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Bericht Nr. 319 Juni 2011

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ON THE ACCURACY OF THE LEVEL SET SUPG METHOD FOR APPROXIMATING INTERFACES

ARNOLD REUSKEN AND EVA LOCH*

Abstract. In this paper we consider a level set equation, the solution of which (called level set function) is used to capture a moving interface denoted by Γ. We assume that this level set function is close to a signed distance function. For discretization of the linear hyperbolic level set equation we use standard polynomial finite element spaces with SUPG stabilization combined with a Crank-Nicolson time differencing scheme. Recently, in [Burmann, Comp. Methods Appl. Mech. Eng. 199, 2010] a discretization error bound for this discretization has been derived. The discretization induces an approximate interface, denoted by Γ_h. Using the discretization error bound, we derive bounds on the distance between Γ and its approximation Γ_h. From this we deduce a quantitative result on the mass conservation quality of the evolving approximate interface Γ_h. Results of numerical experiments are included which illustrate the theoretical error bounds.

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1. Introduction.

Level set methods [8, 9, 6] are very popular for numerically capturing moving surfaces or interfaces and used in many applications, e.g. in two-phase flow simulations [3, 10, 11, 12]. In these methods the (unknown) surface or interface is represented as the zero level of the so-called level set function ϕ. In many applications this function is the solution of the linear hyperbolic equation

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0 \quad \text{for} \quad t \geq 0, \quad x \in \Omega, \tag{1.1}$$

with a given velocity field $\mathbf{u}$. The initial function $\phi_0(x) = \phi(x,0)$, $x \in \Omega$, is taken such that $\phi_0(x) < 0$ for $x \in \Omega_1(0)$, $\phi_0(x) > 0$ for $x \in \Omega_2(0)$, $\phi_0(x) = 0$ for $x \in \Gamma(0)$ and $\Omega_1(0) \cup \Omega_2(0) \cup \Gamma(0) = \Omega$. It is desirable to have the initial level set function ϕ_0 as an approximate signed distance function. In interface capturing methods based on the level set technique one usually wants to have this (approximate) signed distance function property also for $t > 0$ and therefore uses a reparametrization (also called re-initialization) method. Starting from $t = 0$ the time evolution is continued until time $t = t_1$ at which the level set function $\phi(x, t_1)$, or its computed approximation, differs too much from a signed distance function. Then, given this $\phi(x, t_1)$ (or its approximation) a reparametrization results in $\tilde{\phi}(x, t_1)$ which is such that its zero level is (approximately) equal to that of $\phi(x, t_1)$ and, in a neighborhood of the interface, the function $\tilde{\phi}(x, t_1)$ is close to a signed distance function. The function $\tilde{\phi}$ is then used as re-initialization in the evolution of the level set function: $\tilde{\phi}$ is taken as initial data to solve the level set equation for $t \geq t_1$. This procedure is then repeated. Different re-initialization techniques are known in the literature, cf. [8, 9, 4, 13, 7]. We do not address these in this paper.

In the setting described above one has to solve, on each time interval $[t_i, t_{i+1}]$, a level set equation of the form (1.1) for which the solution ϕ can be assumed to be smooth, in the sense that (locally, i.e. in a neighborhood of the interface) it is close to a signed distance function. We consider the level set equation on a time interval

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$[0,T]$ and only consider problems in which the evolving interface $\Gamma(t)$ is a connected smooth hypersurface (i.e. no topological singularities). Furthermore, we assume that T is sufficiently small such that the solution ϕ is close to a signed distance function for $t \in [0,T]$. To simplify the presentation we assume ϕ to be smooth on the whole domain Ω (not only close to the interface). The latter assumption is not essential for our analysis. For the discretization of this problem we apply a standard (popular) method, namely a conforming finite element method with streamline-upwind Petriv-Galerkin (also called streamline diffusion) stabilization combined with a one-step finite difference scheme in time (θ-scheme). Recently, for this full, i.e., space and time, discretization an error analysis has been presented [1]. For the Crank-Nicolson method an error bound of the form $\|\phi_h^N - \phi(T)\|_{L^2} \leq cT(h^{k+\frac{1}{2}} + \Delta t^2)$ is proved, with ϕ_h^N the computed approximation of $\phi(T) = \phi(\cdot, T)$, k the degree of the polynomials used in the finite element space, h the mesh size parameter and Δt the time step. The constant c depends on ϕ, in particular on its smoothness, but is independent of T, h and Δt.

In this paper, based on this L^2-norm discretization error bound and similar bounds proved in [1] we derive bounds on the error between the zero level on ϕ, denoted by Γ, and its approximation Γ_h, which is the zero level of ϕ_h^N. Note that Γ_h depends on h and Δt. Under reasonable assumptions, for example on the choice of Δt and on the smoothness of Γ_h, we show that the distance between Γ and Γ_h, $\mathrm{dist}(\Gamma, \Gamma_h)$, measured in a $L^2(\Gamma_h)$-norm is bounded by ch^k. Furthermore, a bound of the form ch^k on the volume error, $\big||\mathrm{int}(\Gamma)| - |\mathrm{int}(\Gamma_h)|\big|$, is derived. Note that the error measure $\mathrm{dist}(\Gamma, \Gamma_h)$ is stronger than $\big||\mathrm{int}(\Gamma)| - |\mathrm{int}(\Gamma_h)|\big|$ in the sense that an accurate interface approximation implies a small volume error but the reverse does not hold. Our analysis implies that, although the level set method is not strictly volume conserving, the error in the interface approximation and in the volume can be controlled and reduced in a predictable way by refining the mesh or increasing the polynomial degree. In the literature for discretization of the level set equation often finite volume techniques are applied, since these are based on a natural mass conservation property. There are, however, no rigorous analyses in which for these methods bounds for the interface error $\mathrm{dist}(\Gamma, \Gamma_h)$ or the volume error $\big||\mathrm{int}(\Gamma)| - |\mathrm{int}(\Gamma_h)|\big|$ are derived. Furthermore, compared to the finite element methods these finite volume techniques are in general more involved if one wants to use higher order discretizations.

We are not aware of any literature in which for the VOF-method or the level set method rigorous error bounds on the error in the interface approximation are presented.

The remainder of this paper is organized as follows. In the next section we introduce the SUPG combined with Crank-Nicolson discretization of the level set equation. We give a main discretization error result from [1]. In section 3 we collect important assumptions and derive a lemma that we need in our analysis. The main results, namely bounds on the error in the approximation of the interface are given in section 4. Finally in section 5 results of a few numerical experiments are presented.

2. Problem setting and discretization. Let Ω be a domain in $\mathbb{R}^d$ with a polyhedral boundary. To simplify the presentation we restrict ourselves to the from a computational point of view most important case $d = 3$. With some obvious modifications the analysis also applies to the case $d = 2$. The outward pointing unit normal on $\partial\Omega$ is denoted by $\mathbf{n}_\Omega$. The level set function is transported by a given velocity field $\mathbf{u}(x)$, $x \in \Omega$ that is assumed to be bounded, Lipschitz continuous and divergence free, i.e., $\mathrm{div}\,\mathbf{u} = 0$ in Ω. In Remark 3 we comment on the case $\mathrm{div}\,\mathbf{u} \neq 0$. In applications one often has that the velocity also depends on time. We only allow $\mathbf{u} = \mathbf{u}(x)$. The inflow part of the boundary is given by $\partial\Omega^- := \{ x \in \partial\Omega \mid \mathbf{u}(x) \cdot \mathbf{n}_\Omega(x) < 0 \}$. For given sufficiently smooth boundary data g and initial condition ϕ_0 we consider the problem of finding a solution $\phi = \phi(x,t)$, $x \in \Omega,\ t \in [0,T]$, of the level set equation

$$\begin{aligned} \frac{\partial \phi}{\partial \phi} + \mathbf{u} \cdot \nabla \phi = 0 \quad \text{in} \ \ \Omega \\ \phi = g \quad \text{on} \ \ \partial\Omega^- \\ \phi(\cdot, 0) = \phi_0 \quad \text{in} \ \ \Omega. \end{aligned} \tag{2.1}$$

