therefore,

$$\|\mathbf{v}\circ F - \mathbf{v}\|_\Gamma^2 \le \|a\|_{\infty,\Gamma}\int_\Gamma\int_J |D\mathbf{v}(l(s))|^2\, ds\, d\sigma(x).$$

To the double integral, the coarea formula is applied, cf. [Fed69], where the inner integral ranges over the fibers of p. Let $\tilde{U} = \{l(s) \mid s\in J, x\in\Gamma\}\subset U$ be the set of points between Γ and Γ_h, and let $\nu(x) = \prod_{i=1}^{n-1}\big(1 - d(x)\kappa_i(x)\big)$. It follows that

$$\int_\Gamma\int_J |D\mathbf{v}(l(s))|^2\, ds\, d\sigma(x) = \int_{\tilde{U}} \nu\, |D\mathbf{v}|^2.$$

By Hölder's inequality, this is bounded by $\|\nu\|_{\infty,\tilde{U}}\int_{\tilde{U}}|D\mathbf{v}|^2$. The integral is written as sum over integrals on all $T\in\mathcal{T}$ which intersect $\tilde{U}$. Hölder's inequality is applied on each T,

$$\int_{\tilde{U}}|D\mathbf{v}|^2 = \sum_T \int_{T\cap\tilde{U}}|D\mathbf{v}|^2 \le \sum_T \operatorname{meas}(T\cap\tilde{U})\,\|D\mathbf{v}\|_{\infty,T\cap\tilde{U}}^2.$$

Consider a single summand. Let B be the smallest ball enclosing T. From (2.4), one concludes $\mathrm{meas}(T \cap \tilde{U}) \leq \mathrm{meas}(B \cap \tilde{U}) \leq c_m H_T^{n-1} \|a\|_{\infty,\Gamma}$. The inverse inequality (3.13) yields $\|D\mathbf{v}\|^2_{\infty,T\cap\tilde{U}} \leq c_{inv}^2 H_T^{-n} \|D\mathbf{v}\|^2_T$. Collecting the previous estimates yields

$$\|\mathbf{v} \circ F - \mathbf{v}\|^2_\Gamma \leq c_m c_{inv}^2 \|a\|^2_{\infty,\Gamma} \|\nu\|_{\infty,\tilde{U}} \left\| H^{-\frac{1}{2}} D\mathbf{v} \right\|^2_U,$$

and by assumption (6.1), $\|a\|_{\infty,\Gamma} \leq c_d h^{k+1}$. It remains to derive a bound on ν. Let $\xi = p(x)$ for $x \in \tilde{U}$. Equation (2.2) implies $\nu(x) = \left(\prod_{i=1}^{n-1}(1 + d(x)\kappa_i(\xi))\right)^{-1}$. Assumption (6.5) and the definition of $\tilde{U}$ yield $|1 + d(x)\kappa_i(\xi)| \geq 1 - |a(\xi)|\kappa_\Gamma \geq \frac{1}{2}$, $i \in \{1, \ldots, n-1\}$. Therefore, one obtains $\|\nu\|_{\infty,\tilde{U}} \leq 2^{n-1}$. □

To bound term *II* in (6.8), the telescopic sum

$$\begin{aligned} &\mu_*^{-1}(\mathbf{P}DF_*)^T \boldsymbol{\sigma}_*^\Gamma - \tilde{\mathbf{Q}}^T \boldsymbol{\sigma}_h^\Gamma \\ &= \mu_*^{-1}(\mathbf{P}DF_*)^T(\boldsymbol{\sigma}_*^\Gamma - \boldsymbol{\sigma}_h^\Gamma) + (\mu_*^{-1} - 1)(\mathbf{P}DF_*)^T \boldsymbol{\sigma}_h^\Gamma + (\mathbf{P}DF_* - \mathbf{Q})^T \boldsymbol{\sigma}_h^\Gamma \\ &\quad + (\mathbf{Q} - \tilde{\mathbf{Q}})^T \boldsymbol{\sigma}_h^\Gamma \\ &=: A + B + C + D \end{aligned} \tag{6.9}$$

is estimated term by term. In each of the expressions A, B, C, and D, the difference in parentheses is of order $\mathcal{O}(h^{k+1})$, whereas the remaining factors are bounded by constants. That the difference $\boldsymbol{\sigma}_*^\Gamma - \boldsymbol{\sigma}_h^\Gamma$ is of order $\mathcal{O}(h^{k+1})$, is a direct consequence of assumption (6.6). The $\mathcal{O}(h^{k+1})$-bounds for the other differences are proved in Lemma 6.4, 6.5, 6.6. The bounds for the remaining factors are collected in Lemma 6.3.

