CALCULUS ON SURFACES WITH GENERAL CLOSEST POINT FUNCTIONS

THOMAS MÄRZ, COLIN B. MACDONALD [*]

Abstract. The Closest Point Method for solving partial differential equations (PDEs) posed on surfaces was recently introduced by Ruuth and Merriman [J. Comput. Phys. 2008] and successfully applied to a variety of surface PDEs. In this paper we study the theoretical foundations of this method. The main idea is that surface differentials of a surface function can be replaced with Cartesian differentials of its closest point extension, i.e., its composition with a closest point function. We introduce a general class of these closest point functions (a subset of differentiable retractions), show that these are exactly the functions necessary to satisfy the above idea, and give a geometric characterization of this class. Finally, we construct some closest point functions and demonstrate their effectiveness numerically on surface PDEs.

Key words. Closest Point Method, retractions, implicit surfaces, surface-intrinsic differential operators, Laplace–Beltrami operator

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1. Introduction. The Closest Point Method is a set of mathematical principles and associated numerical techniques for solving partial differential equations (PDEs) posed on surfaces. It is an embedding technique and is based on an implicit representation of the surface S. The original method [19] uses a representation induced by Euclidean distance; specifically, for any point x in an embedding space $\mathbb{R}^n$ containing S, a point $\mathrm{ecp}(x) \in S$ is known which is closest to x (hence the term "Closest Point Method"). The function ecp is the Euclidean closest point function.

This kind of representation of a surface S will be generalized: we introduce a general class of *closest point functions* (and denote a member by "cp") within the set of differentiable retractions. The *closest point extension* of a surface function u is given by $u(\mathrm{cp}(x))$. The common feature of all closest point functions cp is that the extension $u(\mathrm{cp}(x))$ locally propagates data u perpendicularly off the surface S into the surrounding space $\mathbb{R}^n$. In this way, closest point extensions lead to simplified derivative calculations in the embedding space—because $u(\mathrm{cp}(x))$ does not vary in the direction normal to the surface. More specifically, we have (for every closest point function):

Gradient Principle: intrinsic gradients of surface functions agree on the surface with Cartesian gradients of the closest point extension.

Divergence Principle: surface divergence operators of surface vector fields agree on the surface with the Cartesian divergence operator applied to the closest point extension of those vector fields.

These are stated more precisely and proven as Principles 3.4 and 3.5. Combinations of these two principles may be made, to encompass higher order differential operators for example the Laplace–Beltrami and surface biharmonic operators. These principles can then be used to replace the intrinsic spatial operators of surface PDEs with Cartesian derivatives in the embedded space.

Numerical methods based on these principles are compelling because they can re-use simple numerical techniques on Cartesian grids such as finite difference methods and standard interpolation schemes [19]. Other advantages include the wide variety of geometry that can be represented, including both open and closed surfaces with or without orientation in general codimension (e.g., filaments in 3D [19] or a Klein bottle in 4D [14]). In this way, the Closest Point Method has been successfully applied to a variety of time-dependent problems including in-surface advection, diffusion, reaction-diffusion, and Hamilton–Jacobi equations [19, 14], where standard time integration schemes are used. It has been shown to achieve high-order accuracy [14, 15]. It has also been used for time-independent problems such as eigenvalue problems on surfaces [13].

The remainder of this paper unfolds as follows. In Section 2, we review both notation and a calculus on embedded surfaces which does not make use of parametrizations. In Section 3, we define our class of closest point functions within the class of differentiable retractions. The key property is that, for points on the surface, the Jacobian matrix of the closest point function is the

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projection matrix onto the tangent space. We show this class of functions gives the desired simplified derivative evaluations and that it is the largest class of retractions that does so. We thus prove all of these functions induce the closest point principles of [19] (in fact, a more general divergence operator is established). Finally, we give a geometric characterization of these functions (namely that the pre-image of the closest point function intersects the surface orthogonally). Section 4 discusses general diffusion operators: these can be treated with the principles established in Section 3 by using two extensions but there are also many interesting cases (including the Laplace–Beltrami operator) where one can simply use a single extension. Section 5 describes one possible construction method for non-Euclidean closest point functions which makes use of a multiple level-set description of S. This construction method can be realized numerically which we demonstrate in an example. Finally, in Section 6 we use the non-Euclidean closest point representation to solve an advection problem and a diffusion problem on a curve embedded in $\mathbb{R}^3$.