The boundary data g may depend on t, and the initial condition ϕ_0 is assumed to satisfy $\phi_0(x) = g(x,0)$ for $x \in \partial\Omega^-$. We use the notation $g(t) = g(\cdot, t)$. For the spatial discretization of this linear hyperbolic problem we use the standard SUPG method (also often called streamline diffusion finite element method). Let $\{\mathcal{T}_h\}_{h>0}$ be a family of shape regular tetrahedral triangulations of Ω. We restrict to triangulations $\mathcal{T}_h$ that are quasi-uniform, cf. Remark 3 for generalizations. The parameter h denotes the maximal diameter: $h = \max_{T \in \mathcal{T}_h} h_T$, with $h_T = \mathrm{diam}(T)$. Let V_h^k be the standard polynomial finite element space:

$$V_h^k = \{ v_h \in C(\Omega) \mid (v_h)_{|T} \in \mathcal{P}_k \ \text{ for all } \ T \in \mathcal{T}_h \}, \quad k \geq 1.$$

For the level set equation one typically has an inhomogeneous boundary condition on the inflow boundary. This can be treated in different ways, for example, as weakly imposed conditions incorporated in the bilinear form (as in [5]) or as essential conditions in the finite element space. We use the latter approach since it fits better to the analysis in [1]. For this we introduce the set of points on the inflow boundary $\partial\Omega^-$ that correspond to degrees of freedom in the finite element space V_h^k. This set is denoted by $\mathcal{V}(\partial\Omega^-)$. For a given $f \in C(\partial\Omega^-)$ we define

$$V_h^k(f) = \{ v_h \in V_h^k \mid v_h(x) = f(x) \quad \text{for all} \ \ x \in \mathcal{V}(\partial\Omega^-) \}.$$

The L^2-scalar product on Ω and corresponding norm are denoted by $(\cdot,\cdot)$ and $\|\cdot\|$, respectively. The SUPG hyperbolic projection operator π_h^f, which corresponds to solving the *stationary* convection problem with Dirichlet boundary condition $\phi = f$ on $\partial\Omega^-$, is defined as follows. For $\phi = \phi(x)$ sufficiently smooth $\pi_h^f \phi \in V_h^k(f)$ is the unique solution of

$$(\mathbf{u} \cdot \nabla(\pi_h^f \phi - \phi), v_h + \delta \mathbf{u} \cdot \nabla v_h) = 0 \quad \text{for all} \ \ v_h \in V_h^k(0).$$

In the remainder, for the stabilization parameter δ we take the value $\delta = \frac{h}{\|\mathbf{u}\|_{L^\infty(\Omega)}}$. Error bounds for $\pi_h^f \phi - \phi$ are derived in [5], cf. Lemma 1 in [1]. The SUPG semi-discretization of the level set equation (2.1) is as follows: For $t \in [0,T]$ determine $\phi_h(\cdot, t) \in V_h^k\big(g(t)\big)$ with $\phi_h(\cdot, 0) = \pi_h^{\phi_0} \phi_0$ such that

$$\Big(\frac{\partial \phi_h}{\partial t} + \mathbf{u} \cdot \nabla \phi_h, v_h + \delta \mathbf{u} \cdot \nabla v_h\Big) = 0 \quad \text{for all} \ \ v_h \in V_h^k(0). \tag{2.2}$$

This space discretization can be combined with finite difference approximations of the time derivative. In [1] the implicit Euler, Crank-Nicolson (CN) and BDF2 time discretizations are analyzed in a general setting. To simplify the presentation, we restrict to the CN method. With obvious modifications the analysis of this paper also applies to the other two methods. Combination of the SUPG spatial discretization with the CN time discretization results in a fully discrete problem with a sequence of finite element functions $\phi_h^n \in V_h^k\big(g(t_n)\big)$, $1 \leq n \leq N$, with $N\Delta t = T$, $t_n := n\Delta t$. The initialization is given by $\phi_h^0 = \pi_h^{\phi_0}\phi_0$, and for $n \geq 1$ the discrete solution $\phi_h^n \in V_h^k\big(g(t_n)\big)$ is defined by

$$\Big(\frac{\phi_h^n - \phi_h^{n-1}}{\Delta t} + \frac{1}{2}\mathbf{u}\cdot\nabla(\phi_h^n + \phi_h^{n-1}), v_h + \delta\mathbf{u}\cdot\nabla v_h\Big) = 0 \quad \text{for all} \;\; v_h \in V_h^k(0).$$

For this method a discretization error bound is derived in Theorem 13 in [1], cf. also Remark 1. It is assumed that the level set function ϕ has sufficient regularity such that higher derivatives of ϕ, that occur in the error bounds, exist (we refer to [1] for precise regularity assumptions). For the SUPG-CN approximation $\phi_h^N \in V_h^k\big(g(T)\big)$ of $\phi(\cdot, T)$ the error bound

$$\|\phi_h^N - \phi(\cdot, T)\| \leq c\, T(h^{k+\frac{1}{2}} + \Delta t^2) \tag{2.3}$$

is proved. The constant c depends on the smoothness of the data g and the solution ϕ, but does not depend on T, h, Δt.

Remark 1. We comment on several aspects related to the error bound (2.3). Firstly, the error analysis in [1] is given for a linear transport equation as in (2.1), but with a source term f in the partial differential equation and *homogeneous* inflow boundary conditions, i.e., $g = 0$. In view of the level set equation we are interested in the *in*homogeneous case $g \neq 0$. Inspection of the analysis in [1] shows that with some modifications the analysis also applies to the inhomogeneous case. We discuss these modifications. The key and main new result of [1] is the stability result given in Proposition 3, which is restricted to the case of homogeneous boundary data $g = 0$. In the discretization error analysis (section 5 in [1]) the discretization error is split as $\phi_h^n - \phi(\cdot, t_n) = \big(\phi_h^n - \pi_h^{g(t_n)}\phi(\cdot, t_n)\big) + \big(\pi_h^{g(t_n)}\phi(\cdot, t_n) - \phi(\cdot, t_n)\big) =: \theta^n + \eta^n$. The term η^n is estimated by using bounds for the hyperbolic projection operator $\pi_h^{g(t_n)}$, which are also valid for the case of inhomogeneous boundary data g. For estimating the term θ^n the stability result is used. From $\phi_h^n \in V_h^k\big(g(t_n)\big)$ and $\pi_h^{g(t_n)}\phi(\cdot, t_n) \in V_h^k\big(g(t_n)\big)$ it follows that $\theta^n \in V_h^k(0)$, i.e. θ^n corresponds to homogeneous boundary data, and hence, the stability result can still be applied to bound this term.

Secondly, in [1] it is proved that if the inverse CFL condition $\Delta t \geq h$ is satisfied, the error bound (2.3) is still correct without the factor T, i.e. one has a quasi-optimal L^2-error bound that is uniform in the length of the time integration interval. In the setting of this paper, where we consider the level set method combined with reparametrization, we typically have "short" time integration intervals and therefore we do not consider this uniform error bound. We (only) use (2.3), which holds without any condition on the relation between h and Δt.

Thirdly, as is typical for the SUPG method, the discretization error is bounded not only in the L^2-norm, but also the error in the streamline derivative can be controlled: the term $\delta\|\mathbf{u}\cdot\nabla(\phi_h^N - \phi(\cdot, T))\|$ can be shown to have the same bound as on the right-hand side in (2.3). This is an important property of the streamline diffusion stabilization method. In our error analysis for the approximate interface, however, we only use the bound in (2.3) and could not obtain better results by using the bound on the error in the streamline derivative. Therefore, in (2.3) we give only the L^2-norm error bound.

Finally, it is known that in general the bound $h^{k+\frac{1}{2}}$ in (2.3) cannot be improved to h^{k+1}, cf. [14]. In many problems, however, one observes the optimal convergence rate of h^{k+1}.

We take Δt such that the two terms in the error bound (2.3) are balanced, i.e. $\Delta t \sim h^{\frac{1}{2}k+\frac{1}{4}}$, implying the error bound

$$\|\phi_h^N - \phi(\cdot, T)\| \leq c\,T h^{k+\frac{1}{2}}. \tag{2.4}$$

In the remainder of this paper, based on this discretization error bound we will derive bounds on the difference between the zero level of $\phi(\cdot, T)$ and of ϕ_h^N. We simplify the notation and write ϕ_h and $\phi(\cdot)$ instead of ϕ_h^N and $\phi(\cdot, T)$, respectively. For the finite element space $V_h^k\big(g(T)\big)$, which contains $\phi_h = \phi_h^N$, we use the notation $V_h^k(g)$. Furthermore, since T is fixed (and "small") we rewrite the estimate (2.4) as

$$\|\phi_h - \phi\| \leq c\, h^{k+\frac{1}{2}}, \tag{2.5}$$

with a constant c that may depend linearly on T but is independent of h and k.