Lemma 6.3. *The following inequalities hold a. e. on* Γ_h*,*

$$|\alpha| \geq \frac{1}{2}, \quad \left|(\mathbf{P}DF_*)^T\right| \leq 3, \quad \text{and} \quad \frac{1}{2^n} \leq |\mu_*| \leq \left(\frac{3}{2}\right)^{n-1}.$$

Proof. Take any $x_h \in \Gamma_h$, where $\mathbf{n}_h$ is single valued. By definition,

$$\alpha(x_h) = \mathbf{n}(x_h)^T \mathbf{n}_h(x_h) = 1 - \tfrac{1}{2} |\mathbf{n}(x_h) - \mathbf{n}_h(x_h)|^2.$$

This is bigger than $1 - \frac{1}{2} c_n^2 h^{2k}$ by (6.2), which is bigger than $\frac{1}{2}$ by (6.5).

Let ξ denote the point on Γ with $x_h = F(\xi)$. From (4.4), one gets $|(\mathbf{P}DF_*)(x_h)^T| \leq |\mathbf{I} + a(\xi)\mathbf{H}(\xi)||\mathbf{Q}(x_h)|$. By (5.2), $|\mathbf{Q}(x_h)| = |\alpha(x_h)|^{-1}$ which less than 2. For the matrix $\mathbf{I} + a\mathbf{H}$, (6.1) and (6.5) lead to $|(\mathbf{I} + a(\xi)\mathbf{H}(\xi))| \leq 1 + \kappa_\Gamma c_d h^{k+1} \leq \frac{3}{2}$.

Instead of $|\mu_*(x_h)|$, one can equivalently consider $|\mu(\xi)|$. The assumptions (6.1) and (6.5) yield

$$\tfrac{1}{2} \leq 1 - |a(\xi)|\kappa_\Gamma \leq |1 + a(\xi)\kappa_i(\xi)| \leq 1 + |a(\xi)|\kappa_\Gamma \leq \tfrac{3}{2}$$

for all $i \in \{1, \ldots, n-1\}$. Using this and $\frac{1}{2} \leq |\alpha(x_h)| \leq 1$, proves the final assertion. □

Lemma 6.4. *Using the constant* $c_\mu = 3^{n-2}\left(4(n-1)c_d\kappa_\Gamma + 3c_n^2 h_0^{k-1}\right)$*, there holds*

$$\left|\mu_*^{-1} - 1\right| \leq c_\mu h^{k+1} \quad \text{a. e. on } \Gamma_h.$$

Proof. One writes $|\mu_*^{-1} - 1|$ as $|\mu|_*^{-1}|1 - \mu_*|$. For the first factor, Lemma 6.3 gives $|\mu_*^{-1}| \leq 2^n$. For the second factor, consider an arbitrary $\xi \in \Gamma$, and let $x_h = F(\xi)$.

Let $g(t) = \prod_{i=1}^{n-1}(1 + sy_i)$ with coefficients $y_i = a(\xi)\kappa_i(\xi)$ for $i \in \{1, \ldots, n-1\}$. Due to (6.1) and (6.5), there holds $\|y\|_\infty \leq \frac{1}{2}$. By definition,

$$\mu_*(x_h) - 1 = \alpha(x_h)g(1) - 1 = g(1) - 1 + g(1)(\alpha(x_h) - 1).$$

From the mean value theorem, one obtains $g(1) - 1 = g(1) - g(0) = g'(s)$ for some $s \in (0, 1)$. Computing the derivative $g'(s) = \sum_{i=0}^{n-1} y_i \prod_{j \neq i}(1 + sy_j)$ gives $|g'(s)| \leq (\frac{3}{2})^{n-2} \sum_{i=1}^{n-1} |y_i|$. Using again (6.1) yields

$$|g(1) - 1| \leq \left(\frac{3}{2}\right)^{n-2} (n-1)\kappa_\Gamma c_d h^{k+1}.$$