2. Calculus on Surfaces without Parametrizations. In this section, we review notation and definitions to form a calculus on surfaces embedded in $\mathbb{R}^n$ (see e.g., [10, 17, 18, 2, 5, 7, 6]).

2.1. Smooth Surfaces. Throughout this paper we consider smooth surfaces S of dimension $\dim S = k$ embedded in $\mathbb{R}^n$ ($k \leq n$) which possess a tubular neighborhood [11]. We refer to this tubular neighborhood as $B(S)$, a *band* around S.

In the case that S has a boundary $\partial S \neq \emptyset$, we identify S with its interior $S = S \setminus \partial S$. Moreover, we assume that S is orientable, i.e., if $\operatorname{codim} S = n - k \neq 0$ there are smooth vector fields $N_i : S \to \mathbb{R}^n$, $i = 1, \ldots, n - k$ which span the normal space $\mathcal{N}_y S = \operatorname{span}\{N_1(y), \ldots, N_{n-k}(y)\}$ (see e.g., [1, Proposition 6.5.8]). The vectors $N_i(y)$ are not required to be pairwise orthogonal, but we require them to be normed $|N_i(y)| = 1$. Finally, we define the $\mathbb{R}^{n \times k}$-matrix $N(y) := (N_1(y)| \ldots |N_{n-k}(y))$ which contains all the normal vectors as columns.

The tubular neighborhood assumption is sufficient for the existence of retractions (see [11]). This is important because the closest point functions defined in Section 3 are retractions. Note that every smooth surface embedded in $\mathbb{R}^n$ without boundary has a tubular neighborhood by [11, Theorem 5.1]. Moreover, the orientability side condition is not restrictive since it will be satisfied locally when referring to sufficiently small subsets of the surface.

The matrix $P(y)$ denotes the orthogonal projector that projects onto the tangent space $\mathcal{T}_y S$ of S at $y \in S$. P as a function of $y \in S$ is a tensor field on the surface and can be written in terms of the normal vectors as

$$P : S \to \mathbb{R}^{n \times n}, \quad P(y) = I - N(y) \cdot N(y)^\dagger$$

where $N(y)^\dagger$ denotes the pseudo-inverse of $N(y)$. If $\operatorname{codim} S = 1$ then P is given by $P(y) = I - N(y) \cdot N(y)^T$ since the matrix $N(y)$ has only a single normed column vector.

Regarding the degree of smoothness: later when we speak about C^l-smooth surface functions and differentials up to order l, we assume that the underlying surface S is at least C^{l+1}-smooth.

2.2. Smooth Surface Functions and Smooth Extensions. Given a surface S, we consider smooth surface functions: a scalar function $u : S \to \mathbb{R}$, vector-valued function $f : S \to \mathbb{R}^m$, and vector field $g : S \to \mathbb{R}^n$. We call g a vector field because it maps to $\mathbb{R}^n$, the embedding space of S, and hence we can define a divergence operation for it. The calculus without parametrizations for such surface functions is based on smooth extensions, defined in the following.

DEFINITION 2.1. *(Extensions) We call $u_E : \Omega_E \to \mathbb{R}$ an extension of the surface function $u : S \to \mathbb{R}$—and likewise for vector-valued surface functions—if the following properties hold:*
- *$\Omega_E \subset \mathbb{R}^n$ is an open subset of the embedding space.*
- *Ω_E contains a surface patch $S \cap \Omega_E \neq \emptyset$.*
- *$u_E|_{S \cap \Omega_E} = u|_{S \cap \Omega_E}$, the extension and the original function coincide on the surface patch.*
- *$u \in C^l(S \cap \Omega_E) \Rightarrow u_E \in C^l(\Omega_E)$, the extension is as smooth as the original function.*

As extensions are not unique, u_E denotes an arbitrary representative of this equivalence class.

Different extensions might have different domains of definition. Here Ω_E is just a generic name for an extension domain that suits the chosen extension and that contains the surface point $y \in S$ which is under consideration.

