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A FINITE ELEMENT LEVEL SET REDISTANCING METHOD BASED ON GRADIENT RECOVERY*

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Abstract. We introduce a new redistancing method for level set functions. This method applies in a finite element setting and uses a gradient recovery technique. Based on the recovered gradient a quasi-normal field on the zero level of the finite element level set function is defined and from this an approximate signed distance function is determined. For this redistancing method rigorous error bounds are derived. For example, the distance between the original zero level and the zero level after redistancing can be shown to be bounded by ch^{k+1}, if finite elements of degree k are used in the discretization.

Key words. level set method, reinitialization, redistancing, gradient recovery

AMS subject classifications. 65M06, 65D05

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1. Introduction.

The level set method is a very popular method for treating problems involving free surfaces or interfaces. We refer to the literature for an explanation of this method and of fields of application, e.g., [17, 18, 13, 19]. Very often in this level set method a so-called reinitialization or redistancing (or reparametrization) procedure is used. Since the introduction of the reinitialization approach in [4] many such methods have been proposed in the literature. Most of these can be classified as either PDE based [20, 15] or geometry based [16, 18, 5]. We refer to the recent paper [3] for a discussion and comparison of these approaches. For an approach based on extension velocities, in which reinitialization is avoided, we refer to [1, 6].

In reinitialization methods, for a *given* discrete approximation ϕ_h of the unknown level set function ϕ one constructs an *approximate signed distance function* $\tilde{d}_h$ to the (only implicitly given) zero level Γ_h of ϕ_h. Let the (implicitly given) zero level of $\tilde{d}_h$ be denoted by $\tilde{\Gamma}_h$. In general, for an approximate signed distance function one has $\text{dist}(\tilde{\Gamma}_h, \Gamma_h) > 0$. In reinitialization methods one tries to construct a function $\tilde{d}_h$ such that, in a neighborhood of Γ_h, this function is "close to" the exact signed distance function to Γ_h, denoted by d_h^{ex}, and such that $\text{dist}(\tilde{\Gamma}_h, \Gamma_h)$ is "small." In numerical analyses of such methods one typically uses numerical experiments, for certain model problems, to investigate and quantify what is meant by "close to" and "small." We are not aware of any paper in which rigorous error bounds for the difference between $\tilde{d}_h$ and d_h^{ex} or for $\text{dist}(\tilde{\Gamma}_h, \Gamma_h) > 0$ are derived.

In this paper we present a new, geometry based, reinitialization method and derive rigorous error bounds for it. Although its error analysis is rather technical, the basic idea of the method is easy to explain. Our method is a geometric one, with a structure that is common in fast marching techniques (FMM), namely, an *initial phase* combined with an *extension phase*. In the initial phase one assigns values to the finite element nodes of the simplices that are intersected by Γ_h. These values are close to (as quantified further on) the signed distance values to Γ_h. Given these values, in the extension phase values are assigned to all other nodes, using, e.g., a

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fast marching sweeping approach. It is well known that in such redistancing methods the initial phase is the critical one and determines the accuracy of the reinitialization method. The method that we introduce is different from the methods known in the literature with respect to its initial phase. For the extension phase one can use any of the extension methods already available in the literature.

We explain the approach used in the initial phase. First consider a point z that is close to the zero level Γ of a smooth level set function ϕ. The normals on Γ are denoted by n. We then have a unique decomposition $z = p(z) + d^{ex}(z)n(p(z))$, with $p(z) \in \Gamma$ the orthogonal projection of z on Γ. By definition, the distance from z to Γ is given by $|d^{ex}(z)| = \|z - p(z)\|$. We adapt this elementary distance characterization to the discrete case. We assume that Γ_h is the zero level of a finite element approximation ϕ_h of ϕ. The function ϕ_h is continuous and a piecewise polynomial of degree k (on simplices). Under weak assumptions, Γ_h is a Lipschitz manifold. We introduce the notion of a *quasi-normal field* n_h on such a Lipschitz manifold, which plays a key role in the new redistancing method. Its essential conditions are that $x \to n_h(x)$, $x \in \Gamma_h$, is locally Lipschitz continuous and that $n_h(x)$ is "close to" orthogonal to Γ_h (cf. Definition 3.3 for a precise formulation). The "close to orthogonal" condition is quantified using a parameter δ; in the case of a smooth manifold one has $\delta = |\cos\theta|$, with θ the angle between $n_h(x)$ and the tangent plane at x. Based on this quasi-normal field, for z sufficiently close to Γ_h there is a unique representation $z = p(z) + d_h(z)n_h(p(z))$, $p(z) \in \Gamma_h$, which induces an *approximate signed distance function* $d_h(z)$. In general $z \to p(z)$ is an oblique projection on Γ_h. In a general analysis, presented in section 4, the difference between $d_h(z)$ and the exact signed distance value $d_h^{ex}(z)$ to Γ_h can be bounded in terms of the orthogonality parameter δ. To be able to apply this abstract approach in a concrete finite element setting we need such a quasi-normal field. The normal field $\nabla\phi_h(x)/\|\nabla\phi_h(x)\|$, $x \in \Gamma_h$, (x not on a simplex boundary) does not satisfy the requirements, since it is *dis*continuous between simplices, hence not Lipschitz. In the finite element literature, however, there are so-called *gradient recovery* techniques which result in approximations of $\nabla\phi_h$ that satisfy the conditions of a quasi-normal field on Γ_h. In this paper, as an example, we consider the polynomial-preserving recovery (PPR) technique introduced in [21]. Using this gradient recovery technique we obtain a quasi-normal field and the general approach then results in an approximate signed distance function d_h. To obtain a feasible method, the nodal interpolation of this d_h in the finite element space, denoted by $\tilde{d}_h = I_h d_h$, is constructed. In the computation of this finite element function $\tilde{d}_h$, which is the output of our initialization phase, we *only need evaluations of* ϕ_h in a small neighborhood of Γ_h. Using error bounds for the recovery technique and (discretization) error bounds for $\phi_h - \phi$ we can quantify statements like "$\tilde{d}_h$ is close to d_h^{ex}" and "$\text{dist}(\tilde{\Gamma}_h, \Gamma_h)$ is small." We prove, for example, that $\text{dist}(\tilde{\Gamma}_h, \Gamma_h) \leq ch^{k+1}$ and $\|\tilde{d}_h - d_h^{ex}\|_{L^\infty(\Omega_{\Gamma_h})} \leq ch^{k+1}$ hold, with Ω_{Γ_h} the neighborhood of Γ_h consisting of all simplices that are intersected by Γ_h. Thus, for quadratic finite elements ($k = 2$) our reinitialization method has accuracy h^3. We include results of a numerical experiment (in three dimensions) that illustrates this h^3 error behavior.

The paper is organized as follows. In sections 2–5 we consider the redistancing method and its analysis in a general setting. In sections 6 and 7 the general results are applied in a finite element setting with a gradient recovery technique that is used for the construction of a quasi-normal field. In section 8 results of a few numerical experiments are presented.

2. Outline of the results in the general setting. We describe the key ideas and main results presented in sections 3–5. Let Γ be a compact $(N-1)$-dimensional

Lipschitz manifold. The exact signed distance function to Γ is denoted by d^{ex}. In section 3 we introduce the notion of a quasi-normal field $n : \Gamma \to \mathbb{R}^N$. The "normality" of this field depends on a parameter $\delta \in (0,1)$ (if $\delta \ll 1$ then n is close to orthogonal to the tangent space on Γ). Based on n we define an oblique projection $p : U \to \Gamma$, with $U \subset \mathbb{R}^N$ a (small) neighborhood of Γ, and a corresponding unique representation for $z \in U$ as $z = p(z) + d(z)n(p(z))$, with $d : U \to \mathbb{R}$. The function d is called the *approximate signed distance function*. For this function the relation $d(z) = \langle z - p(z), n(p(z))\rangle$ holds, which implies that d can evaluated if we know how to evaluate the oblique projection p. By construction we have that $d(z) = 0$ iff $d^{\text{ex}}(z) = 0$, i.e., *the zero level of the approximate signed distance function equals* Γ. In section 4 we derive properties of p and d, for example, $\|\nabla d\| = 1 + \mathcal{O}(\delta)$ almost everywhere in U (Theorem 4.2) and a bound for $|d| - |d^{\text{ex}}|$ on U (Theorem 4.3). In section 5 we study an algorithm for computing the oblique projection $p(z)$ for $z \in U$. The question of *how to obtain* a quasi-normal field is left open in sections 3–5, but is addressed if we apply the general approach in a finite element setting. The construction of a quasi-normal field based on gradient recovery is treated in section 6.2.

3. A Lipschitz continuous local coordinate system.

If Γ is a C^2-manifold then the (oriented) normal field $n(x)$, $x \in \Gamma$, can be used to define a local coordinate system of the form

$$y = p(y) + d(y)n(p(y)), \quad y \in \{y \in \mathbb{R}^N \mid |d(y)| < \epsilon\} \tag{3.1}$$

with $\epsilon > 0$ sufficiently small, $d(\cdot)$ the signed distance function to Γ, and $p(\cdot)$ the orthogonal projection onto Γ. In this section we derive a generalization of this local coordinate system for the case of a Lipschitz manifold.

In the literature there are several (not all equivalent) definitions of k-dimensional Lipschitz manifolds in $\mathbb{R}^N$. A recent overview of the commonly used ones is given in [11]. In this paper we restrict ourselves to the case $k = N - 1$ and use the standard definition of an $(N-1)$-dimensional Lipschitz manifold in graph representation; cf., e.g., [8, 11], which we now recall.

Definition 3.1. *A subset $\mathcal{M} \subset \mathbb{R}^N$ is called an $(N-1)$-dimensional Lipschitz manifold (in graph representation) if for every $x_0 \in \mathcal{M}$ there exists a local Euclidean coordinate system with origin O_{x_0} in x_0 and such that*

1. *there are open subsets $V_1 \in \mathbb{R}^{N-1}$ and $V_2 \subset \mathbb{R}$ with $O_{x_0} \in V := V_1 \times V_2$,*
2. *there exists a Lipschitz mapping $h : V_1 \to V_2$ with*

$$\mathcal{M} \cap V = \{\, (x_1, h(x_1)) \mid x_1 \in V_1 \,\}.$$

In view of our application to the level set function we also introduce the following implicit representation of an $(N-1)$-dimensional Lipschitz manifold which is equivalent to the one given in Definition 3.1; cf. Theorem 2.11 in [11].

Definition 3.2. *A subset $\mathcal{M} \subset \mathbb{R}^N$ is called an $(N-1)$-dimensional Lipschitz manifold (in implicit representation) if for every $x_0 \in \mathcal{M}$ there exists a local Euclidean coordinate system with origin O_{x_0} in x_0 and such that*

1. *there are open subsets $V_1 \in \mathbb{R}^{N-1}$ and $V_2 \subset \mathbb{R}$ with $O_{x_0} \in V := V_1 \times V_2$,*
2. *there exists a scalar function $\phi : V \to \mathbb{R}$ with $\phi(O_{x_0}) = 0$ and there are constants L_ϕ, $K_\phi > 0$ such that*

$$|\phi(x) - \phi(y)| \le L_\phi \|x - y\| \quad \textit{for all} \;\; x, y \in V, \tag{3.2}$$

$$|\phi(x_1, x_2) - \phi(x_1, y_2)| \ge K_\phi |x_2 - y_2| \quad \textit{for all} \;\; x_1 \in V_1,\, x_2, y_2 \in V_2, \tag{3.3}$$

3. $\mathcal{M} \cap V = \{\, x \in V \mid \phi(x) = 0 \,\}$.