From the definition of α, one obtains $\alpha - 1 = \frac{1}{2}|\mathbf{n}_h - \mathbf{n}|^2$, which, by (6.2), gives $|\alpha - 1| \leq \frac{1}{2}c_n^2 h^{2k}$. As $|g(1)| \leq (\frac{3}{2})^{n-1}$, the proof is finished. □

Lemma 6.5. *The inequality* $|\mathbf{P}DF_* - \mathbf{Q}| \leq 2\kappa_\Gamma c_d h^{k+1}$ *holds a. e. on* Γ_h*.*

Proof. Let $x_h = F(\xi) \in \Gamma_h$ be an arbitrary point, where $\mathbf{n}_h$ is defined. By (4.4),

$$(\mathbf{P}DF_* - \mathbf{Q})(x_h) = a(\xi)\mathbf{H}(\xi)\mathbf{Q}(x_h).$$

Equation (5.2) and Lemma 6.3 yield $|\mathbf{Q}(x_h)| \leq 2$. By definition, $|\mathbf{H}(\xi)| \leq \kappa_\Gamma$. Finally, by (6.1), $|a(\xi)| = |d(x_h)| \leq c_d h^{k+1}$. □

Lemma 6.6. *There holds* $\left|\mathbf{Q} - \tilde{\mathbf{Q}}\right| \leq 6c_{\tilde{n}} h^{k+1}$ *a. e. on* Γ_h*.*

Proof. From the definitions of $\mathbf{Q}$ and $\tilde{\mathbf{Q}}$, one infers $\mathbf{Q} - \tilde{\mathbf{Q}} = \mathbf{n}_h \left(\frac{1}{\tilde{\alpha}}\tilde{\mathbf{n}} - \frac{1}{\alpha}\mathbf{n}\right)^T$. Due to (5.1), one has

$$\left|\mathbf{Q} - \tilde{\mathbf{Q}}\right|^2 = \left|\frac{1}{\tilde{\alpha}}\tilde{\mathbf{n}} - \frac{1}{\alpha}\mathbf{n}\right|^2 = \frac{1}{\tilde{\alpha}^2} + \frac{1}{\alpha^2} - 2\frac{\tilde{\mathbf{n}}^T\mathbf{n}}{\alpha\tilde{\alpha}}.$$

Using $\tilde{\mathbf{n}}^T\mathbf{n} = 1 - \frac{1}{2}|\tilde{\mathbf{n}} - \mathbf{n}|^2$, this is $(\frac{1}{\tilde{\alpha}} - \frac{1}{\alpha})^2 + \frac{1}{\tilde{\alpha}\alpha}|\tilde{\mathbf{n}} - \mathbf{n}|^2$. The first summand is considered. From $\alpha = 1 - \frac{1}{2}|\mathbf{n}_h - \mathbf{n}|^2$ one obtains

$$\frac{1}{\tilde{\alpha}} - \frac{1}{\alpha} = \frac{1}{2}\frac{1}{\tilde{\alpha}\alpha}\left(|\tilde{\mathbf{n}} - \mathbf{n}_h| + |\mathbf{n} - \mathbf{n}_h|\right)\left(|\tilde{\mathbf{n}} - \mathbf{n}_h| - |\mathbf{n} - \mathbf{n}_h|\right).$$