An important point is that such extensions exist and may be obtained by using the following feature of a smooth surface: for every $y \in S$ there are open subsets Ω_E, W of $\mathbb{R}^n$, where $y \in \Omega_E$, and a diffeomorphism $\psi : \Omega_E \to W$ (ψ, ψ^{-1} are as smooth as S) that locally flattens S

$$\psi(\Omega_E \cap S) = W \cap \mathbb{R}_0^k , \quad k = \dim S , \quad \mathbb{R}_0^k := \{x \in \mathbb{R}^n : x = (x_1, \ldots, x_k, 0, \ldots, 0)\} ,$$

see e.g., [12, Chapter 3.5]. Now, $\psi^{-1} : W \cap \mathbb{R}_0^k \to \Omega_E \cap S$ parametrizes the patch $\Omega_E \cap S$ of S, so $u \circ \psi^{-1} : W \cap \mathbb{R}_0^k \to \mathbb{R}$ is a smooth function. Let $\tilde{P} \in \mathbb{R}^{n \times n}$ be the projector onto $\mathbb{R}_0^k$. For $x \in \Omega_E$, the function $\tilde{P} \cdot \psi(x)$ maps smoothly onto $W \cap \mathbb{R}_0^k$, hence

$$u_E : \Omega_E \to \mathbb{R} , \quad u_E(x) := u \circ \psi^{-1} \left(\tilde{P} \cdot \psi(x) \right)$$

is smooth and extends u as desired.

2.3. Calculus without Parametrizations. Now, we define the basic first order differential operators on S without the use of parametrizations (compare to e.g., [10, 17, 18, 2, 5, 7, 6]):

DEFINITION 2.2. *Let S be a smooth surface embedded in $\mathbb{R}^n$, $y \in S$ a point on the surface, and $P(y) \in \mathbb{R}^{n \times n}$ the projector (onto $\mathcal{T}_y S$) at this point y. Then the surface gradient ∇_S of a scalar C^1-function u, the surface Jacobian D_S of a vector-valued C^1-function f, and the surface divergence div_S of a C^1 vector field g are given by:*

$$\nabla_S u(y)^T := \nabla u_E(y)^T \cdot P(y) ,$$
$$D_S f(y) := D f_E(y) \cdot P(y) ,$$
$$\mathrm{div}_S g(y) := \mathrm{trace}(D_S g(y)) = \mathrm{trace}(D g_E(y) \cdot P(y)) .$$

Here, ∇ is the gradient and D the Jacobian in the embedding space $\mathbb{R}^n$ applied to the extensions of the surface functions. The extensions are arbitrary representatives of the equivalence classes of Definition 2.1.

Remark. There are other works (see e.g., [3]) that use a variational definition of the surface divergence operator, which we denote by $\mathrm{div}_S^* g$, as

$$\int_\Omega v \, \mathrm{div}_S^* g \, d\mathcal{H}^n(y) = -\int_\Omega \langle \nabla_S v, g \rangle \, d\mathcal{H}^n(y) , \quad \forall \, v \in C_0^1(\Omega) , \quad \Omega \subset S .$$

But this definition applies only to *tangential* vector fields g, because this tangency is required by the surface Gauss–Green Theorem. The connection to our definition is as follows

$$\mathrm{div}_S^* g = \mathrm{div}_S(Pg) ,$$

because div_S^* takes into account only the tangential part Pg of the vector field g. The two are equal if the vector field g is indeed tangential to the surface. The trace-based definition of surface divergence in Definition 3.1 also applies to non-tangential fields [2]. For example when $\mathrm{codim}\, S = 1$ and g is a non-tangential vector field, it can be shown that

$$\mathrm{div}_S g = \mathrm{div}_S(Pg) + \mathrm{div}_S(\langle N, g \rangle \cdot N) = \mathrm{div}_S(Pg) - \langle N, g \rangle \kappa_S ,$$

where N is the normal vector, and $\kappa_S = -\mathrm{div}_S N$ is the mean curvature of S. That is, the surface divergence of g is the surface divergence of the tangential component plus an extra term which depends on the curvature(s) of S.

3. Calculus on Surfaces with Closest Point Functions. Our aim is to compute surface intrinsic derivatives by means of *closest point functions*. For now, we consider only first order derivatives, higher order derivatives are discussed in Section 3.3. By the remark on smoothness in Section 2.1, this means we are considering C^2-smooth surfaces. Closest point functions are retractions with the key property that their Jacobian evaluated on the surface is the projector P.