We use $B(x;r) \subset \mathbb{R}^N$ to denote the open ball with center $x \in \mathbb{R}^N$ and radius $r > 0$ and $B_\Gamma(x;r) := B(x;r) \cap \Gamma$.

In the remainder, Γ is assumed to be a compact $(N-1)$-dimensional Lipschitz manifold.

DEFINITION 3.3. *A quasi-normal field is a mapping $n : \Gamma \to \mathbb{R}^N$, with $\|n(x)\| = 1$ for all x, which has the following properties. For all $x \in \Gamma$ there exist $\delta_x < 1, r_x > 0$, and γ_x, c_x with*

$$\|n(x) - n(y)\| \leq \gamma_x \|x - y\| \quad \text{for all} \quad y \in B_\Gamma(x; r_x), \tag{3.4}$$

$$|\langle n(x), x - y\rangle| \leq \delta_x \|x - y\| + c_x \|x - y\|^2 \quad \text{for all} \quad y \in B_\Gamma(x; r_x), \tag{3.5}$$

$$\text{and} \quad \sup_{x\in\Gamma} \delta_x =: \delta < 1, \quad \sup_{x\in\Gamma} \gamma_x < \infty, \quad \sup_{x\in\Gamma} c_x < \infty, \quad \inf_{x\in\Gamma} r_x > 0. \tag{3.6}$$

The conditions in (3.4) and (3.5) can be interpreted as smoothness and transversality conditions that the field n has to satisfy. For a C^2-manifold these conditions are satisfied for the normal field (with $\delta_x = \mathcal{O}(r_x)$). For a quasi-normal field we can always reduce r_x (if necessary) such that

$$0 < r_x \leq \frac{1 - \delta_x}{4(\gamma_x + c_x)} \tag{3.7}$$

holds. With r_x such that this holds and $y \in B_\Gamma(x; r_x)$, property (3.5) implies that $|\langle n(x), x-y\rangle| \leq \frac{1}{2}(1+\delta)\|x-y\|$ and thus the angle between $n(x)$ and $x-y$ is bounded from below by a strictly positive constant, uniformly in x and y. Given a quasi-normal field n we define

$$F : \Gamma \times \mathbb{R} \to \mathbb{R}^N, \quad F(x,t) := x + t\, n(x). \tag{3.8}$$

We first derive the local injectivity of this function.

LEMMA 3.1. *Given a quasi-normal field with r_x such that* (3.7) *is satisfied, define*

$$D := \left\{ (x,t) \mid x \in \Gamma,\ t \in \left(-\frac{1}{2} r_x, \frac{1}{2} r_x\right) \right\}. \tag{3.9}$$

The function F is injective on D.

Proof. Take $(x,t), (\hat{x}, \hat{t}) \in D$ such that $F(x,t) = F(\hat{x}, \hat{t})$, i.e., $x + t\, n(x) = \hat{x} + \hat{t}\, n(\hat{x})$. If $x = \hat{x}$ it follows that $t = \hat{t}$. Assume that $x \neq \hat{x}$. Note that $\|F(x,t) - \hat{x}\| = |\hat{t}|$ and $\|F(\hat{x}, \hat{t}) - x\| = |t|$. Define $m := \max\{r_x, r_{\hat{x}}\}$. Note that

$$\|x - \hat{x}\| = \|\hat{t}\, n(\hat{x}) - t\, n(x)\| \leq |\hat{t}| + |t| < \frac{1}{2}(r_{\hat{x}} + r_x) \leq m$$

holds. It suffices to consider the case $m = r_x$. Thus $\hat{x} \in B_\Gamma(x, r_x)$ holds. From (3.5) and (3.4) we obtain

$$|\langle n(x), x - \hat{x}\rangle| \leq (\delta_x + c_x r_x)\|x - \hat{x}\| \leq \frac{1}{2}(1 + \delta_x)\|x - \hat{x}\|, \tag{3.10}$$

$$\begin{aligned} |\langle n(\hat{x}), x - \hat{x}\rangle| &\leq |\langle n(\hat{x}) - n(x), x - \hat{x}\rangle| + |\langle n(x), x - \hat{x}\rangle| \\ &\leq (\gamma_x r_x + \delta_x + c_x r_x)\|x - \hat{x}\| \leq \frac{1}{2}(1 + \delta_x)\|x - \hat{x}\|. \end{aligned} \tag{3.11}$$

From $t = \hat{t} = 0$ we obtain the contradiction $x = \hat{x}$. Hence $|t| + |\hat{t}| > 0$ holds. From this and the results in (3.10)–(3.11) it follows that the triangle with vertices x, $\hat{x}$, and $F(x,t) = F(\hat{x},\hat{t})$ is nondegenerated. The inner angle at vertex x is denoted by β. From (3.10) we obtain $|\cos\beta| \leq \frac{1}{2}(1+\delta_x)$ and thus $\sin\beta > 1 - |\cos\beta| \geq \frac{1}{2}(1-\delta_x)$ holds. The inner angle at $F(x,t) = F(\hat{x},\hat{t})$ is denoted by α. The cosine rule implies $\|n(x) - n(\hat{x})\|^2 = 2(1-\cos\alpha) = 4\sin^2(\frac{1}{2}\alpha)$ and thus $\sin\alpha \leq 2\sin(\frac{1}{2}\alpha) = \|n(x) - n(\hat{x})\| \leq \gamma_x\|x-\hat{x}\|$ holds. Due to the sine rule we have $\frac{|\hat{t}|}{\sin\beta} = \frac{\|x-\hat{x}\|}{\sin\alpha}$, and thus $|\hat{t}| = \frac{\sin\beta}{\sin\alpha}\|x-\hat{x}\| > \frac{1}{2}(1-\delta_x)\gamma_x^{-1}$ holds. This yields a contradiction with $|\hat{t}| < \frac{1}{2}r_x \leq \frac{1}{2}(1-\delta_x)\gamma_x^{-1}$; cf. (3.9). Hence $x = \hat{x}$, which implies $t = \hat{t}$, and thus $(x,t) = (\hat{x},\hat{t})$ holds. □

Take $z \in F(D)$, with D as in Lemma 3.1. There are unique $p(z) = x \in \Gamma$, $d(z) \in (-\frac{1}{2}r_x, \frac{1}{2}r_x)$ such that

$$z = p(z) + d(z)n(p(z)). \tag{3.12}$$

THEOREM 3.2. *Take D as in Lemma* 3.1. *Then $F(D) \subset \mathbb{R}^N$ is open. The functions $z \to p(z)$ and $z \to d(z)$ are continuous on $F(D)$.*

Proof. Take $F(x_0,t_0) = x_0 + t_0 n(x_0) \in F(D)$, i.e., $x_0 \in \Gamma$, $-\frac{1}{2}r_{x_0} < t_0 < \frac{1}{2}r_{x_0}$. From the graph representation of Γ (cf. Definition 3.1), it follows that there are open subsets $V_1 \subset \mathbb{R}^{N-1}$, $V_2 \subset \mathbb{R}$ and a Lipschitz function h such that $\Gamma \cap V = \{\,(x_1, h(x_1)) \mid x_1 \in V_1\,\}$ with $V = V_1 \times V_2$. Define $r_{V_1} := \inf\{\, r_x \mid x = (x_1, h(x_1)),\ x_1 \in V_1\,\} > 0$ and the open subset $U := V_1 \times (-\frac{1}{2}r_{V_1}, \frac{1}{2}r_{V_1}) \subset \mathbb{R}^N$. On U we define the continuous mapping $G(x_1,t) := F\big((x_1,h(x_1)),t\big) \in F(D)$. Lemma 3.1 implies injectivity of the function G. From Brouwer's invariant domain theorem it follows that $G(U) \subset F(D)$ is open and the inverse of $G^{-1} : G(U) \to U$ is continuous. Hence, $F(D)$ is open. The inverse is given by $G^{-1}(z) = (x_1,t)$ with x_1 and t such that $z = (x_1, h(x_1)) + t\, n(x_1, h(x_1))$. Continuity of G^{-1} implies that the mapping $z \to t = d(z)$ is continuous. Furthermore, using the continuity of h we also obtain the continuity of $z \to (x_1, h(x_1)) = p(z)$. □

The compact Lipschitz manifold Γ is contained in the open set $F(D)$ and thus for z sufficiently close to Γ we have a unique decomposition $z = p(z) + d(z)\, n(p(z))$. Note that the width of the domain D of the mapping F is determined by r_x, which in turn depends on the parameters δ_x, γ_x, c_x that quantify the local smoothness and transversality of the quasi-normal field n and the local geometry ("curvature") of the manifold Γ.

Based on the representation in (3.12) there is the following natural definition of an approximate distance function.

DEFINITION 3.4. *The function $z \to d(z)$, with d as in* (3.12) *is called the approximate signed distance function.*

Note that this function $d(z)$ gives an approximation of the signed distance, only for z close to the manifold Γ. Below it will be convenient to use the relation

$$d(z) = \langle z - p(z), n(p(z))\rangle, \tag{3.13}$$

which immediately follows form (3.12). The decomposition in (3.12) corresponds to a local Lipschitz continuous coordinate system and is a generalization of the one for a smooth manifold given in (3.1). Note that $z \to p(z)$ is an oblique projection onto Γ.

4. Properties of the approximate signed distance function. In this section we derive some properties of the approximate signed distance function $d(z)$, $z \in F(D)$, defined in (3.12). For convenience we extend the quasi-normal field n, by taking a constant value in the quasi-normal direction, i.e., $n(z) = n(p(z) + d(z)n(p(z)) :=$

$n(p(z))$ for all $z \in D$. The normal field and the manifold Γ are characterized by Lipschitz functions. From a Lipschitz version of the implicit function theorem one can conclude that the functions p and d are not only continuous (cf. Theorem 3.2) but even locally Lipschitz continuous. Instead of applying such a theorem we derive this property directly, using the continuity result from Theorem 3.2 and the properties in (3.4)–(3.5). This derivation yields bounds which show how the local Lipschitz constant depends on the orthogonality parameter δ in (3.5).