With the triangle inequality and letting $\delta = \frac{1}{2}(|\mathbf{n}_h - \mathbf{n}| + |\tilde{\mathbf{n}} - \mathbf{n}|)$, one obtains $|\frac{1}{\tilde{\alpha}} - \frac{1}{\alpha}| \leq \frac{\delta}{\tilde{\alpha}\alpha}|\tilde{\mathbf{n}} - \mathbf{n}|$. Altogether, the bound for $\tilde{\mathbf{Q}} - \mathbf{Q}$ is

$$\left|\mathbf{Q} - \tilde{\mathbf{Q}}\right|^2 \leq \frac{1}{\tilde{\alpha}\alpha}\left(\frac{\delta^2}{\tilde{\alpha}\alpha} + 1\right)|\tilde{\mathbf{n}} - \mathbf{n}|^2 =: \lambda^2 |\tilde{\mathbf{n}} - \mathbf{n}|^2. \tag{6.10}$$

Considering (6.4), it remains to estimate λ. From (6.2) and (6.4), one obtains $\delta \leq \frac{1}{2}(c_n h^k + c_{\tilde{n}} h^{k+1}) \leq \frac{5}{8}$. A lower bound for $\tilde{\alpha}$ is obtained from

$$\tilde{\alpha} = 1 - \frac{1}{2}|\tilde{\mathbf{n}} - \mathbf{n}_h|^2 \geq 1 - \frac{1}{2}(|\tilde{\mathbf{n}} - \mathbf{n}| + |\mathbf{n} - \mathbf{n}_h|)^2 = 1 - 2\delta^2.$$

This is bigger than $1 - 2 \cdot (\frac{5}{8})^2 = \frac{7}{32}$. With the lower bound for α from Lemma 6.3, it follows that $|\lambda| \leq \frac{4}{7}\sqrt{78} < 6$. The conclusion follows from (6.10). □

Remark 6.7. *The projector* $\mathbf{Q}$ *is approximated well by* $\mathbf{P}\mathbf{P}_h$*, namely,* $|\mathbf{P}\mathbf{P}_h - \mathbf{Q}| \in \mathcal{O}(h^{2k})$*. Consider* $\mathbf{P}\mathbf{P}_h - \mathbf{Q} = \mathbf{P}(\mathbf{I} - \mathbf{Q})\mathbf{P}_h = \alpha^{-1}\mathbf{P}\mathbf{n}_h(\mathbf{P}_h\mathbf{n})^T$*. By* (5.1)*,* $|\mathbf{P}\mathbf{P}_h - \mathbf{Q}| = |\alpha|^{-1}|\mathbf{P}\mathbf{n}_h||\mathbf{P}_h\mathbf{n}|$*. Lemma 6.3 yields the upper bound 2 for* $|\alpha|^{-1}$*. To estimate further,* $\mathbf{P}\mathbf{n}_h = \mathbf{n}_h - \alpha\mathbf{n} = \mathbf{n}_h - \mathbf{n} - (\alpha - 1)\mathbf{n}$*. As* $\alpha - 1 = 1 - \frac{1}{2}|\mathbf{n}_h - \mathbf{n}|^2 - 1 =:$

$\frac{1}{2}\delta^2$, *there holds* $|\mathbf{P}\mathbf{n}_h| = \delta + \frac{1}{2}\delta^2$, *which is less than* $\frac{3}{2}\delta$ *by* (6.5). *The term* $|\mathbf{P}_h\mathbf{n}|$ *is bound similarly. Hence, by* (6.2),

$$|\mathbf{P}\mathbf{P}_h - \mathbf{Q}| = |\alpha|^{-1}\,|\mathbf{P}\mathbf{n}_h|\,|\mathbf{P}_h\mathbf{n}| \le \frac{9}{2}c_n^2 h^{2k}.$$

The preceding Lemmas prove a bound for term *II* of (6.8),

Lemma 6.8 (*II*). *There exist positive constants* c_A, $c_{\tilde{II}}$, *and* c_{II} *such that*

$$\begin{aligned}\left|\tilde{f}(\mathbf{v}) - f_h(\mathbf{v})\right| &\le \left(c_A\left\|\boldsymbol{\sigma}_h^\Gamma - \boldsymbol{\sigma}_*^\Gamma\right\|_{\Gamma_h} + c_{\tilde{II}}\left\|\boldsymbol{\sigma}^\Gamma\right\|_\Gamma h^{k+1}\right)\|\mathbf{P}_h D\mathbf{v}\|_{\Gamma_h}\\ &\le c_{II}\,\|\mathbf{P}_h D\mathbf{v}\|_{\Gamma_h} h^{k+1} \quad \textit{for all } \mathbf{v}\in\mathbf{V}_H.\end{aligned}$$