3. Preliminaries. Let

$$\Gamma = \{\, x \in \Omega \mid \phi(x) = 0 \,\}$$

be the zero level of ϕ, which we will also call interface. We assume that Γ is a connected C^2 hypersurface and that for sufficiently small $c_U > 0$ the neighborhood $U := \{x \in \mathbb{R}^3 \mid \mathrm{dist}(x, \Gamma) < c_U\,\}$ is contained in Ω. Let d be the signed distance function

$$d : \Omega \to \mathbb{R}, \qquad |d(x)| := \mathrm{dist}(x, \Gamma) \quad \text{for all } x \in \Omega.$$

Thus, Γ is the zero level set of d. For c_U sufficiently small we have $d \in C^1(U)$. We choose the sign such that $d < 0$ in the interior of Γ. By $\mathbf{n} = \mathbf{n}_\Gamma$ we denote the unit normal on Γ, pointing into the subdomain where $d > 0$ holds. Note that $\mathbf{n}_\Gamma = \nabla d$ on Γ. We define $\mathbf{n}(x) := \nabla d(x)$ for $x \in U$. Thus $\mathbf{n} = \mathbf{n}_\Gamma$ on Γ and $\|\mathbf{n}(x)\|_2 = 1$ for all $x \in U$. Here and in the remainder $\|\cdot\|_2$ denotes the Euclidean vector norm in $\mathbb{R}^3$. For $x \in \Omega$ let $\mathbf{p}(x) \in \Gamma$ be a (possibly nonunique) point such that $d(x) = \|x - \mathbf{p}(x)\|_2$. The identity $\mathbf{p}(x) = x - d(x)\mathbf{n}(\mathbf{p}(x))$ holds. We assume that the neighborhood U is sufficiently small such that $\mathbf{p}(x)$ is unique for all $x \in U$, and thus, we have a well-defined projection $\mathbf{p} : U \to \Gamma$. Note that

$$\mathbf{n}(x) = \mathbf{n}\big(\mathbf{p}(x)\big) \quad \text{for all } x \in U.$$

Hence we have a unique decomposition

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

To formalize the assumption that ϕ is an approximate signed distance function we assume that there are strictly positive constants c_0, c_1, c_2 such that

$$c_0 \leq \|\nabla\phi(x)\|_2 \leq c_1 \quad \text{for all } \ x \in U, \tag{3.1}$$

$$|\phi(x)| \geq c_2 \quad \text{for all } \ x \notin U, \tag{3.2}$$

$$\mathrm{sign}\ \phi(x) = \mathrm{sign}\ d(x) \quad \text{for all } \ x \notin U. \tag{3.3}$$

These assumptions on ϕ and on the existence of such a local coordinate system are reasonable if the level set function ϕ is used for capturing a smooth interface.

The *approximate interface* is given as the zero level of ϕ_h:

$$\Gamma_h = \{\, x \in \Omega \mid \phi_h(x) = 0 \,\}.$$

For the error analysis we need some assumptions on Γ_h, which we now introduce.

ASSUMPTION 1. We introduce three assumptions. The first two are:

(A1) $\Gamma_h \subset U$.

(A2) For $x \in \Gamma$ there is a unique $y = x + \alpha \mathbf{n}(x)$ ($\alpha \in \mathbb{R}$) with $y \in \Gamma_h$.

This second assumption means that Γ_h is the graph of a function on Γ. If these two assumptions are satisfied, the approximate interface is a connected piecewise smooth manifold that can be represented as follows. There is a collection of tetrahedra, denoted by $\mathcal{T}_h^\Gamma \subset \mathcal{T}_h$, such that $\mathrm{meas}_2(T \cap \Gamma_h) > 0$ for $T \in \mathcal{T}_h^\Gamma$ and $\Gamma_h = \cup_{T \in \mathcal{T}_h^\Gamma} \Gamma_T$, with $\Gamma_T := \overline{T \cap \Gamma_h}$. Without loss of generality we can assume $\mathcal{T}_h^\Gamma \subset U$. For almost all $x \in \Gamma_h$ we can define the unit normal at x (with the same orientation as $\mathbf{n}$), denoted by $\mathbf{n}_h(x)$. The third assumption is introduced to exclude a zigzag behavior of the approximate interface:

(A3) $\mathbf{n} \cdot \mathbf{n}_h > 0$ on Γ_h.

In the discussion of these assumptions we use the following elementary result.

LEMMA 3.1. *Assume that ϕ is sufficiently smooth and that* (2.5) *holds. Then we have*

$$\|\phi\|_{L^\infty(\Gamma_h)} \le ch^{k-1}, \tag{3.4}$$

with a constant $c = c(\phi, k)$ independent of h. If the neighborhood U is chosen sufficiently small, then the following holds with $c_0 > 0$ from (3.1) *and suitable $c > 0$ independent of h:*

$$\mathbf{n}(x) \cdot \nabla \phi_h(x) \ge \frac{1}{2} c_0 - ch^{k-2} \quad \text{for all } x \in U \text{ where } \nabla\phi_h(x) \text{ exists.} \tag{3.5}$$

Proof. Let I_h^k be the nodal interpolation operator corresponding to the finite element space $V_h^k(g)$. Due to the smoothness assumption on ϕ we have

$$\|\phi - I_h^k \phi\|_{L^\infty(\Omega)} \le ch^{k+1} \tag{3.6}$$

$$\|\nabla\phi - \nabla I_h^k \phi\|_{L^\infty(\Omega)} \le ch^{k}. \tag{3.7}$$

We use the inverse estimates

$$\|v_h\|_{L^\infty(\Omega)} \le ch^{-1\frac{1}{2}} \|v_h\|, \quad \|\nabla v_h\|_{L^\infty(\Omega)} \le ch^{-2\frac{1}{2}} \|v_h\| \quad \text{for all } \ v_h \in V_h^k(0). \tag{3.8}$$

The following holds:

$$\begin{aligned} \|\phi - \phi_h\|_{L^\infty(\Omega)} &\le \|\phi - I_h^k\phi\|_{L^\infty(\Omega)} + \|\phi_h - I_h^k\phi\|_{L^\infty(\Omega)} \\ &\le ch^{k+1} + ch^{-1\frac{1}{2}} \|\phi_h - I_h^k \phi\| \\ &\le ch^{k+1} + ch^{-1\frac{1}{2}} \|\phi_h - \phi\| + ch^{-1\frac{1}{2}} \|\phi - I_h^k\phi\| \le ch^{k-1}. \end{aligned} \tag{3.9}$$

For $x \in \Gamma_h$ we have $\phi_h(x) = 0$ and thus we obtain

$$\|\phi\|_{L^\infty(\Gamma_h)} \le ch^{k-1},$$

which proves the result (3.4). In a similar way we obtain

$$\begin{aligned} \|\nabla\phi - \nabla\phi_h\|_{L^\infty(U)} &\leq \|\nabla\phi - \nabla I_h^k\phi\|_{L^\infty(\Omega)} + \|\nabla(\phi_h - I_h^k\phi)\|_{L^\infty(\Omega)} \\ &\leq ch^k + ch^{-2\frac{1}{2}}\|\phi_h - I_h^k\phi\| \leq ch^{k-2}. \end{aligned} \tag{3.10}$$

For $x \in U$ we write

$$\begin{aligned} \mathbf{n}(x)\cdot\nabla\phi_h(x) = \mathbf{n}(x)\cdot\nabla\phi(\mathbf{p}(x)) &+ \mathbf{n}(x)\cdot\big(\nabla\phi(x) - \nabla\phi(\mathbf{p}(x))\big) \\ &+ \mathbf{n}(x)\cdot\big(\nabla\phi_h(x) - \nabla\phi(x)\big) \end{aligned}$$

For the last term we have $|\mathbf{n}(x)\cdot\big(\nabla\phi_h(x) - \nabla\phi(x)\big)| \leq \|\nabla\phi - \nabla\phi_h\|_{L^\infty(U)} \leq ch^{k-2}$. If U is chosen sufficiently small, then we have $\big|\mathbf{n}(x)\cdot\big(\nabla\phi(x) - \nabla\phi(\mathbf{p}(x))\big)\big| \leq \frac{1}{2}c_0$. Finally, note that

$$\mathbf{n}(x)\cdot\nabla\phi(\mathbf{p}(x)) = \mathbf{n}(\mathbf{p}(x))\cdot\nabla\phi(\mathbf{p}(x)) = \frac{\nabla\phi(\mathbf{p}(x))}{\|\nabla\phi(\mathbf{p}(x))\|_2}\cdot\nabla\phi(\mathbf{p}(x)) = \|\nabla\phi(\mathbf{p}(x))\|_2 \geq c_0.$$

Combining these results we get the result in (3.5). □

We now comment on Assumption 1. From (3.4) and (3.2) it follows that $\Gamma_h \subset U$ holds for $k \geq 2$ and h sufficiently small, i.e. assumption (A1) is then satisfied.