LEMMA 4.1. *For every $z \in F(D)$ there exists an $\epsilon > 0$ such that for all $z_1, z_2 \in B(z;\epsilon)$ the following hold:*

$$\|p(z_1) - p(z_2)\| \leq \frac{4}{1-\delta_{p(z_1)}}\|z_1 - z_2\|, \tag{4.1}$$

$$|d(z_1) - d(z_2)| \leq \frac{2(1+\delta_{p(z_1)})}{1-\delta_{p(z_1)}}\|z_1 - z_2\|. \tag{4.2}$$

Proof. Take $z_0 = F(x_0, t_0) = x_0 + t_0 n(x_0)$ with $x_0 \in \Gamma$, $t_0 \in (-\frac{1}{2}r_{x_0}, \frac{1}{2}r_{x_0})$. Note that $x_0 = p(z_0)$ and $t_0 = d(z_0)$. Without loss of generality we can assume that for $x \in \Gamma$ the function $x \to r_x$, with r_x as in Definition 3.3, and such that (3.7) holds, is continuous. Due to this and the continuity of the functions p and d there exists an $\epsilon > 0$ such that for all $z \in B(z_0;\epsilon)$ we have $p(z) \in B_\Gamma(x_0; \frac{1}{4}r_{x_0})$, $d(z) \in (-\frac{1}{2}r_{x_0}, \frac{1}{2}r_{x_0})$, and $\max\{\, r_{p(z)} \mid z \in B(z_0;\epsilon)\,\} \leq 2\min\{\, r_{p(z)} \mid z \in B(z_0;\epsilon)\,\}$. Take arbitrary $z_1, z_2 \in B(z_0;\epsilon)$. From

$$\|p(z_1) - p(z_2)\| \leq \|p(z_1) - x_0\| + \|p(z_2) - x_0\| < \frac{1}{2}r_{x_0} \leq r_{p(z_1)}$$

it follows that $p(z_2) \in B_\Gamma(p(z_1); r_{p(z_1)})$ holds. Thus, using (3.4) and (3.5) we get

$$\begin{aligned} |d(z_1) - d(z_2)| &= |\langle z_1 - p(z_1), n(p(z_1))\rangle + \langle z_2 - p(z_2), n(p(z_2))\rangle| \\ &\leq |\langle p(z_2) - p(z_1), n(p(z_1))\rangle| + |\langle p(z_2) - z_2, n(p(z_2)) - n(p(z_1))\rangle| \\ &\quad + |\langle z_1 - z_2, n(p(z_1))\rangle| \\ &\leq \left[\delta_{p(z_1)} + c_{p(z_1)}r_{p(z_1)} + |d(z_2)|\gamma_{p(z_1)}\right]\|p(z_1) - p(z_2)\| + \|z_1 - z_2\|. \end{aligned}$$

Note that $|d(z_2)| \leq \frac{1}{2}r_{x_0} \leq r_{p(z_1)}$, and using (3.7) we get

$$\begin{aligned} |d(z_1) - d(z_2)| &\leq \left[\delta_{p(z_1)} + (c_{p(z_1)} + \gamma_{p(z_1)})r_{p(z_1)}\right]\|p(z_1) - p(z_2)\| + \|z_1 - z_2\| \\ &\leq \frac{1}{4}(1 + 3\delta_{p(z_1)})\|p(z_1) - p(z_2)\| + \|z_1 - z_2\|. \end{aligned} \tag{4.3}$$

Using this we obtain

$$\begin{aligned} \|p(z_1) - p(z_2)\| &= \|z_1 - d(z_1)n(p(z_1)) - z_2 + d(z_2)n(p(z_2))\| \\ &\leq \|z_1 - z_2\| + \|(d(z_1) - d(z_2))n(p(z_1))\| \\ &\quad + \|d(z_2)\,[n(p(z_1)) - n(p(z_2))]\,\| \\ &\leq \|z_1 - z_2\| + |d(z_1) - d(z_2)| + |d(z_2)|\gamma_{p(z_1)}\|p(z_1) - p(z_2)\| \\ &\leq 2\|z_1 - z_2\| + \left[\frac{1}{4}(1 + 3\delta_{p(z_1)}) + \frac{1}{4}(1 - \delta_{p(z_1)})\right]\|p(z_1) - p(z_2)\| \\ &= 2\|z_1 - z_2\| + \frac{1}{2}(1 + \delta_{p(z_1)})\|p(z_1) - p(z_2)\|. \end{aligned}$$

Since $\delta_{p(z_1)} < 1$ we obtain $\|p(z_1) - p(z_2)\| \leq \frac{4}{1-\delta_{p(z_1)}}\|z_1 - z_2\|$, and using this in (4.3) results in $|d(z_1) - d(z_2)| \leq \frac{2+2\delta_{p(z_1)}}{1-\delta_{p(z_1)}}\|z_1 - z_2\|$, which completes the proof. ∎

From Rademacher's theorem it follows that p and d are Frechet differentiable almost everywhere on $F(D)$. Let $N_s \subset F(D)$ be the subset with $|N_s| = 0$ such that d is differentiable at $F(D) \setminus N_s$.

For the *exact* signed distance function to a Lipschitz-manifold, denoted by d^{ex}, it is known that $\|\nabla d^{\mathrm{ex}}(z)\| = 1$ almost everywhere in a neighborhood of the manifold. From (4.2) it follows that for $z \in F(D) \setminus N_s$ we have $\|\nabla d(z)\| \leq 2(1+\delta_{p(z)})(1-\delta_{p(z)})^{-1}$, i.e., $\|\nabla d(z)\| \lesssim 2$ for $\delta_{p(z)} \ll 1$. In the next theorem we derive $\|\nabla d(z)\| \approx 1$ if $\delta_{p(z)} \ll 1$.

THEOREM 4.2. *The following holds, with $\delta_{p(z)} < 1$ as in* (3.5),

$$1 - \frac{16\delta_{p(z)}}{7 + 9\delta_{p(z)}} \leq \|\nabla d(z)\| \leq 1 + \frac{16}{7}\frac{\delta_{p(z)}}{1 - \delta_{p(z)}} \quad \textit{for all} \quad z \in F(D) \setminus N_s. \tag{4.4}$$

Proof. The Frechet derivative of a function $G : \mathbb{R}^N \to \mathbb{R}^N$ is denoted by DG, and its representation at $x \in \mathbb{R}^N$ by the Jacobian matrix $DG(x) \in \mathbb{R}^{N\times N}$. From $\|n(z)\| = 1$ for all $z \in D$ it follows that

$$Dn(z)^T n(z) = 0 \quad \text{for all} \quad z \in F(D) \setminus N_s \tag{4.5}$$

holds. From the relation (3.13) we obtain, for $z \in F(D) \setminus N_s$,

$$\begin{aligned}\nabla d(z) &= D(id - p)(z)^T n(p(z)) + D(n \circ p)(z)^T (z - p(z))\\ &= (I - Dp(z)^T) n(p(z)) + Dp(z)^T Dn(p(z))^T (z - p(z)).\end{aligned}$$

Using (3.12), (4.5) we get $Dn(p(z))^T (z - p(z)) = d(z) Dn(p(z))^T n(p(z)) = 0$ and

$$\nabla d(z) = n(p(z)) - Dp(z)^T n(p(z)), \quad z \in F(D) \setminus N_s.$$

Hence,

$$\|\nabla d(z) - n(p(z))\| \leq \|Dp(z)^T n(p(z))\|, \quad z \in F(D) \setminus N_s. \tag{4.6}$$

For $w \in \mathbb{R}^N$ and $|\epsilon|$ sufficiently small we obtain, due to (3.5),

$$|\langle n(p(z)), p(z) - p(z + \epsilon w)\rangle| \leq \delta_{p(z)} \|p(z) - p(z + \epsilon w)\| + c_{p(z)} \|p(z) - p(z + \epsilon w)\|^2,$$

and thus, for $z \in F(D) \setminus N_s$,

$$\begin{aligned}\|Dp(z)^T n(p(z))\| &= \max_{\|w\|=1} \langle w, Dp(z)^T n(p(z))\rangle\\ &= \max_{\|w\|=1} \langle n(p(z)), Dp(z) w\rangle \leq \delta_{p(z)} \|Dp(z)\|\end{aligned}$$

holds. Relation (3.12) implies $Dp(z) = I - d(z) Dn(p(z)) Dp(z) - n(p(z)) \nabla d(z)^T$, and thus $[I + d(z) Dn(p(z))]\, Dp(z) = I - n(p(z)) \nabla d(z)^T$. From (3.4) we get $\|Dn(p(z))\| \leq \gamma_{p(z)}$ for $z \in F(D) \setminus N_s$, and due to $|d(z)| \leq \frac{1}{2} r_{p(z)}$ and the condition (3.7) we get $|d(z)| \|Dn(p(z))\| \leq \frac{1}{8}(1 - \delta_{p(z)})$ and thus the matrix $I + d(z) Dn(p(z))$ is invertible and we have the estimate $\| [I + d(z) Dn(p(z))]^{-1} \| \leq 8(7 + \delta_{p(z)})^{-1}$. Combining these results we get

$$\begin{aligned}\|\nabla d(z) - n(p(z))\| &\leq \|Dp(z)^T n(p(z))\| \leq \delta_{p(z)} \|Dp(z)\|\\ &\leq \delta_{p(z)} \| [I + d(z) Dn(p(z))]^{-1} \| \|I - n(p(z)) \nabla d(z)^T\|\\ &\leq 8\delta_{p(z)} (7 + \delta_{p(z)})^{-1} (1 + \|\nabla d(z)\|).\end{aligned}$$

Using $\|n(p(z))\| = 1$ and $8\delta_{p(z)}(7+\delta_{p(z)})^{-1} < 1$ this implies

$$1 - \frac{16\delta_{p(z)}}{7+9\delta_{p(z)}} \leq \|\nabla d(z)\| \leq 1 + \frac{16}{7}\frac{\delta_{p(z)}}{1-\delta_{p(z)}},$$

i.e., the result in (4.4). ∎

Note that the bounds in (4.4) are determined (only) by the quantity $\delta_{p(z)}$ from (3.5). For a "close to orthogonal" quasi-normal field we have $\delta_{p(z)} \ll 1$ and thus $\|\nabla d(z)\| \approx 1$ as quantified in (4.4). In our application below we have $\delta_{p(z)} = \mathcal{O}(h^k) \ll 1$, with h a (local) mesh size parameter and k related to the degree of the finite elements used.

The next result quantifies in which sense the function d is close to the exact signed distance function d^{ex}.

THEOREM 4.3. *Take $z \in F(D), z \notin \Gamma$ and let $x_0 \in \Gamma$ be such that $|d^{\text{ex}}(z)| = \min_{x\in\Gamma}\|z-x\| = \|z-x_0\|$. Define $L_{x_0,z} := \{\, x_0 + t(z-x_0) \mid 0 \leq t \leq 1 \,\}$ and assume that $L_{x_0,z} \cap N_s$ has one-dimensional measure zero. Then*

$$0 \leq \frac{|d(z)| - |d^{\text{ex}}(z)|}{|d^{\text{ex}}(z)|} \leq \frac{16}{7}\frac{\delta_L}{1-\delta_L} \tag{4.7}$$

holds, with $\delta_L := \max\{\delta_{p(y)} \mid y \in L_{x_0,z}\} < 1$.

Proof. From $|d(z)| = \|z-p(z)\|$, with $p(z) \in \Gamma$, it follows that $|d(z)| \geq |d^{\text{ex}}(z)|$ and thus the left inequality in (4.7) holds. Using the mean value theorem and $d(x_0) = 0$ we get

$$d(z) = \int_0^1 \nabla d(x_0 + t(z-x_0)) \cdot (z-x_0)\, dt.$$

Hence, using Theorem 4.2 we obtain

$$\begin{aligned} |d(z)| &\leq \max_{y\in L_{x_0,z}} \|\nabla d(y)\| \|z-x_0\| \leq \max_{y\in L_{x_0,z}} \left(1 + \frac{16}{7}\frac{\delta_{p(y)}}{1-\delta_{p(y)}}\right) |d^{\text{ex}}(z)| \\ &= \left(1 + \frac{16}{7}\frac{\delta_L}{1-\delta_L}\right)|d^{\text{ex}}(z)|, \end{aligned}$$

which proves the right inequality in (4.7). ∎

5. A method for computing $p(z)$. In this section we introduce a simple iterative procedure for computing the oblique projection $p(z)$. If for a given z the oblique projection $p(z) \in \Gamma$ is known, the value for $d(z)$ can directly be determined from $d(z) = \langle z - p(z), n(p(z))\rangle$. Let z sufficiently close to Γ ($z \in F(D)$) be given. We propose the following scheme:

$$\begin{aligned} &\text{let } x^0 \in \Gamma \;\; \text{(close to } p(z)) \text{ be given. For } k \geq 0: \\ &x^{k+1} := z - \alpha\, n(x^k) \;\; \text{with} \;\; \alpha \in \mathbb{R} \text{ such that } x^{k+1} \in \Gamma \text{ and } |\alpha| \text{ minimal.} \end{aligned} \tag{5.1}$$

The following theorem shows that this method is well defined and converges locally.