DEFINITION 3.1. *(Closest Point Functions) We call a map $B(S) \to S$ a closest point function* cp, *if*
1. cp *is a C^1-retraction, i.e.,* cp $: B(S) \to S$ *features the properties*

a) $\mathrm{cp} \circ \mathrm{cp} = \mathrm{cp}$ *or equivalently* $\mathrm{cp}\,|_S = \mathrm{id}_S$,[1]
   b) cp *is continuously differentiable.*
2. $D\,\mathrm{cp}(y) = P(y)$ *for all* $y \in S$.

   If cp belongs to this class of closest point functions, we recover surface differential operators (those in Definition 2.2) by standard Cartesian differential operators applied to the closest point extensions $u \circ \mathrm{cp}$. This fundamental point is the basis for the Closest Point Method and is established by the following theorem:

   THEOREM 3.2. *(Closest Point Theorem) If* $\mathrm{cp} : B(S) \to S$ *is a closest point function according to Definition 3.1, then the following rule*

$$D[f \circ \mathrm{cp}](y) = D_S f(y)\,, \quad y \in S, \tag{3.1}$$

holds for the surface Jacobian $D_S f$ *of a continuously differentiable vector-valued surface function* $f : S \to \mathbb{R}^m$.

   We also show that any C^1-retraction that satisfies the relation in (3.1) must be a closest point function satisfying Definition 3.1.

   THEOREM 3.3. *Let* $r : B(S) \to S$ *be a* C^1-*retraction (i.e., only part 1 of Definition 3.1 is required). If for every continuously differentiable surface function* $f : S \to \mathbb{R}^m$ *the following holds*

$$D[f \circ r](y) = D_S f(y)\,, \quad y \in S, \tag{3.2}$$

then r satisfies also part 2 of Definition 3.1

$$Dr(y) = P(y) \quad \textit{for all} \quad y \in S,$$

and is thus a closest point function.

   Proof. Ad Theorem 3.2: the closest point extension can be written in terms of an arbitrary extension f_E:

$$f \circ \mathrm{cp}(x) = f_E \circ \mathrm{cp}(x)\,, \quad x \in B(S)\,.$$

Now, we expand the differential using the chain rule[2]

$$D[f \circ \mathrm{cp}](x) = Df_E \circ \mathrm{cp}(x) \cdot D\,\mathrm{cp}(x)\,, \quad x \in B(S)\,.$$

Next we set $x = y \in S$, a point on the surface, and by Definition 3.1 we have $\mathrm{cp}(y) = y$ and $D\,\mathrm{cp}(y) = P(y)$. Finally, using the surface differential in Definition 2.2 gives

$$D[f \circ \mathrm{cp}](y) = Df_E(y) \cdot P(y) = D_S f(y)\,, \quad y \in S\,.$$

   Ad Theorem 3.3: we consider the identity map on S, $\mathrm{id}_S : S \to S$, $\mathrm{id}_S(y) = y$. The simplest extension of id_S is given by the identity map on the embedding space, $\mathrm{id} : \mathbb{R}^n \to \mathbb{R}^n$. By Definition 2.2, the surface Jacobian of the surface identity is

$$D_S\,\mathrm{id}_S(y) = D\,\mathrm{id}(y) \cdot P(y) = P(y)\,, \quad y \in S\,. \tag{3.3}$$

By assumption, (3.2) is true for every smooth surface function. And so with $f = \mathrm{id}_S$ and the previous result we have

$$Dr(y) = D[\mathrm{id}_S \circ r](y) = D_S\,\mathrm{id}_S(y) = P(y)\,, \quad y \in S\,.$$

$\square$

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[1] Here $\mathrm{id}_S : S \to S$ with $\mathrm{id}_S(y) = y$ denotes the identity map on the surface S.
[2] In this paper, we follow the convention that differential operators occur before composition in the order of operations. For example, $Df_E \circ \mathrm{cp}(x)$ means differentiate f_E and then compose with $\mathrm{cp}(x)$.

Direct consequences of the Closest Point Theorem 3.2 are the gradient and the divergence principles below.

PRINCIPLE 3.4. *(Gradient Principle) If* cp $: B(S) \to S$ *is a closest point function according to Definition 3.1, then*

$$\nabla[u \circ \mathrm{cp}](y) = \nabla_S u(y) , \quad y \in S, \tag{3.4}$$

holds for the surface gradient $\nabla_S u$ of a continuously differentiable scalar surface function $u : S \to \mathbb{R}$.