Take a fixed $y \in \Gamma$ and consider the line in normal direction $l(y) = \{\, y + \alpha\mathbf{n}(y) \mid \alpha \in \mathbb{R}\,\}$. From the smoothness of ϕ and (3.2), (3.3) it follows that there exist $x_1, x_2 \in l(y)\cap U$ with $\phi(x_1) < 0, \phi(x_2) > 0$. There exists $\beta > 0$ such that $x_2 - x_1 = \beta\mathbf{n}(y)$ holds. From (3.9) it follows that for $k \geq 2$ and h sufficiently small $\phi_h(x_1) < 0, \phi_h(x_2) > 0$ holds. On the line segment connecting x_1 and x_2 the finite element function ϕ_h is continuous and piecewise polynomial. For the directional derivative along the line segment we get, with $x_\alpha := x_1 + \alpha(x_2 - x_1)$,

$$\frac{\partial}{\partial\alpha}\phi_h(x_\alpha) = \nabla\phi_h(x_\alpha)\cdot(x_2 - x_1) = \beta\nabla\phi_h(x_\alpha)\cdot\mathbf{n}(y) = \beta\nabla\phi_h(x_\alpha)\cdot\mathbf{n}(x_\alpha).$$

Using this and (3.5) it follows that for $k \geq 3$ and h sufficiently small ϕ_h is monotonic on the line segment $l(y)\cap U$. Hence, ϕ_h has a unique zero on this line segment, i.e. assumption (A2) is satisfied.

From (3.10) and (3.1) it follows that for $k \geq 3$ and h sufficiently small $\|\nabla\phi_h(x)\|_2 > 0$ holds for all $x \in U$ where $\nabla\phi_h(x)$ is defined. Using this and the result in (3.5) we get that for $k \geq 3$ and h sufficiently small,

$$\mathbf{n}(x)\cdot\mathbf{n}_h(x) = \mathbf{n}(x)\cdot\frac{\nabla\phi_h(x)}{\|\nabla\phi_h(x)\|_2} > 0 \quad \text{for almost all} \quad x \in \Gamma_h,$$

i.e. (A3) is satisfied.

Remark 2. If instead of the 3D case we consider the 2D level set equation the inverse estimates in (3.8) can be sharpened to $\|v_h\|_{L^\infty(\Omega)} \leq ch^{-1}\|v_h\|$, $\|\nabla v_h\|_{L^\infty(\Omega)} \leq ch^{-2}\|v_h\|$ and hence the bounds in (3.4), (3.5) can be modified to $ch^{k-\frac{1}{2}}$ and $\frac{1}{2}c_0 - ch^{k-1\frac{1}{2}}$, respectively. These (better) bounds influence the discussion on Assumption 1 in a positive way; for example, (A1) is now satisfied already for $k \geq 1$ (instead of $k \geq 2$ in the 3D case discussed above). A similar improvement occurs, if instead of the rigorous bound $\|\phi_h - \phi\| \leq c\,h^{k+\frac{1}{2}}$ in (2.5), we would use the estimate $\|\phi_h - \phi\| \leq c\,h^{k+1}$

which appears to be correct in many cases.

Summarizing, we conclude that the assumptions (A1)–(A3) are reasonable, in particular if for the discretization of the level set equation higher order finite elements are used. We use these assumptions in the error analysis presented in section 4.

We will also need two trace type inequalities that are given in the next lemma.

LEMMA 3.2. *Let (A1), (A2) be satisfied. There exists a constant c independent of h such that for all* $v_h \in V_h^k(0)$ *the following holds:*

$$\|v_h\|_{L^2(\Gamma_h)} \leq c\, h^{-\frac{1}{2}} \|v_h\|_{L^2(U)} \tag{3.11}$$

$$\|\nabla v_h\|_{L^2(\Gamma_h)} \leq c\, h^{-1\frac{1}{2}} \|v_h\|_{L^2(U)}. \tag{3.12}$$

Proof. The approximate interface Γ_h can be represented as $\Gamma_h = \cup_{T \in \mathcal{T}_h^\Gamma} \Gamma_T$ for a suitable collection of tetrahedra $\mathcal{T}_h^\Gamma$ contained in U. Take $T \in \mathcal{T}_h^\Gamma$ and the corresponding $\Gamma_T = \overline{T \cap \Gamma_h} \subset \Gamma_h$. Let $F(x) = \mathbf{A}x + b$ be the affine mapping such that $F(\hat{T}) = T$, with $\hat{T}$ the unit tetrahedron. Let Γ_T be parameterized by a (local) curvilinear coordinate system $x = x(s,t)$, $(s,t) \in S$. Hence,

$$\int_{\Gamma_T} v_h(x)^2 \, dx = \iint_S v_h(s,t)^2 \, \|\frac{\partial x}{\partial s} \times \frac{\partial x}{\partial t}\|_2 \, ds\, dt.$$

The transformed surface $\hat{\Gamma}_T = F^{-1}(\Gamma_T)$ can be parameterized by $\hat{x}(s,t) := \mathbf{A}^{-1}x(s,t) - \mathbf{A}^{-1}b$. Using $(\mathbf{M}a) \times (\mathbf{M}b) = (\det \mathbf{M})\mathbf{M}^{-T}(a \times b)$ for $a, b \in \mathbb{R}^3$, $\mathbf{M} \in \mathbb{R}^{3\times 3}$ we get

$$\begin{aligned}
\|\frac{\partial \hat{x}}{\partial s} \times \frac{\partial \hat{x}}{\partial t}\|_2 &= \|\mathbf{A}^{-1}\frac{\partial x}{\partial s} \times \mathbf{A}^{-1}\frac{\partial x}{\partial t}\|_2 = |\det \mathbf{A}|^{-1} \|\mathbf{A}^T (\frac{\partial x}{\partial s} \times \frac{\partial x}{\partial t})\|_2 \\
&\geq |\det \mathbf{A}|^{-1} \|\mathbf{A}^{-1}\|_2^{-1} \|\frac{\partial x}{\partial s} \times \frac{\partial x}{\partial t}\|_2
\end{aligned}$$

Hence, with $\hat{v}_h = v_h \circ F$ we obtain

$$\begin{aligned}
\int_{\Gamma_T} v_h(x)^2 \, dx &\leq |\det \mathbf{A}| \|\mathbf{A}^{-1}\|_2 \int_{\hat{\Gamma}_T} \hat{v}_h(\hat{x})^2 \, d\hat{x} \leq |\det \mathbf{A}| \|\mathbf{A}^{-1}\|_2 |\hat{\Gamma}_T| \max_{\hat{x} \in \hat{\Gamma}_T} |\hat{v}_h(\hat{x})|^2 \\
&\leq c |\det \mathbf{A}| \|\mathbf{A}^{-1}\|_2 \max_{\hat{x} \in \hat{T}} |\hat{v}_h(\hat{x})|^2.
\end{aligned}$$

Due to equivalence of norms we have $\max_{\hat{x} \in \hat{T}} |\hat{v}_h(\hat{x})|^2 \leq c \int_{\hat{T}} \hat{v}_h(\hat{x})^2 \, d\hat{x}$ with a constant c independent of $\hat{v}_h$ and h. Transformation from $\hat{T}$ back to T results in

$$\begin{aligned}
\int_{\Gamma_T} v_h(x)^2 \, dx &\leq c \|\mathbf{A}^{-1}\|_2 \int_{\hat{T}} \hat{v}_h(\hat{x})^2 |\det \mathbf{A}| \, d\hat{x} \\
&= c \|\mathbf{A}^{-1}\|_2 \int_T v_h(x)^2 \, dx.
\end{aligned}$$