THEOREM 5.1. *Let $z \in F(D)$ with $|d(z)| < \frac{3}{4}\frac{1-\delta_{p(z)}}{\gamma_{p(z)}}$ be given. For $x^0 \in \Gamma$ sufficiently close to $p(z)$ the iteration* (5.1) *is well defined and the following holds:*

$$\|x^{k+1} - p(z)\| \leq \frac{4}{3}\frac{\gamma_{p(z)}}{1-\delta_{p(z)}} |d(z)| \|x^k - p(z)\|, \quad k = 0, 1 \ldots. \tag{5.2}$$

Proof. Take z as specified above. In a sufficiently small neighborhood $V = V_1 \times V_2$ of $p(z) \in \Gamma$, as in the Definitions 3.1, 3.2, we can use both the graph representation and level set representation of Γ:

$$\Gamma \cap V = \{ (x_1, h(x_1)) \mid x_1 \in V_1 \} = \{ x \in V \mid \phi(x) = 0 \}.$$

The function $f : V_1 \times V_2 \to \mathbb{R}$ given by $f(x_1, \alpha) = \phi(z - \alpha\, n(x_1, h(x_1)))$ has a zero $(x_1^*, \alpha^*) \in V_1 \times V_2$, with x_1^* such that $(x_1^*, h(x_1^*)) = p(z)$ and $\alpha^* = d(z)$. From a Lipschitz version of the implicit function theorem (cf. [7]), it follows that there exists a neighborhood W of x_1^* and a function $\alpha : W \to V_1$ such that $f(x_1, \alpha(x_1)) = 0$ for all $x_1 \in W$ and $\Gamma \cap (W \times V_2) = \{ f(x_1, \alpha(x_1)) = 0 \mid x_1 \in W \}$. This implies that for $x^0 \in \Gamma$ sufficiently close to $p(z)$ there is a unique $\alpha_1 = \alpha_1(x^0) \in V_1$ such that

$$x^1 = z - \alpha_1\, n(x^0) \in \Gamma. \tag{5.3}$$

We conclude that for $k = 0$ the iteration (5.1) is well defined for all $x^0 \in \Gamma$ with $\|x^0 - p(z)\| < \xi$ and ξ sufficiently small. From a continuity argument it follows that for $\xi > 0$ sufficiently small we have $x^k \in B_\Gamma(p(z); r_{p(z)})$ for $k = 0, 1$. We use the notation $e^k = x^k - p(z)$. From (5.3) and $p(z) = z - d(z)n(p(z))$ it follows that

$$e^1 = d(z)n(p(z)) - \alpha_1 n(x^0) = d(z)\big(n(p(z)) - n(x^0)\big) + \big(d(z) - \alpha_1\big)n(x^0)$$

holds, and thus

$$\|e^1\|^2 \le |d(z)|\gamma_{p(z)}\|e^0\|\|e^1\| + |d(z) - \alpha_1||\langle n(x^0), e^1\rangle|. \tag{5.4}$$

Note that $|d(z) - \alpha_1| = \big|\|p(z) - z\| - \|x^1 - z\|\big| \le \|p(z) - x^1\| = \|e^1\|$. Hence, $\|e^1\| \le |d(z)|\gamma_{p(z)}\|e^0\| + |\langle n(x^0), e^1\rangle|$ holds. Using $x^k \in B_\Gamma(p(z); r_{p(z)})$ and the conditions (3.4)–(3.5) we get

$$\begin{aligned} |\langle n(x^0), e^1\rangle| &= |\langle n(x^0), p(z) - x^1\rangle| \\ &\le |\langle n(x^0) - n(p(z)), p(z) - x^1\rangle| + |\langle n(p(z)), p(z) - x^1\rangle| \\ &\le \gamma_{p(z)} r_{p(z)}\|e^1\| + \big(\delta_{p(z)} + c_{p(z)} r_{p(z)}\big)\|e^1\|. \end{aligned} \tag{5.5}$$

Using this we obtain $\|e^1\| \le |d(z)|\gamma_{p(z)}\|e^0\| + \big[\delta_{p(z)} + (c_{p(z)} + \gamma_{p(z)})r_{p(z)}\big]\|e^1\|$, and using (3.7) this yields $\big(1 - \frac{1}{4}(1 + 3\delta_{p(z)})\big)\|e^1\| \le |d(z)|\gamma_{p(z)}\|e^0\|$. Hence, the result (5.2) holds for $k = 0$. From the assumption $|d(z)| < \frac{3}{4}\frac{1-\delta_{p(z)}}{\gamma_{p(z)}}$ it follows that $\|e^1\| < \|e^0\|$ and thus the same argument can be applied for $k \ge 1$. ∎

It remains to determine the value of α such that $x^{k+1} = z - \alpha\, n(x^k) \in \Gamma$ holds; cf. (5.1). In our applications the manifold Γ is represented as the zero level of a level set function ϕ. In that case the value of α can be determined by a line search algorithm applied to $g_k(\alpha) = 0$, with $g_k(\alpha) := \phi(z - \alpha\, n(x^k))$. If g_k is (only) Lipschitz, special algorithms should be used; cf. [7, 14].

6. Application to the reinitialization of finite element level set functions. In this section we explain how the approximate signed distance function introduced above (cf. Definition 3.4), can be used in a reinitialization method. For a general discussion of the role of reinitialization techniques in level set methods we refer to the literature; cf. [12, 16, 17, 18].

We consider a finite element setting and a standard level set description of a smooth manifold (interface) in $\mathbb{R}^N$ $(N = 2, 3)$. Let $\phi : \Omega \to \mathbb{R}$ be a smooth function and $\Omega \subset \mathbb{R}^N$, $\Omega = \Omega_1 \cup \Omega_2$, $\Gamma = \bar{\Omega}_1 \cap \bar{\Omega}_2 = \{ x \in \Omega \mid \phi(x) = 0 \}$, $\phi(x) < 0$ for $x \in \Omega_1$, $\phi(x) > 0$ for $x \in \Omega_2$.

In applications one typically only has a finite element approximation ϕ_h of ϕ available. Let $\{\mathcal{T}_h\}_{h>0}$ be a family of shape regular simplicial triangulations of Ω, and V_h the corresponding standard finite element space of continuous piecewise polynomials of degree $k \geq 1$:

$$V_h = \{\, \psi \in C(\Omega) \mid \psi_{|T} \in \mathcal{P}_k \ \text{ for all } \ T \in \mathcal{T}_h \,\}. \tag{6.1}$$

The function $\phi_h \in V_h$ is a given (sufficiently accurate) approximation of ϕ. We define

$$\Gamma_h = \{\, x \in \Omega \mid \phi_h(x) = 0 \,\}. \tag{6.2}$$

Note that the zero level set Γ_h is only *implicitly* described and except for the case $k = 1$ (linear finite elements) it can generally *not* be represented in an explicit form.

We need some further notation. Let $\mathcal{T}_{\Gamma_h}$ be the set of all simplices that are intersected by Γ_h. This set is called *local triangulation*. The corresponding local domain is denoted by $\Omega_{\Gamma_h} = \overline{\cup_{T \in \mathcal{T}_{\Gamma_h}} T}$. To avoid technical details, we assume the generic situation that the intersection of any simplex $T \in \mathcal{T}_{\Gamma_h}$ with Γ_h divides T into two subsets with nonzero N-dimensional measure. For a collection of simplices A let $V(A)$ be the set of all vertices of the simplices contained in A and $N(A)$ the set of all finite element nodes of the simplices contained in A. Hence, for $k = 1$ we have $V(A) = N(A)$ and $V(A) \subset N(A)$ for $k \geq 2$. For a vertex v the union of all simplices that have v as a vertex is denoted by $\omega(v)$. The local triangulation is enlarged by adding the neighboring simplices, resulting in the set

$$\mathcal{T}^e_{\Gamma_h} ; = \cup_{v \in V(\mathcal{T}_{\Gamma_h})} \omega(v),$$

which is called the *extended local triangulation*. The corresponding domain is denoted by $\Omega^e_{\Gamma_h}$. The finite element space V_h restricted to the local triangulation is denoted by $V_h(\Omega_{\Gamma_h}) := \{\, \psi_{|\Omega_{\Gamma_h}} \mid \psi \in V_h \,\}$. We define $V_h(\Omega^e_{\Gamma_h})$ similarly.

6.1. Outline of the results in the finite element setting. We are interested in a reinitialization of the finite element function $\phi_h \in V_h$. We only consider the *initialization* phase. Given this initialization phase, any of the (many) known variants of the fast marching *extension* algorithms can be applied.

The initialization phase that we present in section 6.3 is based on an application of the approach studied in sections 3–5. The Lipschitz manifold is given by Γ_h from (6.2). For the given ϕ_h its gradient field $\nabla \phi_h$ cannot be used as a quasi-normal field on Γ_h since it is *discontinuous* (at the faces between simplices). In the finite element literature there are well-established *gradient recovery* techniques. Such methods result in *Lipschitz continuous* gradient approximations. In section 6.2 we present one particular technique, namely, the PPR method. The output of such a gradient recovery method can (after scaling) be used as a quasi-normal field n_h on Γ_h. The corresponding oblique projection and approximate signed distance function are denoted by p_h and d_h, respectively. We recall that, by construction, the zero level of d_h equals Γ_h. Using the method given in section 5, for z sufficiently close to Γ_h the value of $p_h(z)$, and thus of $d_h(z)$, can be determined. This leads to the final step in our approximation process, namely, the *nodal interpolation* of d_h in vertices $v \in V(\mathcal{T}_{\Gamma_h})$ in the finite element space $V_h(\Omega_{\Gamma_h})$. The result is denoted by $\tilde{d}_h = I_h d_h$ and for the zero level of $\tilde{d}_h$ we use the notation $\tilde{\Gamma}_h$. The finite element function $\tilde{d}_h$ is the output of our initialization phase. We emphasize that for computing $\tilde{d}_h$ *we only need evaluations of* ϕ_h on the neighborhood $\Omega^e_{\Gamma_h}$ of Γ_h. Hence, we do *not* construct an approximation of the zero level Γ_h.

In section 7.1 we show that the scaled recovered gradient forms a quasi-normal field on Γ_h and that for the orthogonality measure δ_x in (3.5) we have $\delta_x \lesssim h^k$. Using this and the analysis in section 4 we derive an estimate that quantifies in which sense the output $\tilde{d}_h = I_h d_h$ of the initialization phase is "close to" the *exact* signed distance function to Γ_h; cf. Theorem 7.3. Furthermore, we show that $\tilde{\Gamma}_h$ has optimal accuracy, namely, $\text{dist}(\tilde{\Gamma}_h, \Gamma_h) \lesssim h^{k+1}$. The precise result is given in Theorem 7.7.

6.2. The polynomial-preserving recovery (PPR) method. Gradient recovery techniques are often used in error estimators; cf., e.g., [2]. A famous example is the gradient recovery method introduced by Zienkiewicz and Zhu (ZZ) [22, 23], known as the superconvergence patch recovery (SPR), which forms the basis of the ZZ error estimator. Basically, the SPR uses a least squares fit to the *gradient* of the finite element function to recover a *continuous* gradient. Another method, the so-called PPR is introduced in [21] and analyzed in [10]. In PPR one applies a least squares fit *directly to the finite element function* and based on this fit a *continuous* gradient is determined. The reason that we use PPR is that for this method more theoretical analyses, e.g., error bounds as in [10], are known. We emphasize, however, that in the initialization method, presented in section 6.3, one could replace the PPR method by another gradient recovery algorithm. The general description (i.e., $N = 2, 3,\ k \geq 1$) of the PPR method is given in [10]. To simplify the presentation, we restrict ourselves to the cases $N = 3,\ k = 1, 2$.