Proof. By direct computation, one finds $\tilde{\mathbf{Q}} = \tilde{\mathbf{Q}}\mathbf{P}_h$. Using this, (4.3), and the Cauchy-Schwarz inequality, the term *II* is bound by

$$\left|\tilde{f}(\mathbf{v}) - f_h(\mathbf{v})\right| \le \|A+B+C+D\|_{\Gamma_h}\,\|\mathbf{P}_h D\mathbf{v}\|_{\Gamma_h}.$$

Hölder's inequality is applied to the first factor on the right-hand side. Term A yields $\|A\|_{\Gamma_h} \le \|\mu_*^{-1}(\mathbf{P}DF_*)^T\|_{L^\infty(\Gamma_h)}\|\boldsymbol{\sigma}_h^\Gamma - \boldsymbol{\sigma}_*^\Gamma\|_{\Gamma_h} \le 3\cdot 2^n\|\boldsymbol{\sigma}_h^\Gamma - \boldsymbol{\sigma}_*^\Gamma\|_{\Gamma_h}$ by Lemma 6.3. The contribution from any term $T\in\{B,C,D\}$ is bound as $\|T\|_{\Gamma_h} \le c_T\left\|\boldsymbol{\sigma}_h^\Gamma\right\|_{\Gamma_h} h^{k+1}$, where the constants c_T follow from the Lemma 6.3, 6.4, 6.5, and 6.6:

$$c_A = 3\cdot 2^n, \quad c_B = 3c_\mu, \quad c_C = 2\kappa_\Gamma c_d, \quad c_D = 6c_{\tilde{n}}.$$

A bound for $\|\boldsymbol{\sigma}_h^\Gamma\|_{\Gamma_h}$ follows from (6.6), the triangle inequality, and (4.6),

$$\|\boldsymbol{\sigma}_h^\Gamma\|_{\Gamma_h} \le \|\boldsymbol{\sigma}_h^\Gamma - \boldsymbol{\sigma}_*^\Gamma\|_{\Gamma_h} + \|\mu\|_{\infty,\Gamma}^{1/2}\|\boldsymbol{\sigma}^\Gamma\|_\Gamma.$$

The upper bound for $|\mu|$ from Lemma 6.3 concludes the proof. □

The estimate in Lemma 6.8 is with respect to the L^2-norm of $\mathbf{P}_h D\mathbf{v}$ on Γ_h. To estimate the discretization error in (3.15), the $H^1(\Omega)$-norm is required. A trace theorem is needed to convert the former to the latter. Such a theorem is [GR07, Thm. 4.6] which is proved for $n=3$ ibidem. A simpler proof for general n is given below. The simplification comes through the use of a well-known inverse inequality which removes the necessity to transform the interfacial quantities to the reference simplex.

Theorem 6.9. *Let* $(\mathcal{T}_H)_{H>0}$ *be a shape-regular family of triangulations of* Ω, *and let the inverse inequality* (3.13) *hold. Let* (6.1), (6.5), *and* (6.3) *be satisfied. There is a positive constant* c_{tr} *such that*

$$\|\mathbf{P}_h D\mathbf{v}\|_{T\cap\Gamma_h} \le c_{tr} H_T^{-\frac{1}{2}}\,\|D\mathbf{v}\|_T \quad \textit{for all } \mathbf{v}\in\mathbf{V}_H, T\in\mathcal{T}_H, H>0. \tag{6.11}$$

Proof. Take any $T\in\mathcal{T}_H$, $\mathbf{v}\in\mathbf{V}_H$. By Hölder's inequality and $|\mathbf{P}_h|\le 1$ one has

$$\|\mathbf{P}_h D\mathbf{v}\|_{T\cap\Gamma_h}^2 \le \|D\mathbf{v}\|_{\infty,T\cap\Gamma_h}^2 \operatorname{meas}(T\cap\Gamma_h) \le \|D\mathbf{v}\|_{\infty,T}^2 \operatorname{meas}(T\cap\Gamma_h).$$