PRINCIPLE 3.5. *(Divergence Principle) If* cp $: B(S) \to S$ *is a closest point function according to Definition 3.1, then*

$$\mathrm{div}[g \circ \mathrm{cp}](y) = \mathrm{div}_S g(y) , \quad y \in S, \tag{3.5}$$

holds for the surface divergence $\mathrm{div}_S g$ of a continuously differentiable surface vector field $g : S \to \mathbb{R}^n$. Notably the vector field g need not be tangential to S.

3.1. Geometric Characterization of Closest Point Functions. A further characteristic feature of closest point functions is that the pre-image $\mathrm{cp}^{-1}(y)$ of a closest point function must intersect the surface S orthogonally. This fact will be established in Theorem 3.7, for which we will need smoothness of the pre-image.

LEMMA 3.6. *Let $r : B(S) \to S$ be a C^1-retraction and let $y \in S$. The pre-image $r^{-1}(y)$ is (locally around y) a C^1-manifold.*

Proof. By differentiation of the equation $\mathrm{id}_S \circ r(x) = r(x)$ and setting $x = y \in S$ thereafter, we get

$$P \circ r(x) \cdot Dr(x) = Dr(x) \quad \Rightarrow \quad P(y) \cdot Dr(y) = Dr(y) . \tag{3.6}$$

We see that the range of the Jacobian matrix $Dr(y)$ is contained in the tangent space $\mathcal{T}_y S$. On the other hand, we can differentiate $r \circ \mathrm{id}_S(y) = \mathrm{id}_S(y)$ with respect to $y \in S$ and right-multiply by a matrix $T(y) \in \mathbb{R}^{n \times k}$ which consists of an orthonormal basis of $\mathcal{T}_y S$ to get

$$Dr(y) \cdot P(y) = P(y) \quad \Rightarrow \quad Dr(y) \cdot T(y) = T(y) . \tag{3.7}$$

Equation (3.6) shows that the linear operator $Dr(y) : \mathbb{R}^n \to \mathbb{R}^n$ is rank deficient while $Dr(y) : \mathcal{T}_y S \to \mathcal{T}_y S$ is full rank by (3.7) and the rank is $k = \dim S$. Now, we can apply the Implicit Function Theorem to

$$f_y(x) = T(y)^T \cdot (r(x) - y) = 0$$

where $f_y : \mathbb{R}^n \to \mathbb{R}^k$ is a C^1-mapping and $r^{-1}(y)$ is the set of solutions. The preceding discussion shows that $Df_y(y) = T(y)^T \cdot Dr(y)$ is full rank, and hence $r^{-1}(y)$ is (locally around y) a C^1-manifold. □

THEOREM 3.7. *Let $r : B(S) \to S$ be a C^1-retraction and let $y \in S$. The retraction r has the property $Dr(y) = P(y)$ (and hence r is a closest point function according to Definition 3.1), if and only if for every $y \in S$ the C^1-manifold $r^{-1}(y)$ intersects S orthogonally, i.e.,*

$$\mathcal{T}_y r^{-1}(y) = \mathcal{N}_y S .$$

Proof. Let $y \in S$ and assume that the pre-image $r^{-1}(y)$ intersects S orthogonally. Let $\xi : (-\varepsilon, \varepsilon) \to r^{-1}(y)$, $\varepsilon > 0$, be a regular C^1-curve in $r^{-1}(y)$ with $\xi(0) = y$. As $r^{-1}(y)$ is a C^1-manifold by Lemma 3.6 such curves ξ exist. Because $\xi(t) \in r^{-1}(y)$, r maps every point $\xi(t)$ to y:

$$r \circ \xi(t) = y , \quad \text{for all} \quad t \in (-\varepsilon, \varepsilon).$$

Differentiation of the latter equation with respect to t and the substitution of $t = 0$ yield

$$Dr(y) \cdot \xi'(0) = 0 \,. \tag{3.8}$$

By assumption $\xi'(0)$ is an arbitrary vector of the normal space $\mathcal{N}_y S$. Let (here) $N(y) \in \mathbb{R}^{n \times (n-k)}$ be a matrix where the columns form an orthonormal basis of $\mathcal{N}_y S$, then (3.8) implies

$$Dr(y) \cdot N(y) = 0 \,.$$

By the latter result combined with (3.7) the product of $Dr(y)$ with the $n \times n$ orthogonal matrix $(T(y)|N(y))$ (the matrix $T(y) \in \mathbb{R}^{n \times k}$ consists of an orthonormal basis of $\mathcal{T}_y S$) is

$$Dr(y) \cdot (T(y)|N(y)) = (T(y)|0) \quad \Rightarrow \quad Dr(y) = T(y) \cdot T(y)^T = P(y) \,.$$

This proofs the first direction.