For $v \in N(\mathcal{T}_h)$ let ψ_v be the corresponding nodal finite element basis function. Below we explain how, given the set of function values $\{\, \phi_h(v) \mid v \in N(\mathcal{T}_h) \,\}$, the gradient recovery vectors $\{\, (G_h\phi_h)(v) \mid v \in N(\mathcal{T}_h) \,\}$ are constructed. The induced continuous gradient recovery finite element vector function is given by the operator $G_h : V_h \to V_h^3$:

$$G_h\phi_h := \sum_{v \in N(\mathcal{T}_h)} (G_h\phi_h)(v)\psi_v \in V_h^3. \tag{6.3}$$

The function $G_h\phi_h$ is a continuous finite element approximation of the gradient $(G_h\phi_h)(x) \approx \nabla\phi(x)$. In the application of the PPR method in section 6.3 we use the gradient recovery only "close to Γ_h." More precisely, we only need

$$(G_h\phi_h)_{|\Omega_{\Gamma_h}} = \sum_{v \in N(\mathcal{T}_{\Gamma_h})} (G_h\phi_h)(v)\psi_v. \tag{6.4}$$

It remains to explain how the vectors $(G_h\phi_h)(v),\ v \in N(\mathcal{T}_{\Gamma_h})$ are determined. We first consider $k = 1$. In this case the set of finite element nodes and the set of vertices coincide: $V(\mathcal{T}_{\Gamma_h}) = N(\mathcal{T}_{\Gamma_h})$. Take $v \in V(\mathcal{T}_{\Gamma_h})$ and the corresponding neighborhood $\omega(v)$. Let p_v be the polynomial of degree 2 that fits ϕ_h in a least-squares sense:

$$\sum_{z \in V(\omega(v))} |(\phi_h(z) - p_v(z)|^2 = \min_{p \in \mathcal{P}_2} \sum_{z \in V(\omega(v))} |(\phi_h(z) - p(z)|^2.$$

We assume that this least-squares problem has a unique solution p_v and define $(G_h\phi_h)(v) := \nabla p_v(v)$. Note that the polynomial p_v is uniquely defined if we have at least 10 independent conditions. In our applications this holds, since we typically have 11–14 edges that have v as a vertex. If there are not enough independent conditions one can enlarge the neighborhood $\omega(v)$ by including further neighboring simplices. This approach is explained in [10]. For ease of implementation we propose to use a simpler (but theoretically less favorable) approach. In the case of fewer than

10 independent conditions we fit a polynomial of degree 2 (or 1) with fewer degrees of freedom. For example, we set the coefficient corresponding to xy and/or xz and/or yz to zero. Another possibility is to use a local refinement of one or more of the $T \in \omega(v)$ and thus create more conditions.

We now consider $k = 2$, and thus $V(\mathcal{T}_{\Gamma_h}) \neq N(\mathcal{T}_{\Gamma_h})$. We first take $v \in V(\mathcal{T}_{\Gamma_h})$. The approach is the same as above: we fit a polynomial p_v of degree 3 to the values in all *nodes* in $\omega(v)$:

$$\sum_{z \in N(\omega(v))} |(\phi_h(z) - p_v(z)|^2 = \min_{p \in \mathcal{P}_3} \sum_{z \in N(\omega(v))} |(\phi_h(z) - p(z)|^2. \tag{6.5}$$

We assume a unique solution p_v (which is generally true in our applications) and define $(G_h\phi_h)(v) := \nabla p_v(v)$. We now consider $v \in N(\mathcal{T}_{\Gamma_h}) \setminus V(\mathcal{T}_{\Gamma_h})$. Let v be the midpoint of an edge with vertices v_1 and v_2. We define $(G_h\phi_h)(v) := \frac{1}{2}\big(\nabla p_{v_1}(v) + \nabla p_{v_1}(v)\big)$, where p_{v_i} are the least-squares polynomials defined in (6.5).

6.3. The initialization phase. As *input* for the method we need (only) $\mathcal{T}^e_{\Gamma_h}$ and $\{\, \phi_h(v) \mid v \in N(\mathcal{T}^e_{\Gamma_h}) \,\}$. Note that we do *not* need an approximation of Γ_h. The output is a finite element function $I_h d_h \in V_h(\mathcal{T}_{\Gamma_h})$ that is "close to" the (local) signed distance function to Γ_h.

Given $\{\, \phi_h(v) \mid v \in N(\mathcal{T}^e_{\Gamma_h}) \,\}$, the PPR method described in (6.4) results in $G_h\phi_h \in V_h(\mathcal{T}^e_{\Gamma_h})^3$, with $(G_h\phi_h)(x) \approx \nabla\phi(x)$ for $x \in \Omega_{\Gamma_h}$ (cf. section 7). We define

$$n_h(x) = \|(G_h\phi_h)(x)\|^{-1}(G_h\phi_h)(x), \quad x \in \Omega_{\Gamma_h}. \tag{6.6}$$

As we will indicate in section 7, it is reasonable to assume that this function satisfies the conditions of a quasi-normal field on Γ_h as formulated in Definition 3.3. Hence, for z close to Γ_h the approximate signed distance function $d(z)$ (cf. Definition 3.4), is well defined. To emphasize the dependence on the triangulation $\mathcal{T}_h$, we write d_h instead of d. For $h \downarrow 0$ the points $z \in \Omega_{\Gamma_h}$ can be forced to be sufficiently close to Γ_h. We assume that h is small enough such that the approximate signed distance function $d_h(z)$ is well defined for $z \in \Omega_{\Gamma_h}$. Note that the function d_h is close to the exact signed distance function to Γ_h (cf. Theorems 4.2 and 4.3), and it *has* Γ_h *as its zero level*:

$$\{\, x \in \Omega_{\Gamma_h} \mid d_h(x) = 0 \,\} = \Gamma_h.$$

Clearly, $d_h(z),\ z \in \Omega_{\Gamma_h}$, is not explicitly available. Therefore we introduce a nodal interpolation $I_h d_h \in V_h(\Omega_{\Gamma_h})$ of d_h given by

$$I_h d_h(v) = d_h(v) \quad \text{for all} \ \ v \in N(\mathcal{T}_{\Gamma_h}). \tag{6.7}$$

This finite element function $I_h d_h$ is the output of our initialization phase. Clearly, the interpolation procedure introduces an interpolation error that causes a change in the zero level, i.e.,

$$\tilde{\Gamma}_h := \{\, x \in \Omega_{\Gamma_h} \mid (I_h d_h)(x) = 0 \,\} \approx \Gamma_h. \tag{6.8}$$

The error in the approximation $\tilde{\Gamma}_h \approx \Gamma_h$ will be analyzed in the next section. It remains to discuss how $d_h(v),\ v \in N(\mathcal{T}_{\Gamma_h})$, can be computed. For this we use an obvious variant of the method explained in section 5. Given a node $v \in N(\mathcal{T}_{\Gamma_h})$ and $x^k \in \Gamma_h$, $x^k \approx p(v)$, we have to determine the zero of

$$\phi_h(v - \alpha\, n_h(x^k)) = 0; \tag{6.9}$$

cf. (5.1). This can be realized by, for example, the following *approximate* Newton line search: $\alpha_0 := 0$ and

$$\alpha_{n+1} = \alpha_n + \frac{\phi_h(v - \alpha_n n_h(x^k))}{(G_h\phi_h)(v - \alpha_n n_h(x^k)) \cdot n_h(x^k)}, \quad n = 0, 1, \dots. \tag{6.10}$$

The iteration in (5.1) takes the form

$$x^{k+1} = v - \alpha\, n_h(x^k) \tag{6.11}$$

with an α that solves (6.9). A starting vector $x^0 \in \Gamma_h$ can be determined as follows. Notice that the quasi-normal field n_h is defined not only on Γ_h but also on Ω_{Γ_h}. Hence, one can define $x^0 := v - \alpha\, n_h(v)$, with α such that $\phi_h(v - \alpha\, n_h(v)) = 0$ holds.

In the iterations (6.10), (6.11) the work per iteration is "low" since one only has to evaluate the known finite element functions ϕ_h, $G_h\phi_h$, and n_h. These iterations converge if v is sufficiently close to Γ_h; cf. section 5. Furthermore, the contraction of the iteration (6.11) can be bounded by $c|d(v)|$; cf. Theorem 5.1 for the precise statement. In the initialization phase we have $v \in N(\mathcal{T}_{\Gamma_h})$ and thus $|d(v)| = \mathcal{O}(h)$, i.e., we have "fast" convergence for small h.

The iteration (6.11) is stopped when a suitable tolerance criterion is satisfied. The oblique projection of v is then given by $p_h(v) = x^{k+1}$, and the value of $d_h(v)$ follows from the relation $d_h(v) = \langle v - p_h(v), n_h(p_h(v))\rangle$.

Concerning the practical realization of the algorithm there are several issues that should be addressed. For example. it might be better to replace (6.10) by a damped variant to guarantee that the iterates remain in Ω_{Γ_h}. Furthermore it might be necessary to choose a better starting value than $x^0 := v - \alpha\, n_h(v)$ proposed above. These and other numerical issues will be investigated in a forthcoming paper.

7. Analysis of the PPR based initialization phase. In this section we use the results derived in section 4 to analyze the initialization phase presented in section 6.3. We consider the following setting. We assume that Γ is the zero level of a level set function ϕ, i.e., $\Gamma = \{\, x \in \Omega \mid \phi(x) = 0 \,\}$. The analysis is restricted to a (small) neighborhood $U \subset \Omega$ of Γ. We assume that ϕ is smooth on U ($\phi \in C^{k+1}(U)$) and that there are constants $c_L > 0$ and c_U such that

$$c_L \le \|\nabla\phi(x)\| \le c_U \quad \text{for all} \;\; x \in U. \tag{7.1}$$

Let there be given a finite element function $\phi_h \in V_h$ that is an optimal approximation of ϕ in the neighborhood U, in the sense that

$$\|\phi - \phi_h\|_{L^\infty(U)} + h\|\phi - \phi_h\|_{W^{1,\infty}(U)} \lesssim h^{k+1} \tag{7.2}$$

holds. Here and in the remainder we use the notation $a \lesssim b$ to denote $a \le cb$ with a constant c independent of h. In applications, the finite element function ϕ_h is known and used as input for the initialization phase. Recall that the zero level of ϕ_h, which for $k \ge 2$ cannot be determined explicitly, is denoted by Γ_h; cf. (6.2). As output of the initialization phase we obtain $I_h d_h \in V_h$ as in (6.7), with a zero level denoted by $\tilde\Gamma_h$; cf. (6.8). Note that $\tilde\Gamma_h$ can also not be determined explicitly for $k \ge 2$.

7.1. Recovered gradient as a quasi-normal field on Γ_h. In this section we assume that (7.1) and (7.2) hold and we show that the scaled recovered gradient (6.6) is a quasi-normal field on Γ_h (but not necessarily on Γ!). In the analysis we also need certain properties of the PPR gradient recovery operator $G_h : V_h \to V_h^N$. This operator has been analyzed in [21, 10]. In our analysis we need the following two approximation and stability properties:

$$\|G_h(I_h\phi) - \nabla\phi\|_{L^\infty(U)} \lesssim h^{k+1}, \tag{7.3}$$

$$\|G_h v_h\|_{L^\infty(U)} \le c\|v_h\|_{W^{1,\infty}(U^e)} \quad \text{for all } \ v_h \in V_h, \tag{7.4}$$

with a constant c independent of v_h and h. Here U^e denotes the neighborhood U extended with a suitable patch of surrounding elements (we refer to [10] for the details). The approximation result (7.3) follows from the Bramble–Hilbert lemma and the fact that G_h has the consistency property $G_h(I_h p) = \nabla p$ for all $p \in \mathcal{P}_k$. The stability property (7.4) is proved for $N = 2$ (under mild assumptions on the triangulation $\mathcal{T}_h$) in [10]. A proof of this property for $N = 3$ is not known to us.