The inverse estimate (3.13) is applied to $\|D\mathbf{v}\|_{\infty,T}$ producing a factor H_T^{-n} among others. It remains to show that $\operatorname{meas}(T\cap\Gamma_h) \le cH_T^{n-1}$ for some constant c. The transformation rule (4.6) gives

$$\operatorname{meas}(T\cap\Gamma_h) = \int_{T\cap\Gamma_h} 1 = \int_{F^{-1}(T\cap\Gamma_h)} \mu.$$

From Lemma 6.3, the upper bound $\|\mu\|_{L^\infty(\Gamma)} = \|\mu_*\|_{L^\infty(\Gamma_h)} \le (\frac{3}{2})^{n-1}$ is taken. The patch $T \cap \Gamma_h$ is contained in a ball of radius $\frac{1}{2}H_T$. Due to (6.1), the distance between any $F(\xi)$ and ξ is bounded by $c_d h^{k+1}$ on Γ. Hence, the patch $F^{-1}(T \cap \Gamma_h) \subset \Gamma$ is contained in a ball B of radius less than $\frac{1}{2}H_T + 2c_d h^{k+1}$. By (6.3), this is less than $(\frac{1}{2} + 2c_d c_{\mathcal{T}} h^k)H_T$. From (2.4), one obtains

$$\operatorname{meas}(T \cap \Gamma_h) \le \left(\frac{3}{2}\right)^{n-1} \operatorname{meas}(B \cap \Gamma) \le c H_T^{n-1}$$

with $c = (\frac{3}{2})^{n-1} c_m (\frac{1}{2} + 2c_d c_{\mathcal{T}} h_0^k)^{n-1}$. □

The main result on the discretization error of the variable interfacial tension functional is

THEOREM 6.10. *Let $(\mathcal{T}_H)_{H>0}$ be a shape-regular family of triangulations of Ω, and let (3.13) and (6.1) – (6.6) hold. There are positive constants c_0, c_1, c such that*

$$\begin{aligned}|f(\mathbf{v}) - f_h(\mathbf{v})| &\le \left(c_0 \left\|\boldsymbol{\sigma}^\Gamma\right\|_{div} h^{k+1} + c_1 \left\|\boldsymbol{\sigma}_h^\Gamma - \boldsymbol{\sigma}_*^\Gamma\right\|_{\Gamma_h}\right) \left\|H^{-\frac{1}{2}}\mathbf{v}\right\|_{\mathbf{V}} \\ &\le c h^{k+\frac{1}{2}} \|\mathbf{v}\|_{\mathbf{V}} \quad \textit{for all } \mathbf{v} \in \mathbf{V}_H.\end{aligned}$$

Proof. The result is an immediate consequence of the splitting (6.8) of $f - f_h$. The constituents are bound in Lemma 6.2 and Lemma 6.8; for term II, Theorem 6.9 is used as well. □

COROLLARY 6.11. *Under the premises of Theorem 6.10, there is a positive constant c such that*

$$\sup_{\mathbf{v} \in \mathbf{V}_H} \frac{f(\mathbf{v}) - f_h(\mathbf{v})}{\|\mathbf{v}\|_{\mathbf{V}_H}} \le c h^{k+\frac{1}{2}}.$$

An important property of the bound in Corollary 6.11 is that it only depends on the mesh width of Γ_h.

7. Consequences of Strang's lemma. A bound for the discretization error $\|\mathbf{u} - \mathbf{u}_H\|_{\mathbf{V}}$ which uses Strang's lemma contains the terms

$$\inf_{\mathbf{v}_H \in \mathbf{V}_H} \|\mathbf{u} - \mathbf{v}_H\|_{\mathbf{V}} \quad \text{and} \quad \|f - f_h\|_{\mathbf{V}_H'}.$$

Let the first term be of order $\mathcal{O}(H^{l+1})$, $l \ge 1$. For example, this can be achieved with the Hood-Taylor P_{l+1}-P_l-pair, if $\mathbf{u}$ is smooth enough. To balance the order of magnitude of the terms in Strang's lemma, the relation

$$h^{k+1} \le c H^{l+\frac{3}{2}}$$

is required by Theorem 6.10. Some ways to achieve this in a numerical method are discussed. For simplicity, it is assumed that Γ_h is the zero level of $I_h^m d$ where I_h^m is the nodal interpolation operator of the continuous finite elements of degree m.