The mesh regularity assumption implies $\|\mathbf{A}^{-1}\|_2 \leq ch^{-1}$. Summing over $T \in \mathcal{T}_h^\Gamma$ yields

$$\int_{\Gamma_h} v_h(x)^2 \, dx \leq ch^{-1} \sum_{T \in \mathcal{T}_h^\Gamma} \int_T v_h(x)^2 \, dx \leq ch^{-1} \|v_h\|_{L^2(U)}^2$$

and thus the result in (3.11). The same arguments can be used with v_h replaced by $\frac{\partial v_h}{\partial x_i}$, resulting in

$$\|\nabla v_h\|_{L^2(\Gamma_h)} \leq ch^{-\frac{1}{2}} \|\nabla v_h\|_{L^2(\mathcal{T}_h^\Gamma)},$$

and combining this with the standard inverse estimate for finite element functions proves that (3.12) also holds. ▯

4. Interface approximation error bounds. In this section we derive bounds on quantities that measure the quality of Γ_h as an approximation of Γ. We start with bounds on norms of the signed distance function d, namely $\|d\|_{L^\infty(\Gamma_h)}$ and $\|d\|_{L^2(\Gamma_h)}$.

THEOREM 4.1. *Let the neighborhood U be sufficiently small and ϕ be sufficiently smooth. Assume that* (2.5), (3.1) *hold and the assumptions (A1) and (A2) are satisfied. Then,*

$$\|d\|_{L^\infty(\Gamma_h)} \leq ch^{k-1} \tag{4.1}$$

holds, with a constant c independent of h.

Proof. Take $x \in \Gamma_h$ and introduce the notation $y = \mathbf{p}(x) = x - d(x)\mathbf{n}(y)$. For suitable s with $|s| \leq |d(x)|$ and $\tilde{y} = y + s\mathbf{n}(y)$ we get

$$\begin{aligned}\phi(x) &= \phi(x) - \phi(y) = \phi(y + d(x)\mathbf{n}(y)) - \phi(y) = d(x)\nabla\phi(y + s\mathbf{n}(y)) \cdot \mathbf{n}(y) \\ &= d(x)\big[\big(\nabla\phi(\tilde{y}) - \nabla\phi(y)\big) \cdot \mathbf{n}(y) + \nabla\phi(y) \cdot \mathbf{n}(y)\big].\end{aligned}$$

Note that using (3.1) we get

$$\nabla\phi(y) \cdot \mathbf{n}(y) = \nabla\phi(y) \cdot \frac{\nabla\phi(y)}{\|\nabla\phi(y)\|_2} = \|\nabla\phi(y)\|_2 \geq c_0.$$

If U is sufficiently small we have

$$|\big(\nabla\phi(\tilde{y}) - \nabla\phi(y)\big) \cdot \mathbf{n}(y)| \leq \frac{1}{2}c_0$$

and thus, we get

$$|d(x)| \leq 2c_0^{-1}|\phi(x)|. \tag{4.2}$$

Using the result in (3.4) completes the proof. ▯

Starting from the L^2-error bound in (2.5) it is natural to consider the error in the interface approximation also in the L^2-norm. Such a result is given in the following theorem.

THEOREM 4.2. *Let the assumptions be as in Theorem 4.1. The following holds:*

$$\|d\|_{L^2(\Gamma_h)} \leq ch^k, \tag{4.3}$$

with a constant c independent of h.

Proof. Using the interpolation error bound (3.6), the bounds in (2.5) and (4.2) and the trace inequality in (3.11) we obtain

$$\begin{aligned}\|d\|_{L^2(\Gamma_h)} &\le c\|\phi\|_{L^2(\Gamma_h)} = c\|\phi-\phi_h\|_{L^2(\Gamma_h)} \le c\|\phi - I_h^k\phi\|_{L^2(\Gamma_h)} + c\|\phi_h - I_h^k\phi\|_{L^2(\Gamma_h)}\\ &\le c\|\phi - I_h^k\phi\|_{L^\infty(\Gamma_h)} + ch^{-\frac12}\|\phi_h - I_h^k\phi\|_{L^2(U)}\\ &\le c\|\phi - I_h^k\phi\|_{L^\infty(\Omega)} + ch^{-\frac12}\big(\|\phi - I_h^k\phi\| + \|\phi_h-\phi\|\big) \le ch^k.\end{aligned}$$

Hence, the inequality (4.3) holds. □

We conclude that Γ_h is "close to" Γ in a sense as described in the above two theorems. In assumption (A3) we introduced a condition on the discrete normal $\mathbf{n}_h(x)$, $x \in \Gamma_h$. A natural question is whether $\mathbf{n}_h(x)$ is "close to" $\mathbf{n}(x)$. An answer to this can be derived along the same lines as in the previous theorem:

THEOREM 4.3. *Let the assumptions as in Theorem 4.1 be fulfilled. In addition we assume that there exists a constant $\hat{c}_0 > 0$ independent of h such that*

$$\hat{c}_0 \le \|\nabla\phi_h(x)\|_2 \quad \textit{for all } x \in U \textit{ where } \nabla\phi_h(x) \textit{ exists.} \tag{4.4}$$

The following holds:

$$\|\mathbf{n}-\mathbf{n}_h\|_{L^2(\Gamma_h)} \le ch^{k-1}, \tag{4.5}$$

with a constant c independent of h.

Proof. For $a, b \in \mathbb{R}^n$, $a \neq 0$, $b \neq 0$ the identity

$$\Big\|\frac{a}{\|a\|_2} - \frac{b}{\|b\|_2}\Big\|_2^2 = \frac{\|a-b\|_2^2}{\|a\|_2\|b\|_2} - \frac{\big(\|a\|_2 - \|b\|_2\big)^2}{\|a\|_2\|b\|_2}$$

holds, and thus,

$$\Big\|\frac{a}{\|a\|_2} - \frac{b}{\|b\|_2}\Big\|_2^2 \le \frac{\|a-b\|_2^2}{\|a\|_2\|b\|_2}.$$

For $x \in \Gamma_h$ (x not on an edge of the triangulation) and $y = \mathbf{p}(x) \in \Gamma$ we have $\mathbf{n}(x) - \mathbf{n}_h(x) = \mathbf{n}(y) - \mathbf{n}_h(x)$ and thus,

$$\|\mathbf{n}-\mathbf{n}_h\|_{L^2(\Gamma_h)} \le \Big\|\frac{\nabla\phi(\mathbf{p}(\cdot))}{\|\nabla\phi(\mathbf{p}(\cdot))\|_2} - \frac{\nabla\phi}{\|\nabla\phi\|_2}\Big\|_{L^2(\Gamma_h)} + \Big\|\frac{\nabla\phi}{\|\nabla\phi\|_2} - \frac{\nabla\phi_h}{\|\nabla\phi_h\|_2}\Big\|_{L^2(\Gamma_h)}. \tag{4.6}$$

We consider the first term on the right-hand side in (4.6). Using the result of Theorem 4.1 and (3.1) we get, for $x \in \Gamma_h$,

$$\Big\|\frac{\nabla\phi(\mathbf{p}(x))}{\|\nabla\phi(\mathbf{p}(x))\|_2} - \frac{\nabla\phi(x)}{\|\nabla\phi(x)\|_2}\Big\|_2 \le c_0^{-1}\|\nabla\phi(\mathbf{p}(x)) - \nabla\phi(x)\|_2 \le c|d(x)| \le ch^{k-1}.$$

For the second term on the right-hand side in (4.6) we use (3.1), (3.12), (4.4) and obtain

$$\begin{aligned}\Big\|\frac{\nabla\phi}{\|\nabla\phi\|_2} - \frac{\nabla\phi_h}{\|\nabla\phi_h\|_2}\Big\|_{L^2(\Gamma_h)} &\le c\|\nabla\phi - \nabla\phi_h\|_{L^2(\Gamma_h)}\\ &\le c\|\nabla\phi - \nabla I_h^k\phi\|_{L^2(\Gamma_h)} + c\|\nabla(\phi_h - I_h^k\phi)\|_{L^2(\Gamma_h)}\\ &\le c\|\nabla\phi - \nabla I_h^k\phi\|_{L^\infty(\Gamma_h)} + ch^{-1\frac12}\|\phi_h - I_h^k\phi\|_{L^2(U)}\\ &\le c\|\nabla\phi - \nabla I_h^k\phi\|_{L^\infty(\Omega)} + ch^{-1\frac12}\big(\|\phi - I_h^k\phi\| + \|\phi_h - \phi\|\big)\\ &\le ch^{k-1}.\end{aligned}$$

Hence, the result in (4.5) holds. □

For $k \geq 3$ and h sufficiently small the assumption in (4.4) is satisfied due to (3.1) and the result in (3.10).