In the remainder we assume that (7.3) and (7.4) hold. In the following two lemmas, we show that the scaled recovered gradient n_h defined in (6.6) satisfies the two conditions (3.4) and (3.5) for a quasi-normal field on Γ_h.

LEMMA 7.1. *Consider n_h as in (6.6). There exist constants c and $h_0 > 0$ such that for all $h \le h_0$ the following holds:*

$$\|n_h(x) - n_h(y)\| \le c\|x - y\| \quad \textit{for all } \ x \in \Gamma_h, \quad y \in B(x; r_x), \tag{7.5}$$

with r_x sufficiently small such that $B(x; r_x) \subset U$.

Proof. Take $x \in \Gamma_h$ and $y \in B(x; r_x) \subset U$. Inserting the definition we get

$$\begin{aligned} \|n_h(x) - n_h(y)\| &= \left\| \frac{(G_h\phi_h)(x)}{\|(G_h\phi_h)(x)\|} - \frac{(G_h\phi_h)(y)}{\|(G_h\phi_h)(y)\|} \right\| \\ &\le 2\frac{\|(G_h\phi_h)(x) - (G_h\phi_h)(y)\|}{\|(G_h\phi_h)(x)\|}. \end{aligned} \tag{7.6}$$

We write $G_h\phi_h = G_h(\phi_h - I_h\phi) + (G_h(I_h\phi) - \nabla\phi) + \nabla\phi$, and using (7.3), (7.4), (7.1), (7.2), and the interpolation bound $\|\phi - I_h\phi\|_{W^{1,\infty}(U^e)} \lesssim h^k$ we get

$$\begin{aligned} \|(G_h\phi_h)(x)\| &\ge \|\nabla\phi(x)\| - c\|\phi_h - I_h\phi\|_{W^{1,\infty}(U^e)} - c\|G_h(I_h\phi) - \nabla\phi\|_{L^\infty(U)} \\ &\ge c_L - ch^k. \end{aligned}$$

Hence, for h sufficiently small we have

$$\|(G_h\phi_h)(x)\| \ge \frac{1}{2}c_L. \tag{7.7}$$

The vector function $G_h v_h \in V_h^3$ is Lipschitz continuous and

$$\|(G_h\phi_h)(x) - (G_h\phi_h)(y)\| \le \int_0^1 \|\nabla(G_h\phi_h)(x + t(x - y))\|\, dt\|x - y\| \tag{7.8}$$

holds. We write $z := x + t(x - y) \in B(x; r_x)$ and note that

$$\|\nabla(G_h\phi_h)(z)\| \le \|\nabla\big(G_h\phi_h - I_h(\nabla\phi)\big)\|_{L^\infty(U)} + \|\nabla I_h(\nabla\phi)\|_{L^\infty(U)}.$$

Using an inverse inequality and the boundedness of I_h on $W^{1,\infty}(U)$ we get

$$\|\nabla(G_h\phi_h)(z)\| \lesssim h^{-1}\|G_h\phi_h - I_h(\nabla\phi)\|_{L^\infty(U)} + 1,$$

and using (7.3), (7.4) results in

$$\begin{aligned}\|\nabla(G_h\phi_h)(z)\| &\lesssim h^{-1}\|G_h(\phi_h - I_h\phi)\|_{L^\infty(U)} + h^{-1}\|G_h(I_h\phi) - \nabla\phi\|_{L^\infty(U)} \\ &\quad + h^{-1}\|\nabla\phi - I_h(\nabla\phi)\|_{L^\infty(U)} + 1 \\ &\lesssim h^{-1}\|\phi_h - I_h\phi\|_{W^{1,\infty}(U^e)} + h^k + 1 \lesssim h^{k-1} + 1 \lesssim 1.\end{aligned} \tag{7.9}$$

Using this result in (7.8), in combination with (7.7) and (7.6) completes the proof. □

LEMMA 7.2. *There exist constants c_1, c_2 and $h_0 > 0$ such that for $h \le h_0$ and all $x \in \Gamma_h$, $y \in \Gamma_h \cap B(x; r_x)$, with r_x sufficiently small such that $B(x; r_x) \subset U$, the following holds:*

$$|\langle n_h(x), x - y\rangle| \le c_1 h^k \|x - y\| + c_2\|x - y\|^2.$$

Proof. Using the definition of n_h and the lower bound in (7.7) results in

$$|\langle n_h(x), x - y\rangle| \le \frac{2}{c_L}|\langle(G_h\phi_h)(x), x - y\rangle|. \tag{7.10}$$

Since $x, y \in \Gamma_h$ we have $0 = \phi_h(x) - \phi_h(y) = \int_0^1 \langle\nabla\phi_h(x + t(y - x)), x - y\rangle\, dt$. Using this relation we obtain

$$\begin{aligned}\langle(G_h\phi_h)(x), x - y\rangle &= \int_0^1 \langle(G_h\phi_h)(x) - (G_h\phi_h)(x + t(y - x)), x - y\rangle\, dt \\ &\quad + \int_0^1 \langle(G_h\phi_h)(x + t(y - x)) - \nabla\phi_h(x + t(y - x)), x - y\rangle\, dt.\end{aligned} \tag{7.11}$$

From the Lipschitz continuity estimate (7.8)–(7.9), with y replaced by $x + t(y - x) \in B(x, r_x)$, we get

$$|\langle(G_h\phi_h)(x) - (G_h\phi_h)(x + t(y - x)), x - y\rangle| \le c\|x - y\|^2. \tag{7.12}$$

For the second term on the right-hand side in (7.11) we get

$$\begin{aligned}&|\langle(G_h\phi_h)(x + t(y - x)) - \nabla\phi_h(x + t(y - x)), x - y\rangle| \\ &\quad \le \|G_h\phi_h - \nabla\phi_h\|_{L^\infty(U)}\|x - y\| \\ &\quad \le \Big(\|G_h(\phi_h - I_h\phi)\|_{L^\infty(U)} + \|G_h(I_h\phi) - \nabla\phi\|_{L^\infty(U)} + \|\nabla\phi - \nabla\phi_h\|_{L^\infty(U)}\Big)\|x - y\| \\ &\quad \lesssim \big(\|\phi_h - I_h\phi\|_{W^{1,\infty}(U^e)} + h^{k+1} + h^k\big)\|x - y\| \lesssim h^k\|x - y\|.\end{aligned}$$

Using this and (7.12) in (7.11) in combination with (7.10) completes the proof. □

From the lemmas above we conclude that indeed n_h defines a quasi-normal field on Γ_h and that for the parameter δ_x in (3.5) we have $\delta_x \le ch^k$ with a constant c independent of $x \in \Gamma_h$.

7.2. Accuracy of the initialization phase. In this section, we use the properties of n_h derived in the previous section and apply the results of section 4 to derive properties of the signed distance function d_h and the zero level $\tilde{\Gamma}_h$ given in (6.8).

The results in section 4, e.g., in Theorems 4.2 and 4.3, hold in a neighborhood $F(D)$ of the manifold. Using the fact that $\lim_{h\to 0} \operatorname{dist}(\Gamma_h, \Gamma) = 0$ (follows from

(7.2)) and the results in Lemmas 7.1 and 7.2 one can check that the width of this neighborhood $F(D)$ around Γ_h is bounded from below by a strictly positive constant uniformly for $h \to 0$. Hence, for h sufficiently small the local neighborhood Ω_{Γ_h}, that has width $\mathcal{O}(h)$ is contained in the neighborhood $F(D)$.

Let d_h^{ex} denote the *exact* signed distance function to Γ_h. As output of the initialization phase we obtain $I_h d_h$; cf. (6.7). In the next theorem, which is an immediate consequence of Theorem 4.3, we quantify the statement that $I_h d_h$ is "close to" the exact signed distance function to d_h^{ex}.

THEOREM 7.3. *There exist constants c and $h_0 > 0$ such that for $h \leq h_0$ the following holds:*

$$0 \leq \frac{|I_h d_h(v)| - |d_h^{ex}(v)|}{|d_h^{ex}(v)|} \leq ch^k \tag{7.13}$$

for all nodes $v \in N(\mathcal{T}_{\Gamma_h})$, $v \notin \Gamma_h$, that fulfill the condition, specified in Theorem 4.3, *that $L_{x_0,v} \cap N_s$ has one-dimensional measure zero.*

Proof. We apply Theorem 4.3. For h sufficiently small we have $v \in F(D)$. For $v \in N(\mathcal{T}_{\Gamma_h})$ we have $I_h d_h(v) = d_h(v)$. Due to Lemma 7.2 the parameter δ_L in Theorem 4.3 is bounded by ch^k. ◻

In the generic case the condition "$L_{x_0,v} \cap N_s$ has one-dimensional measure zero" used in the theorem above is satisfied. In the remainder of this section we analyze the accuracy of the perturbed zero level $\tilde{\Gamma}_h$ compared to that of Γ_h. We start with the accuracy of the latter as an approximation of the zero level Γ of the "exact" level set solution ϕ. The exact signed distance function to Γ is denoted by d^{ex}. The exact normal field on Γ is denoted by $n_\Gamma(x)$, $x \in \Gamma$. We take a (sufficiently small) neighborhood U of Γ such that for all $z \in U$ there exists a unique $p(z) = x \in \Gamma$ such that $z = p(z) + d^{ex}(z) n_\Gamma(p(z))$; cf. (3.12). Furthermore, to simplify the analysis, we assume that $\Gamma_h \subset U$ is the graph of a function on Γ in the following sense: there exists a function $g : \Gamma \to \mathbb{R}$ such that $\Gamma_h = \{\, x + g(x) n_\Gamma(x) \mid x \in \Gamma \,\}$. Then $d^{ex}(z) = g(p(z))$ holds for all $z \in \Gamma_h$.

LEMMA 7.4. *Define $c_H := \max_{z \in \bar{U}} \|\nabla^2 \phi(z)\| < \infty$ Assume that* (7.1) *and* (7.2) *are satisfied and that $|d^{ex}(z)| \leq c_L c_H^{-1}$ holds for all $z \in \Gamma_h$. For $h_0 > 0$ sufficiently small and $h \leq h_0$ the following holds:*

$$\operatorname{dist}(\Gamma_h, \Gamma) := \max_{z \in \Gamma_h} |d^{ex}(z)| \lesssim h^{k+1}. \tag{7.14}$$

Proof. Take $z = p(z) + d^{ex}(z) n_\Gamma(p(z)) \in \Gamma_h$. Hence, $|d^{ex}(z)| = \|z - p(z)\|$ holds. From a Taylor expansion we obtain, for suitable ξ,

$$\phi(z) - \phi(p(z)) = \nabla \phi(p(z))^T (z - p(z)) + \frac{1}{2}(z - p(z))^T \nabla^2 \phi(\xi)(z - p(z)).$$

Since $\nabla \phi(p(z))$ and $z - p(z)$ are aligned we obtain, using $\phi(p(z)) = \phi_h(z) = 0$,

$$\begin{aligned}
&\|\nabla \phi(p(z))\| \|z - p(z)\| \\
&\quad = |\nabla \phi(p(z))^T (z - p(z))| \leq \|\phi(z) - \phi(p(z))\| + \frac{1}{2} c_H \|z - p(z)\|^2 \\
&\quad = \|\phi(z) - \phi_h(z)\| + \frac{1}{2} c_H \|z - p(z)\|^2 \leq ch^{k+1} + \frac{1}{2} c_H \|z - p(z)\|^2.
\end{aligned}$$

From (7.1), (7.2), and $\|z - p(z)\| \leq c_L c_H^{-1}$ we then get $\|z - p(z)\| \lesssim h^{k+1}$. ◻

In the next lemma we show that from the result in (7.14) it follows that the signed distance functions d_h^{ex} and d^{ex} to Γ_h and Γ, respectively, are close.