The obvious choice $h = H$ requires $k = l + 1$. Hence, Γ_h is the zero level of $I_H^{l+1} d$. To satisfy (6.4), the interpolant $I_H^{l+2} d$ is required to compute the improved normal $\tilde{\mathbf{n}}$ as the gradient $D(I_H^{l+2} d)$ which is rescaled to unit length. An advantage of this choice is that only a single mesh is required; a disadvantage is that Γ_h is composed of curved pieces which are the zero levels of polynomials of degree $l + 1$. This complicates the numerical integration over Γ_h.

r	0	1	2	3	4	5	6
s	1	2	2	2	2	3	3

TABLE 7.1
The mesh-width $h = H/s$ of a piecewise linear Γ_h for $H = 2^{-r}$.

Another choice is $k = 1$ which requires two meshes satisfying $h \leq cH^{l/2+3/4}$. The resulting piecewise linear discrete interface admits standard numerical integration schemes. To satisfy (6.4), the interpolant $I_h^2 d$ is required on the fine mesh to compute the improved normal as the gradient $D(I_h^2 d)$ which is rescaled to unit length. Assume $H = 2^{-r}$ for $\mathcal{T}_H$ and a mesh width $h = H/s$, $s \in \mathbb{N}$, for Γ_h, which could be obtained by subdividing the elements of $\mathcal{T}_H$. For $c = 1$, the requirement $h \leq cH^{l/2+3/4}$ becomes $s \geq 2^{r(l/2-1/4)}$. For the low order case $l = 1$, which corresponds to the P_2-P_1-Hood-Taylor pair, the dependence of s on the refinement level r of $\mathcal{T}_H$ is shown in Table 7.1. For typical mesh-widths in 3-dimensional flow simulations, s increases slowly with r.

8. Numerical experiments. Let Ω be the cube $(-1,1)^3$. The initial mesh is the uniform subdivision of Ω into $10 \times 10 \times 10$ cubes, each of which is subdivided into 6 tetrahedra. This results in a Kuhn-triangulation $\mathcal{T}$ with initial mesh width $H_0 = \frac{1}{5}$. To obtain finer meshes $\mathcal{T}_H$, adaptive refinement is applied in the vicinity of Γ, such that it is embedded in a mesh with local mesh width $H = H(i) = 2^{-i}H_0$ for $i \in \{0, 1, 2, \dots\}$. The discrete interface Γ_h is constructed as the zero level of $I_H^1 d$. The operator I_H^1 is the standard nodal interpolation operator for the continuous, piecewise linear finite elements on $\mathcal{T}_H$ which corresponds to the choices $k = 1$ and $h = H$. Let $\tilde{d} = I_H^2 d$ be the nodal interpolant of d with continuous, piecewise quadratic finite elements. The improved approximation $\tilde{\mathbf{n}}$ is constructed as $D\tilde{d}/|D\tilde{d}|$.

Let $\mathbf{V}_H$ be the finite element space of continuous, vector-valued, piecewise quadratic functions on the mesh $\mathcal{T}_H$. Let $\mathcal{B}$ be the standard nodal basis, let $\mathbf{G}$ be the Grammian matrix of the $\mathbf{V}$-inner-product on $\mathbf{V}_H$, and let the tuple $\underline{v}$ denote the representation of $\mathbf{v} \in \mathbf{V}_H$ in $\mathcal{B}$. The dual norm of the $\mathbf{V}_H$-norm is required, cf. (3.15),

$$\|f\|_{\mathbf{V}_H'} = \sup\{f(\mathbf{v}) \mid \mathbf{v} \in \mathbf{V}_H, \|\mathbf{v}\|_{\mathbf{V}} = 1\}.$$