Before we turn to an analysis of mass (or volume) conservation, we first consider the distance error in the $L^2(\Gamma)$-norm instead of the $L^2(\Gamma_h)$-norm, which is used in Theorem 4.2. For this we need a suitable extension (or lifting) of functions defined on Γ_h. Below *we assume that the assumptions* (A1), (A2), (A3) *are satisfied*. Let ψ be a continuous scalar function on Γ_h. We define its extension $\psi^e : U \to \mathbb{R}$ as follows. For $x \in \Gamma_h$, and $\alpha \in \mathbb{R}$ such that $x + \alpha\mathbf{n}(x) \in U$ we define $\psi^e(x + \alpha\mathbf{n}(x)) := \psi(x)$, i.e., ψ has a constant value along each normal $\mathbf{n}(x)$, $x \in \Gamma_h$. To relate the integral of ψ over Γ_h to the integral of ψ^e over Γ we use an integral transformation result that is derived in [2] (for this result to hold we need $\mathbf{n} \cdot \mathbf{n}_h > 0$ on Γ_h, i.e. assumption (A3)). For $x \in U$ let $\mathbf{H}(x) = D^2 d(x) \in \mathbb{R}^{3\times 3}$ be the Weingarten map and $\kappa_i(x)$, $i = 1, 2$, the two nonzero eigenvalues of $\mathbf{H}(x)$. For $x \in \Gamma$, $\kappa_1(x)$ and $\kappa_2(x)$ are the principal curvatures. We assume that the neighborhood U is sufficiently small such that $\|d\kappa_i\|_{L^\infty(U)} < 1$ for $i = 1, 2$. The following integral transformation rule holds, cf. [2]:

$$\begin{gathered}\int_\Gamma \psi^e(z)\,dz = \int_{\Gamma_h} \psi(x)\mu_h(x)\,dx, \\ \mu_h(x) := \mathbf{n}(x)\cdot\mathbf{n}_h(x)\big(1 - d(x)\kappa_1(x)\big)\big(1 - d(x)\kappa_2(x)\big),\end{gathered} \tag{4.7}$$

with dz and dx the surface measures on Γ and Γ_h, respectively.

Using this we easily obtain a distance measure on Γ. Let d^e be the extension of the signed distance function d, as defined above. The bijective mapping

$$\delta : \Gamma \to \Gamma_h, \qquad \delta(z) := z + d^e(z)\mathbf{n}(z),$$

describes Γ_h as the graph of a function δ on Γ. The distance between Γ and Γ_h can be measured by $\|\delta(z) - z\|_2 = |d^e(z)|$, $z \in \Gamma$. For the error measure $\|d^e\|_{L^2(\Gamma)}$ we have the following bound.

Corollary 1. Let the assumptions of Theorem 4.1 be satisfied. The following holds:

$$\|d^e\|_{L^2(\Gamma)} \leq c\|d\|_{L^2(\Gamma_h)} \leq ch^k. \tag{4.8}$$

Proof. Direct consequence of Theorem 4.2 and the formula in (4.7). □

Based on this we can derive a bound for the error in the approximation of an important quantity, namely the volume of the domain in the interior of Γ. We return to the time dependent setting outlined in section 2 and define

$$\Omega_1(t) := \{\, x \in \Omega \mid \phi(x,t) \leq 0 \,\}.$$

The volume of $\Omega_1(t)$ is denoted by $V(t) := \int_{\Omega_1(t)} 1\,dx$. From $\operatorname{div}\mathbf{u} = 0$ and Reynolds transport theorem it follows that

$$V'(t) = \frac{d}{dt}\int_{\Omega_1(t)} 1\,dx = \int_{\Omega_1(t)} \operatorname{div}\mathbf{u}\,dx = 0,$$

and thus $V(t)$ is a conserved quantity: $V(T) = V(0) =: V$. In applications from fluid dynamics this usually corresponds to a mass conservation property. The discrete interface Γ_h, which approximates $\Gamma = \Gamma(T)$, has an interior with volume

$$V_h := \int_{\Omega_{1,h}} 1\, dx, \quad \Omega_{1,h} := \{\, x \in \Omega \mid \phi_h(x) \leq 0 \,\}.$$

We investigate the error $|V - V_h|$.

THEOREM 4.4. *Let the assumptions be as in Theorem 4.1. The following holds:*

$$|V - V_h| \leq c\|d\|_{L^2(\Gamma_h)} \leq ch^k, \tag{4.9}$$

with a constant c independent of h.

Proof. Let Γ be parameterized by $z = z(\sigma)$, $\sigma = (s,t) \in S \subset \mathbb{R}^2$, a (local) system of curvilinear coordinates. Then

$$\int_\Gamma \psi(z)\, dz = \iint_S \psi(z(s,t))\, \|\frac{\partial z}{\partial s} \times \frac{\partial z}{\partial t}\|_2\, ds\, dt =: \int_S \psi(z(\sigma))\, \|\frac{\partial z}{\partial s} \times \frac{\partial z}{\partial t}\|_2\, d\sigma.$$

On U we introduce a transformed coordinate system $(\sigma, \alpha) = (s, t, \alpha)$, given by

$$x = x(\sigma, \alpha) = z(\sigma) + \alpha \mathbf{n}(z(\sigma)), \quad \sigma \in S,\ |\alpha| \leq c_U.$$

For the Jacobian of this coordinate transformation we have, with $\mathbf{H} = \nabla \mathbf{n} = D^2 d$,

$$\mathbf{J} = \mathbf{J}(\sigma, \alpha) = \frac{dx}{d(\sigma, \alpha)} = \left((\mathbf{I} + \alpha \mathbf{H})\tfrac{\partial z}{\partial s} \quad (\mathbf{I} + \alpha \mathbf{H})\tfrac{\partial z}{\partial t} \quad \mathbf{n} \right),$$

where $\mathbf{H} = \mathbf{H}(z(\sigma))$, $\frac{\partial z}{\partial s} = \frac{\partial z(\sigma)}{\partial s}$, $\frac{\partial z}{\partial t} = \frac{\partial z(\sigma)}{\partial t}$ and $\mathbf{n} = \mathbf{n}(z(\sigma))$. The Weingarten mapping $\mathbf{H}$ is symmetric and satisfies $\mathbf{Hn} = 0$. Furthermore, $\frac{\partial z}{\partial s} \cdot \mathbf{n} = \frac{\partial z}{\partial t} \cdot \mathbf{n} = 0$. Hence, both $(\mathbf{I} + \alpha \mathbf{H})\frac{\partial z}{\partial s}$ and $(\mathbf{I} + \alpha \mathbf{H})\frac{\partial z}{\partial t}$ are orthogonal to $\mathbf{n}$. The Jacobian determinant $|\det(\mathbf{J})|$ equals the volume of the parallelepiped spanned by the columns of $\mathbf{J}$. From the orthogonality property and $\|\mathbf{n}\|_2 = 1$ it follows that this volume is equal to the area of the parallelogram spanned by the first two columns of $\mathbf{J}$, which is given by $\left\|(\mathbf{I} + \alpha \mathbf{H})\frac{\partial z}{\partial s} \times (\mathbf{I} + \alpha \mathbf{H})\frac{\partial z}{\partial t}\right\|_2$. Hence, we obtain

$$|\det(\mathbf{J}(\sigma, \alpha))| = \left\|(\mathbf{I}+\alpha \mathbf{H})\frac{\partial z}{\partial s} \times (\mathbf{I}+\alpha \mathbf{H})\frac{\partial z}{\partial t}\right\|_2 = |\det(\mathbf{I}+\alpha \mathbf{H})| \left\|(\mathbf{I}+\alpha \mathbf{H})^{-1}\left(\frac{\partial z}{\partial s} \times \frac{\partial z}{\partial t}\right)\right\|_2.$$