LEMMA 7.5. *Let the assumptions as in Lemma* 7.5 *be fulfilled. For* $h_0 > 0$ *sufficiently small and* $h \le h_0$ *the following holds:*

$$\|d_h^{ex} - d^{ex}\|_{L^\infty(U)} \lesssim h^{k+1}. \tag{7.15}$$

Proof. Take $z \in U$. First we consider the case that $d_h^{ex}(z)$ and $d^{ex}(z)$ have the same sign. Then $|d_h^{ex}(z) - d^{ex}(z)| = \big||d_h^{ex}(z)| - |d^{ex}(z)|\big|$ holds. Let $z_h^* \in \Gamma_h$ be such that $|d_h^{ex}(z)| = \|z - z_h^*\|$. Since $p(z_h^*) \in \Gamma$, we get, using (7.14),

$$|d^{ex}(z)| - |d_h^{ex}(z)| \le \|z - p(z_h^*)\| - \|z - z_h^*\| \le \|z_h^* - p(z_h^*)\| = |d^{ex}(z_h^*)| \lesssim h^{k+1}.$$

Take $y_h^* := p(z) + g(p(z))n_\Gamma(p(z)) \in \Gamma_h$. With (7.14) we obtain

$$\begin{aligned}|d_h^{ex}(z)| - |d^{ex}(z)| &\le \|z - y_h^*\| - \|z - p(z)\| \\ &\le |g(p(z))| = |g(p(y_h^*))| = |d^{ex}(y_h^*)| \lesssim h^{k+1}.\end{aligned}$$

Now we treat the case that $d_h^{ex}(z)$ and $d^{ex}(z)$ have opposite sign. With y_h^* as defined above we get

$$|d_h^{ex}(z) - d^{ex}(z)| = \|z - p(z)\| + \min_{x \in \Gamma_h} \|z - x\| \le \|z - p(z)\| + \|z - y_h^*\|.$$

Due to the sign property, z is located on the line segment that connects $p(z)$ with y_h^*. Hence,

$$|d_h^{ex}(z) - d^{ex}(z)| \le \|p(z) - y_h^*\| = |g(p(z))| = |g(p(y_h^*))| = |d^{ex}(y_h^*)| \lesssim h^{k+1}$$

holds. ∎

We are now in a position to derive a bound for the difference between the interpolated approximate signed distance function $I_h d_h \in V_h$, that results from the initialization phase, and the signed distance functions d^{ex} and d_h^{ex} to the zero levels Γ and Γ_h, respectively.

LEMMA 7.6. *Let the assumptions as in Lemma* 7.5 *be satisfied. In addition we assume (the generic case) that all* $v \in N(\mathcal{T}_{\Gamma_h})$ *fulfill the condition that* $L_{x_0,v} \cap N_s$ *has one-dimensional measure zero (cf. Theorem* 4.3*). For* $h_0 > 0$ *sufficiently small and* $h \le h_0$ *the following hold:*

$$\|I_h d_h - d^{ex}\|_{L^\infty(\Omega_{\Gamma_h})} \lesssim h^{k+1}, \tag{7.16}$$

$$\|I_h d_h - d_h^{ex}\|_{L^\infty(\Omega_{\Gamma_h})} \lesssim h^{k+1}. \tag{7.17}$$

Proof. From Theorem 4.3 it follows that $\big||I_h d_h(v)| - |d_h^{ex}(v)|\big| \lesssim h^{k+1}$ holds, uniformly for $v \in N(\mathcal{T}_{\Gamma_h})$. Since per construction $I_h d_h(v)$ and $d_h^{ex}(v)$ have the same sign, we get $\max_{v \in N(\mathcal{T}_{\Gamma_h})} |d_h(v) - d_h^{ex}(v)| \lesssim h^{k+1}$, and thus,

$$\|I_h(d_h - d_h^{ex})\|_{L^\infty(\Omega_{\Gamma_h})} \le c \max_{v \in N(\mathcal{T}_{\Gamma_h})} |d_h(v) - d_h^{ex}(v)| \lesssim h^{k+1}.$$

From the smoothness of d^{ex} (close to Γ) we get $\|I_h d^{ex} - d^{ex}\|_{L^\infty(\Omega_{\Gamma_h})} \lesssim h^{k+1}$. Combining these results with the result in (7.15) we get

$$\begin{aligned}\|I_h d_h - d^{ex}\|_{L^\infty(\Omega_{\Gamma_h})} &\le \|I_h(d_h - d_h^{ex})\|_{L^\infty(\Omega_{\Gamma_h})} + \|I_h(d_h^{ex} - d^{ex})\|_{L^\infty(\Omega_{\Gamma_h})} \\ &\quad + \|I_h d^{ex} - d^{ex}\|_{L^\infty(\Omega_{\Gamma_h})} \lesssim h^{k+1} + \|d_h^{ex} - d^{ex}\|_{L^\infty(\Omega_{\Gamma_h})} \\ &\lesssim h^{k+1},\end{aligned}$$

hence (7.16) holds. The result in (7.17) follows from (7.15) and (7.16). ∎

As a direct consequence of Lemma 7.6 we obtain a result on the accuracy of the zero level $\tilde{\Gamma}_h$ of $I_h d_h$; cf. (6.8).

THEOREM 7.7. *Let the assumptions of Lemma* 7.6 *be fulfilled. For* $h_0 > 0$ *sufficiently small and* $h \le h_0$ *the following hold:*

$$\operatorname{dist}(\tilde{\Gamma}_h, \Gamma) := \max_{z \in \tilde{\Gamma}_h} |d^{ex}(z)| \lesssim h^{k+1}, \tag{7.18}$$

$$\operatorname{dist}(\tilde{\Gamma}_h, \Gamma_h) := \max_{z \in \tilde{\Gamma}_h} |d_h^{ex}(z)| \lesssim h^{k+1}. \tag{7.19}$$

Proof. Take $z \in \tilde{\Gamma}_h$, hence $(I_h d_h)(z) = 0$. Using (7.16) we obtain

$$|d^{ex}(z)| = |(I_h d_h)(z) - d^{ex}(z)| \le \|I_h d_h - d^{ex}\|_{L^\infty(\Omega_{\Gamma_h})} \lesssim h^{k+1},$$

which proves the result in (7.18). Using (7.17) the same argument can be applied to prove (7.19). ∎

We conclude that under reasonable assumptions the PPR based initialization phase results in a reinitialization $I_h d_h \in V_h$, which locally (i.e., on Ω_{Γ_h}) differs at most $\mathcal{O}(h^{k+1})$ from the exact signed distance function d_h^{ex} to Γ_h. Furthermore, the perturbation of the zero level caused by the reinitialization is also at most $\mathcal{O}(h^{k+1})$.

8. Numerical experiments. In this section we present results of numerical experiments. Related to the PPR based initialization algorithm introduced in section 6.3 there are several numerical issues that need further investigations; cf. section 9. Here we consider only a few relatively simple test problems and illustrate the theoretical accuracy bounds derived in section 7.2.

Example 1. For the manifold Γ we take the torus, characterized by the distance function

$$d^{ex}(x) = \sqrt{x_3^2 + \left(\sqrt{x_1^2 + x_2^2} - R\right)^2} - r,$$

with radii $r = 0.2$ and $R = 0.4$. For computations Γ is embedded in $\Omega := [-1, 1]^3$.

Example 2. We consider a manifold Γ illustrated in Figure 8.1, which we call the apple. It consists of the combination of a half-sphere with a large radius, a half-torus, and a half-sphere with a small radius. For this manifold a formula for the exact distance function d^{ex} can be derived. In this example the variation of the curvature is significantly larger than for the torus in Example 1. The manifold is embedded in $\Omega := [-1.5, 1.5]$.

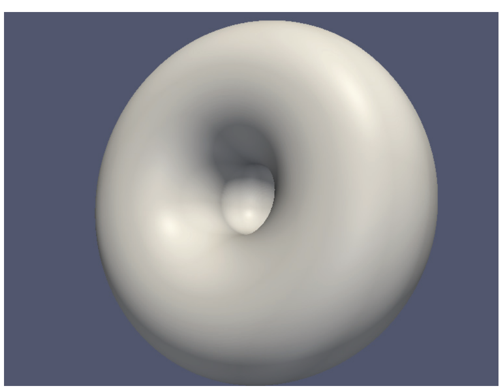

FIG. 8.1. *Manifold* Γ *in Example* 2*: the apple.*

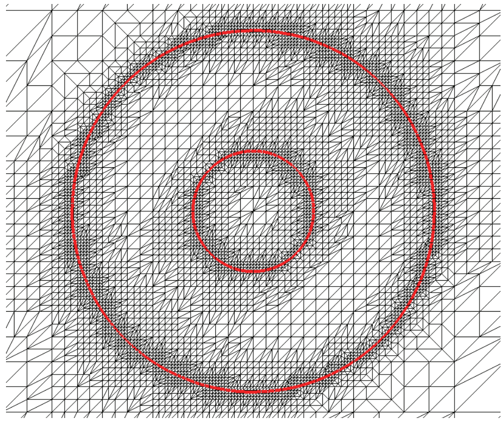

FIG. 8.2. *Cross section of tetrahedral triangulation on level $\ell = 5$.*

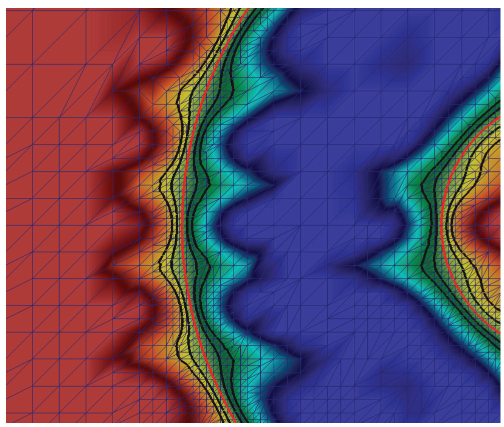

FIG. 8.3. *Level lines of function $\phi^{(\alpha)}$ for $\alpha = 50$.*

We construct finite element spaces as follows. First a uniform tetrahedral triangulation of Ω with mesh size parameter $h_0 = 2/3$ (Example 1) or $h_0 = 1.0$ (Example 2) is constructed. This uniform grid is locally refined in a neighborhood of Γ by using a red-green procedure. This results in triangulations with mesh size parameters $h_\ell = 2^{-\ell}h_0$, $\ell = 1, 2, \ldots 8$, close to Γ. These triangulations are denoted by $\mathcal{T}_\ell$. A cross section of the level $\ell = 5$ triangulation in Example 1 is given in Figure 8.2.