By elementary linear algebra,

$$\|f\|_{\mathbf{V}_H'} = \sqrt{\underline{f}\mathbf{G}^{-1}\underline{f}},$$

where $f_j = f(\mathbf{v}^j)$ with the nodal basis function $\mathbf{v}^j \in \mathcal{B}$. Hence, the $\mathbf{V}_H'$-norm can be evaluated by solving a linear system with the Grammian. This is done up to floating point precision. In the implementation of (4.7), a 5th-order accurate quadrature rule is used on the triangles which constitute Γ_h.

For the first experiment, let Ω^1 be the ball $\{x \in \Omega \mid |x| \leq R\}$ with $R = \frac{1}{2}$, $\Gamma = \partial\Omega^1$. Constant interfacial tension $\tau \equiv 1$ is prescribed, and f_h is compared to the 'improved' discretization of [GR07] which is denoted as g_h. The results are shown in Table 8.1. They show that g_h is an $\mathcal{O}(h^{3/2})$-approximation of f_h. This can be explained by a variation of our analysis and Remark 6.7 because, for constant interfacial tension and $k = 1$, the improved approximation from [GR07] is equivalent to (4.7) after substituting $\tilde{\mathbf{P}}\mathbf{P}_h$ for $\tilde{\mathbf{Q}}$.

i	0	1	2	3	4	5
$\|f_h - g_h\|_{\mathbf{V}_H'}$	0.03227	0.008206	0.002241	6.241e-4	1.816e-4	5.743e-5
Order		1.98	1.87	1.84	1.78	1.66

TABLE 8.1
Comparison of f_h and g_h for constant interfacial tension.

i	0	1	2	3	4	5
$\|f_h - \tilde{f}\|_{\mathbf{V}_H'}$	0.1150	0.03532	0.009634	0.002510	6.485e-4	1.696e-4
Order		1.70	1.87	1.94	1.95	1.93
$\|f_h - f_7\|_{\mathbf{V}_H'}$	0.2471	0.1195	0.04720	0.01710	0.006068	0.002048
Order		1.05	1.34	1.46	1.49	1.57

TABLE 8.2
Variable interfacial tension.

For the second experiment, the variable interfacial tension

$$\tau(x) = 1 + \cos(2\pi x^1)$$

is taken. Despite the simple geometry, it is difficult to evaluate f exactly. Instead, the auxiliary functional $\tilde{f}$ in (6.7) is considered which has an exact representation as integral over Γ_h. By Lemma 6.2 and (6.3), it is an $\mathcal{O}(h^{\frac{3}{2}})$-approximation of f. In the present example, the integrand of the right-hand side of (6.7) can be evaluated exactly using the expressions

$$\mathbf{n}(x) = \frac{x}{|x|}, \qquad F^{-1}(x_h) = R\mathbf{n}(x_h),$$

$$\mu_*(x_h) = \alpha(x_h)\left(1 + \frac{d(x_h)}{R}\right)^2, \qquad \mathbf{P}DF(x_h) = \left(1 + \frac{d(x_h)}{R}\right)\mathbf{Q}(x_h).$$

This yields a piecewise analytic integrand. Therefore, approximating the integral over Γ_h in (6.7) with a fifth order accurate quadrature rule on the triangles of Γ_h yields an $\mathcal{O}(h^{\frac{3}{2}})$ approximation to which f_h is compared. Additionally, f_h is compared to f_7 which is the evaluation of f_h on level 7.

The results are shown in Table 8.2. One can conclude from the data for $f_h - \tilde{f}$ that f_h is an $\mathcal{O}(h^2)$-approximation of $\tilde{f}$ as predicted by Lemma 6.8. One cannot conclude the same approximation property with respect to f as $\tilde{f}$ is only an $\mathcal{O}(h^{\frac{3}{2}})$-approximation of f. On the other hand, the results for $f_h - f_7$ in Table 8.2 reflect the $\mathcal{O}(h^{\frac{3}{2}})$-error-bound in Corollary 6.11.

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