The eigenvalues of the matrix $\mathbf{H}$ are given by the principal curvatures κ_1, κ_2 and 0. Hence, for $|\alpha| \leq c_U$ and c_U sufficiently small we have $|\det(\mathbf{I} + \alpha \mathbf{H})| \leq c$, $\|(\mathbf{I} + \alpha \mathbf{H})^{-1}\|_2 \leq c$ for all (σ, α) with $x(\sigma, \alpha) \in U$. Thus, we get

$$|\det(\mathbf{J}(\sigma, \alpha))| \leq c\left\|\frac{\partial z}{\partial s} \times \frac{\partial z}{\partial t}\right\|_2 \quad \text{for} \quad \sigma \in S,\ |\alpha| \leq c_U.$$

We analyze the volume difference using this variable transformation. We write $\Omega_1 = \{\, x \in \Omega \mid \phi(x) \leq 0 \,\}$, i.e. $V = \int_{\Omega_1} 1\, dx$. Recall $V_h = \int_{\Omega_{1,h}} 1\, dx$. Since both Γ and Γ_h are contained in U, we get

$$V - V_h = \int_{\Omega_1 \cap U} 1\, dx - \int_{\Omega_{1,h} \cap U} 1\, dx$$

In the transformed coordinates we have

$$\Omega_1 \cap U = \{\, (\sigma, \alpha) \mid \sigma \in S,\ \alpha \in [-c_U, 0] \,\}$$
$$\Omega_{1,h} \cap U = \{\, (\sigma, \alpha(\sigma)) \mid \sigma \in S,\ \alpha(\sigma) \in [-c_U, d^e(z(\sigma))] \,\}.$$

Hence, we obtain

$$\begin{aligned}
|V - V_h| &= \Big| \int_S \int_{-c_U}^{0} |\det(\mathbf{J}(\sigma,\alpha))| \, d\alpha \, d\sigma - \int_S \int_{-c_U}^{d^e(z(\sigma))} |\det(\mathbf{J}(\sigma,\alpha))| \, d\alpha \, d\sigma \Big| \\
&= \Big| \int_S \int_{d^e(z(\sigma))}^{0} |\det(\mathbf{J}(\sigma,\alpha))| \, d\alpha \, d\sigma \Big| \\
&\le c \int_S |d^e(z(\sigma))| \, \Big\| \frac{\partial z}{\partial s} \times \frac{\partial z}{\partial t} \Big\|_2 \, d\sigma = c \int_\Gamma |d^e(z)| \, dz \qquad (4.10) \\
&\le c \|d^e\|_{L^2(\Gamma)} \le c \|d\|_{L^2(\Gamma_h)} \le c h^k,
\end{aligned}$$

where in the last inequality we used Corollary 1. □

The inequality in (4.10) is expected to be *very pessimistic*, since it does not take into account cancellation effects that occur between error contributions coming from parts with $d^e(\sigma(z)) < 0$ and $d^e(\sigma(z)) > 0$.

We summarize and discuss the results derived in this section. Based on the discretization error bound in (2.5) and (reasonable) assumptions, in particular (3.1)–(3.3) and (A1)–(A3), we proved error bounds for the (signed) distance function and the discrete normals on Γ_h, namely $\|d\|_{L^2(\Gamma_h)} \le ch^k$ and $\|\mathbf{n} - \mathbf{n}_h\|_{L^2(\Gamma_h)} \le ch^{k-1}$ in Theorem 4.2 and Theorem 4.3. Furthermore, in Theorem 4.4 we derived a (pessimistic) volume error bound $|V - V_h| \le ch^k$. The constants c are independent of h but may depend on the smoothness of ϕ and k. There can be a mild (namely linear) dependence of the constants on the length T of the time integration interval. In the 2D case, cf. Remark 2, these error bounds improve in the sense that a factor $\frac{1}{2}$ can be added to the exponents. The same improvement occurs (in 2D and 3D) if the bound $ch^{k+\frac{1}{2}}$ in (2.5) is replaced by the (often observed) bound ch^{k+1}.

We conclude that the level set method combined with SUPG-CN discretization results in an accurate (in the sense as discussed above) interface capturing method. In general there is no exact volume conservation (which is often claimed to be a disadvantage in comparison with the VOF approach), but the volume error is bounded by ch^k (or even $ch^{k+\frac{1}{2}}$). This (pessimistic) bound predicts that, in particular if one uses higher order finite elements, the volume approximation accuracy will be satisfactory in many applications.

Remark 3. In [1] a discretization error bound for the case $\operatorname{div} \mathbf{u} \neq 0$ is discussed, namely the same as in (2.3), but under the additional inverse CFL condition $h \le \Delta t$. For $\Delta t \sim h$ we obtain, instead of (2.5), the bound $\|\phi_h - \phi\| \le ch^{\min\{k+\frac{1}{2},2\}}$. Note that this bound does not get better for increasing $k \ge 3$. Starting from this bound the analysis presented above can be applied with only minor changes and results in interface approximation bounds that are modified in an obvious manner, e.g., the estimate in Theorem 4.2 is replaced $\|d\|_{L^2(\Gamma_h)} \le ch^{\min\{k,1\frac{1}{2}\}}$. For the case $\operatorname{div} \mathbf{u} \neq 0$ the issue of volume conservation becomes more delicate, because the continuous level set function $\phi(x,t)$ is not necessarily volume conserving.

In the SUPG method on nonuniform meshes one typically uses a local stabilization parameter $\delta = \delta_T$. In the spatial discretization one then uses the following generalization of (2.2):

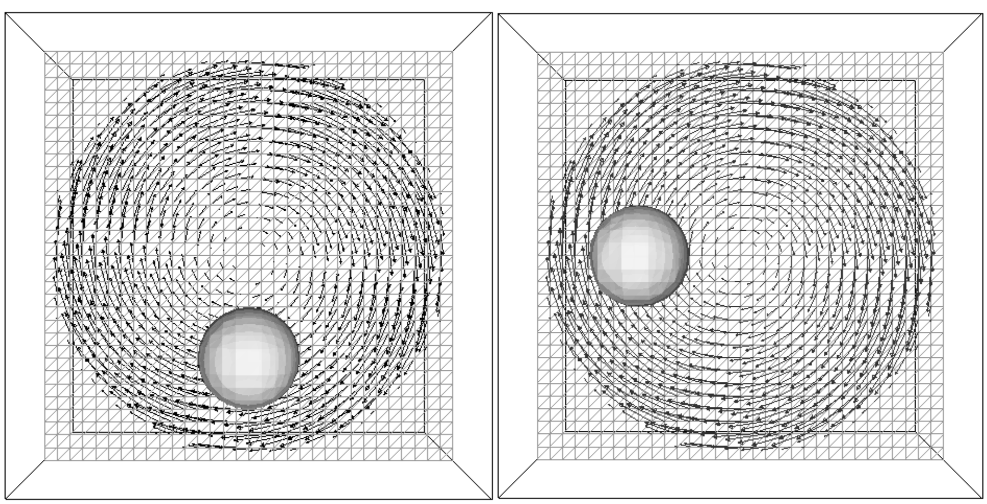
$$\sum_{T\in\mathcal{T}_h}(\frac{\partial\phi_h}{\partial t}+\mathbf{u}\cdot\nabla\phi_h, v_h+\delta_T\mathbf{u}\cdot\nabla v_h)_{L^2(T)}=0 \quad \text{for all} \quad v_h\in V_h^k(0).$$

with $\delta_T = h_T/\|\mathbf{u}\|_{L^\infty(T)}$ if $\|\mathbf{u}\|_{L^\infty(T)} > 0$ and $\delta_T = 0$ otherwise. In practice such a localized stabilization often performs much better than the one with a global stabilization parameter. Concerning the theoretical analysis we note that based on the results in [1] an error bound as in (2.5) is expected to hold for the case of quasi-uniform triangulations. Given this bound, the analysis of this paper still applies.