We use standard finite element spaces with polynomials of degree $k = 1$ and $k = 2$:

$$V_\ell^k = \{\, \psi \in C(\Omega) \mid \psi_{|T} \in \mathcal{P}_k \;\text{ for all }\; T \in \mathcal{T}_\ell \,\}, \quad k = 1, 2.$$

The nodal interpolation corresponding to this space is denoted by I_h, with $h = h_\ell$. As exact level set function we take a perturbation of d^{ex}, given by $\phi^{(\alpha)} = d^{ex} q^{(\alpha)}$, with

$$q^{(\alpha)}(x) = 9.0 + 4.0 \cos\left(\alpha x_1 x_2 / ||x||_2\right), \quad \alpha \in \{1, 10, 50\}.$$

Note that $\phi^{(\alpha)}$ has Γ as its zero level, it has a large gradient, and for increasing α it becomes more and more distorted. For $\alpha = 50$ the level lines of $\phi^{(\alpha)}$ on the same cross section as in Figure 8.2 are illustrated in Figure 8.3. The four level lines shown in the figure correspond to the values $\phi^{(\alpha)} = -0.2, \ -0.1, \ 0.1, \ 0.2$.

As input for the initialization phase we take $\phi_h^{(\alpha)} = I_h \phi^{(\alpha)}$. Note that for $k = 2$ the zero level Γ_h of $\phi_h^{(\alpha)}$ can not be constructed explicitly. We implemented the initialization phase described in section 6.3. We summarize its main components as follows.

- Based on sign properties the local triangulation $\mathcal{T}_{\Gamma_h}$ that contains Γ_h is determined.
- The recovered gradient $G_h\phi_h^{(\alpha)} \in V_\ell^k(\mathcal{T}_{\Gamma_h}^e)^3$ and its normalization $n_h(v) = \|(G_h\phi_h^{(\alpha)})(v)\|^{-1}(G_h\phi_h^{(\alpha)})(v)$, $v \in N(\mathcal{T}_{\Gamma_h})$ are determined.
- For $v \in N(\mathcal{T}_{\Gamma_h})$ the approximate signed distance value $d_h^{(\alpha)}(v)$ is determined by using (6.10)–(6.11).
- Nodal interpolation results in the finite element function $I_h d_h^{(\alpha)} \in V_h^k(\Omega_{\Gamma_h})$, which is the output of the initialization phase.

Since the signed distance function d_h^{ex} to Γ_h (the zero level of $\phi_h^{(\alpha)}$) is not known, we compare the output $I_h d_h^{(\alpha)}$ to the *exact signed distance function* d^{ex} to Γ. We use the following error measure:

$$e_\infty := \max_{v \in N(\mathcal{T}_{\Gamma_h})} |I_h d_h(v) - d^{\mathrm{ex}}(v)|.$$

Furthermore, to measure the size of the gradient of $I_h d_h$ on Ω_{Γ_h} we determine

$$e_\infty^\nabla := \max_{T \in \mathcal{T}_{\Gamma_h}} \left| \sqrt{\frac{1}{|T|}\int_T ||\nabla(I_h d_h)(s)||^2\, ds} - 1 \right|.$$

The results for Example 1 are shown in the Tables 8.1, 8.2, and 8.3, for the cases $\alpha = 1, 10, 50$, respectively.

TABLE 8.1
Example 1: Errors and order of convergence for $\alpha = 1$.

ℓ	$k=1$ e_∞	order	$k=1$ e_∞^∇	order	ℓ	$k=2$ e_∞	order	$k=2$ e_∞^∇	order
3	1.21*e*-2	-	2.50*e*-1	-	3	5.73*e*-4	-	1.66*e*-2	-
4	3.01*e*-3	2.00	1.53*e*-1	0.71	4	7.21*e*-5	2.99	3.46*e*-3	2.26
5	7.54*e*-4	2.00	8.32*e*-2	0.87	5	9.94*e*-6	2.86	8.70*e*-4	1.99
6	1.90*e*-4	1.99	4.25*e*-2	0.97	6	1.24*e*-6	3.01	2.13*e*-4	2.03
7	4.68*e*-5	2.02	2.12*e*-2	1.00	7	1.58*e*-7	2.96	5.31*e*-5	2.01
8	1.19*e*-5	1.98	1.07*e*-2	0.99	8	2.07*e*-8	2.93	1.34*e*-5	1.98

TABLE 8.2
Example 1: Errors and order of convergence for $\alpha = 10$.

ℓ	$k=1$ e_∞	order	$k=1$ e_∞^∇	order	ℓ	$k=2$ e_∞	order	$k=2$ e_∞^∇	order
3	1.15*e*-2	-	2.40*e*-1	-	3	7.16*e*-4	-	1.77*e*-2	-
4	3.24*e*-3	1.82	1.61*e*-1	0.57	4	1.04*e*-4	2.78	3.78*e*-3	2.23
5	7.91*e*-4	2.03	8.02*e*-2	1.00	5	1.56*e*-5	2.75	1.10*e*-3	1.78
6	2.07*e*-4	1.94	4.32*e*-2	0.89	6	1.87*e*-6	3.06	3.10*e*-4	1.83
7	5.18*e*-5	2.00	2.24*e*-2	0.95	7	2.44*e*-7	2.94	7.32*e*-5	2.08
8	1.32*e*-5	1.97	1.11*e*-2	1.01	8	3.09*e*-8	2.98	1.91*e*-5	1.94

TABLE 8.3
Example 1: Errors and order of convergence for $\alpha = 50$.

ℓ	$k=1$ e_∞	order	$k=1$ e_∞^∇	order
3	4.07e-2	-	6.23e-1	-
4	1.05e-2	1.95	2.32e-1	1.42
5	2.91e-3	1.86	1.01e-1	1.21
6	7.63e-4	1.93	5.76e-2	0.80
7	1.94e-4	1.98	3.04e-2	0.92
8	4.84e-5	2.00	1.58e-2	0.94

ℓ	$k=2$ e_∞	order	$k=2$ e_∞^∇	order
3*	7.47e-2	-	8.10e-1	-
4*	2.86e-2	1.38	3.10e-1	1.39
5*	5.66e-4	5.66	1.63e-2	4.25
6	6.87e-5	3.04	2.48e-2	-0.61
7	7.21e-6	3.25	1.52e-3	4.03
8	8.78e-7	3.04	3.90e-4	1.97

TABLE 8.4
Example 2: Errors and order of convergence for $\alpha = 10$.

ℓ	$k=1$ e_∞	order	$k=1$ e_∞^∇	order
4	6.20e-3	-	2.11e-1	-
5	1.61e-3	1.94	1.21e-1	0.81
6	4.20e-4	1.94	6.26e-2	0.95
7	1.06e-4	1.99	3.17e-2	0.98
8	2.67e-5	1.98	1.64e-2	0.95

ℓ	$k=2$ e_∞	order	$k=2$ e_∞^∇	order
4	4.37e-4	-	8.69e-3	-
5	5.49e-5	2.99	2.33e-3	1.90
6	7.52e-6	2.87	6.08e-4	1.94
7	9.36e-7	3.01	1.54e-4	1.98
8	1.20e-7	2.97	3.90e-5	1.98

In the cases indicated with $*$ in Table 8.3 there were convergence problems in the sense that the approximate Newton line search (6.10) did not satisfy its tolerance criterion.

The results in the tables show an error reduction behavior that is consistent with the theoretical results derived in Lemma 7.6 for the error measure e_∞ and with the results on the size of the gradient of the approximate signed distance function in Theorem 4.2. In the application of the latter theorem to our method we have $\delta_{p(z)} \leq ch^k$; cf. section 7.1.

The same experiment is repeated for the apple manifold of Example 2. It turns out that the behavior of the method remains essentially the same if we change from the torus to the apple manifold. In Table 8.4 we show the results for the case $\alpha = 10$.

Repeated reparametrization: Volume conservation. As a final test we consider the method *repeatedly* applied to a sphere with radius $r = 0.25$, in order to investigate whether "drifting" or "shrinking" occurs. The exact distance function is denoted by d^{ex}. As input for the reparametrization we use the interpolation in the finite element space V_ℓ^k, which is denoted by $\tilde{d}_h := I_h d^{ex}$ (recall that $h = h_\ell$). We repeated the reparametrization 100 times resulting in approximate distance functions $\tilde{d}_h^0 = \tilde{d}_h$, $\tilde{d}_h^n :=$ reparametrization of $\tilde{d}_h^{n-1}$, $n = 1, \ldots 100$. We determined (with sufficient accuracy) the volume inside the approximate manifold induced by $\tilde{d}_h^n$, i.e., $V^n := \mathrm{Vol}(\mathrm{int}((\tilde{\Gamma}_h^n))$, where $\tilde{\Gamma}_h^n$ is the zero level of the finite element function $\tilde{d}_h^n$. The corresponding relative volume error is denoted by

$$e_{\mathrm{Vol}}^n := \left| \frac{V^n - 4/3\pi r^3}{4/3\pi r^3} \right| .$$

In Figure 8.4 we plot this error over the number of reparametrizations for two levels of refinement, $\ell = 5, 6$. We observe a mild shrinking effect with increasing n and this effect becomes weaker if we change from $k = 1$ to $k = 2$.

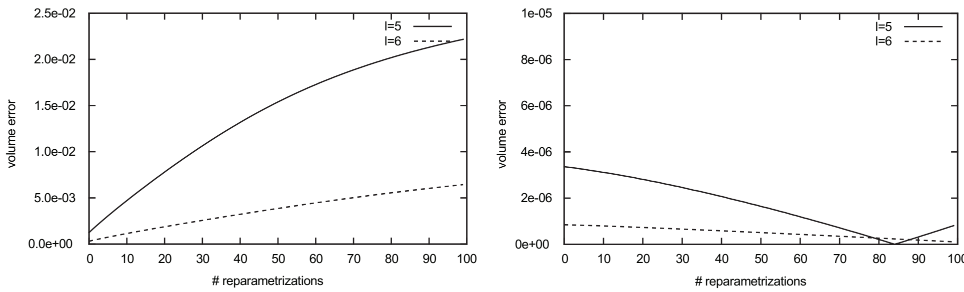

FIG. 8.4. *Relative volume error. Left:* $k = 1$*, right:* $k = 2$*.*

9. Discussion and outlook. In this paper we introduce a new level set redistancing method. The method is based on well-known finite element gradient recovery techniques. Such a gradient recovery technique can be used to determine a quasi-normal field on the (only implicitly given) zero level of a finite element level set function ϕ_h. This quasi-normal field induces a natural approximate signed distance function. The output of the initialization phase of the redistancing method is the nodal interpolation (in a neighborhood of the zero level) of this approximate signed distance function. This redistancing method does not need a reconstruction of the zero level of ϕ_h. We present an error analysis of this new method. A key assumption in the analysis is that the underlying level set function ϕ (that is approximated by the finite element level set function ϕ_h) is sufficiently smooth such that error bounds as in (7.2) and (7.3) hold.

A topic for further research is whether this approach (or a modification of it) is also applicable for redistancing of a level set function ϕ_h that approximates a *non*smooth level set function ϕ, e.g., a ϕ with a zero level that has corners or edges. Related to the PPR based initialization algorithm introduced in section 6.3 there are several numerical issues that have to be studied further; for example, the computational work needed in the PPR method and in the iterations (6.10)–(6.11), the robustness of these iterations w.r.t. the choice of the starting value, and the rate of convergence of these iterations. The performance of the new redistancing method in more challenging applications has to be investigated. We are particularly interested in applications in two-phase incompressible flow simulations (where often the interface is smooth); cf. [9]. A further issue that will be addressed in future work is the combination of this new initialization method with a standard (FMM based) extension phase and the comparison of the resulting reinitialization method with other methods known in the literature.

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