5. Numerical experiments. Consider the domain $\Omega = [0,1]^3$ and an initial interface $\Gamma(0)$ given by the sphere $B_{r_0}(m) \subset \Omega$ with centre $m = (0.5, 0.25, 0.5)$ and radius $r_0 = 0.125$. The initial condition $\phi(x, 0)$ is given by the signed distance function to this sphere. A divergence free velocity field $\mathbf{u}(x) = \mathbf{u}(x_1, x_2, x_3)$ is defined as follows. For $r \geq 0$ let $c(r)$ be a smooth function with $c(0) = 0$, monotonically increasing for $0 \leq r \leq 0.05$, $c(r) = \frac{\pi}{2}$ for $0.05 \leq r \leq 0.45$, monotonically decreasing for $0.45 \leq r \leq 0.5$ and $c(r) = 0$ for $r \geq 0.5$. The velocity field is defined by

$$\begin{aligned}\mathbf{u}(x) &= c(r)(x_2 - 0.5, -(x_1 - 0.5), 0)\\ r &:= \|(x_1, x_2, x_3) - (0.5, 0.5, 0.5)\|_2,\end{aligned}$$

which describes a clockwise rotation around the point $(0.5, 0.5, 0.5)$ in the x, y-plain, cf. Fig. 5.1. Note that $\mathbf{u} = 0$ on $\partial\Omega$. This velocity field is chosen such that in the region $U := B_{0.45}(0.5) \setminus B_{0.05}(0.5)$ the initial function $\phi(x, 0)$ and its zero level $\Gamma(0)$ are simply advected by $\mathbf{u}$, and thus for $x \in U$ the level set function $\phi(x, t)$ is the signed distance function to $\Gamma(t)$, where the latter is obtained by a rotation of $\Gamma(0)$, cf. Fig. 5.1. We take the time interval $[0, T]$ with $T = 1$, which corresponds to a quarter of one complete rotation.



(a) $t = 0$ (b) $t = T$

FIG. 5.1. *Velocity field and* $\Gamma(t)$.

In this test problem the exact solution $\phi(x, t)$ and its zero level $\Gamma(t)$ are known and thus discretization errors can, in principle, be computed. For the finite element discretization we construct an initial (= level 0) triangulation by subdividing Ω into 8^3 sub-cubes, each of which is further subdivided into 8 tetrahedra. The corresponding mesh size is $h_0 = \frac{1}{8}$. This initial tetrahedral triangulation is uniformly refined l times, $l = 1, 2, 3$. For the discretization we use piecewise quadratics with streamline diffusion stabilization as in (2.2) and stabilization parameter $\delta \sim \frac{h}{\|\mathbf{u}\|_{L^\infty(\Omega)}}$. Since there is no inflow boundary we use the space V_h^2 for trial and test functions. In the Crank-Nicolson method the time-step size Δt is such that $N\Delta t = T$ and $\Delta t \approx h^{1\frac{1}{4}}$, with $h = h_l$. The time step sizes that we use on level l are given by $\Delta t(l) = 0.0625$ ($N = 16$), 0.03125 ($N = 32$), 0.0125 ($N = 80$), 0.005 ($N = 200$) for $l = 0, 1, 2, 3$. The computed discrete approximation of $\phi(\cdot, t_n)$ is given by ϕ_h^n, $0 \leq n \leq N$.

We computed the L^2-norm discretization error on a subdomain, denoted by $\omega(t)$, such that $\Gamma(t) \subset \omega(t) \subset U$ and $\phi(\cdot, t)$ has high smoothness in $\omega(t)$. The reason for introducing this subdomain is that since ϕ is a signed distance function it has low regularity ($\phi \in H^1(\Omega)$), due to the singularity at the centre of the sphere. The subdomain is taken as follows. Let $\mathcal{T}_{h_0}$ be the level 0 triangulation. The subdomain $\omega(t)$ is formed by the union of all tetrahedra in $\mathcal{T}_{h_0}$ which are contained in U and do not contain the centre of the sphere $\Gamma(t)$. This technical detail related to $\omega(t)$ can be avoided if instead of the signed distance initialization $\phi(\cdot, 0)$ we would use a modification of it that is smooth at the centre of the sphere.

For $n = 0$ and $n = N$ the discretization errors $\|\phi_h^n - \phi(\cdot, t_n)\|_{L^2(\omega(t_n))}$ are given in Table 5.1

	$n = 0$		$n = N$	
level	error	order	error	order
0	1.53 e-4	-	2.01 e-3	-
1	2.43 e-5	2.66	3.97 e-4	2.34
2	3.06 e-6	2.99	6.13 e-5	2.70
3	3.86 e-7	2.99	1.03 e-5	2.57

Table 5.1
Error $\|\phi_h^n - \phi(\cdot, t_n)\|_{L^2(\omega(t_n))}$

For $n = 0$ we only have the interpolation error of the inital data in the space of piecewise quadratics. We clearly observe the expected third order convergence. For $n = N$ we expect, due to (2.3) and the choice of Δt, an $h^{2\frac{1}{2}}$ error behavior, as confirmed by the results in the last column of Table 5.1.

We now consider the (interface) error quantity $\|d\|_{L^2(\Gamma_h)}$, which is a measure for the difference between the exact interface $\Gamma(t)$ and its approximation $\Gamma_h(t)$, at a given time t. We note that although the signed distance function $d(\cdot, t)$ is known, this error quantity can not be determined directly, since the discrete interface $\Gamma_h(t_n)$, which is the zero level of ϕ_h^n is not available. We use a procedure in which the given piecewise quadratic finite element function ϕ_h^n is approximated by a sequence of piecewise *linear* interpolations on nested successively refined meshes. The zero level of these piecewise linears can be determined easily. Using this and a standard extrapolation technique the quantity $\|d\|_{L^2(\Gamma_h)}$ can be determined with sufficient accuracy. Results for $\|d(\cdot, t_n)\|_{L^2(\Gamma_h(t_n))}$, $n = 0$, $n = N$ are given in Table 5.2

The results in the last column of Table 5.2 are consistent with the theoretical error bound ch^2 derived in Theorem 4.2. At initialization ($n = 0$) we only have interpolation errors and therefore a better bound for the discretization error, cf. Table 5.1, which implies a better bound (of order $h^{2.5}$ instead of h^2) for $\|d(\cdot, 0)\|_{L^2(\Gamma_h(0))}$. This better

level	$n=0$ error	$n=0$ order	$n=N$ error	$n=N$ order
0	6.34 e-4	-	4.00 e-3	-
1	1.10 e-4	2.53	4.25 e-4	3.23
2	1.21 e-5	3.19	1.03 e-4	2.04
3	1.20 e-6	3.33	1.93 e-5	2.42

TABLE 5.2
Error $\|d(\cdot,t_n)\|_{L^2(\Gamma_h(t_n))}$

convergence behavior is reflected in the results for $n=0$ in Table 5.2.

Finally we consider the volume error $|V-V_h|$. The exact volume of $\Gamma(t)$ is $V=\frac{4}{3}\pi\cdot r^3 \overset{r=0.125}{\approx} 8.181231$ e-3. The discrete volume V_h, i.e. the volume of the interior of $\Gamma_h(t_n)$, is determined by using an approximation procedure with piecewise linears, as outlined above for the computation of $\|d(\cdot,t_n)\|_{L^2(\Gamma_h(t_n))}$. Results are presented in Table 5.3.

level	$n=0$ error	$n=0$ order	$n=N$ error	$n=N$ order
0	6.82 e-5	-	1.03 e-4	-
1	6.64 e-6	3.36	5.15 e-7	7.65
2	5.21 e-7	3.67	9.85 e-7	-0.94
3	2.20 e-7	4.11	7.00 e-8	3.81

TABLE 5.3
Volume error $|V-V_h|$

In Theorem 4.4 we derived the bound $|V-V_h(t_n)|\leq c\|d(\cdot,t_n)\|_{L^2(\Gamma_h(t_n))}$. As noted after the proof of that theorem, this bound is expected to be pessimistic, due to cancellation effects that are not taken into account. In view of this the results for $n=0$ in Tabel 5.3 are in good agreement with those in Table 5.2. For $n=N$ we observe a very irregular behavior. This can be due to a strong cancellation effect that (accidentally) occurs on level 1. Note that the volume conservation of the discretization method is very good in the sense that the volume errors for $n=N$ are not significantly larger than those for $n=0$ (caused by interpolation).

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