Let now $Dr(y) = P(y)$ for all $y \in S$, i.e., the retraction r is already a closest point function. Let again $\xi : (-\varepsilon, \varepsilon) \to r^{-1}(y)$ be a regular C^1-curve in $r^{-1}(y)$ with $\xi(0) = y$. We consider again (3.8) but this time we replace $Dr(y)$ with $P(y)$:

$$P(y) \cdot \xi'(0) = 0 \,.$$

The latter tells us that every vector of $\mathcal{T}_y r^{-1}(y)$ is perpendicular to $\mathcal{T}_y S$, in other words $r^{-1}(y)$ intersects S orthogonally.   ☐

3.2. The Euclidean Closest Point Function. The class of closest point functions from Definition 3.1 is not empty. We show that the Euclidean closest point function ecp

$$\mathrm{ecp}(x) = \arg\min_{y \in S} |x - y| \,, \qquad x \in B(S) \tag{3.9}$$

—which is well-defined by our assumptions on surfaces in Section 2.1—belongs to this class. However, this is not just a corollary of the last theorem, we have to show that ecp is continuously differentiable on the surface S.

THEOREM 3.8. *The Euclidean closest point function* ecp *is a closest point function satisfying Definition 3.1.*

Proof. The proof is instructive in the special case of codim $S = 1$ and we begin with that case: The Euclidean closest point function ecp $: B(S) \to S$ is a continuous retraction and can be written in terms of the Euclidean distance map d as

$$\mathrm{ecp}(x) = x - d(x) \cdot \nabla d(x) \,. \tag{3.10}$$

Because codim $S = 1$, we can replace d with a signed Euclidean distance sd which on $B(S)$ is a classical solution of the Eikonal equation, where sd is as smooth as S and where $\nabla \, \mathrm{sd}(y) = N(y)$, for $y \in S$, is one of the two possible choices of the surface normal. So ecp is continuously differentiable with Jacobian

$$D \, \mathrm{ecp}(x) = I - \nabla \, \mathrm{sd}(x) \cdot \nabla \, \mathrm{sd}(x)^T - \mathrm{sd}(x) \cdot D^2 \, \mathrm{sd}(x) \,,$$

and, as sd vanishes on S, we get

$$D \, \mathrm{ecp}(y) = I - N(y) \cdot N(y)^T = P(y) \,, \quad y \in S \,,$$

which proves the statement in this case.

If S is of higher codimension, we cannot use this argument since d is not differentiable on the surface S. But it is continuously differentiable off the surface and so is ecp by (3.10). We prove now that $D \, \mathrm{ecp}$ extends continuously onto S and equals the projector P there.

Let $\gamma : U \subset \mathbb{R}^k \to \Omega_S$, $\theta_1 \to \gamma(\theta_1)$ be a regular parametrization of a surface patch $\Omega_S \subset S$, ($k = \dim S$). Then, by adding the normal space

$$\Phi(\theta) = \gamma(\theta_1) + N \circ \gamma(\theta_1) \cdot \theta_2 \,,$$

(3.11)

$$\Phi : \Omega \subset \mathbb{R}^n \to B(S) \,, \quad \theta = (\theta_1, \theta_2) \to \Phi(\theta) \,,$$

we get a coordinate system on a corresponding subset of $B(S)$. $N(y) = (N_1(y)| \ldots |N_{n-k}(y))$ is a matrix formed of the normal space basis and $\theta_2 \in \mathbb{R}^{n-k}$. Now, we have

$$\gamma(\theta_1) = \text{ecp} \circ \Phi(\theta) \,.$$

(3.12)

As long as $\theta_2 \neq 0$ (i.e., off the surface) we can differentiate (3.12) using the chain rule:

$$(D_{\theta_1}\gamma \mid 0) = D\,\text{ecp} \circ \Phi \cdot D_\theta \Phi = D\,\text{ecp} \circ \Phi \cdot (D_{\theta_1}\gamma + D_{\theta_1}(N \circ \gamma) \cdot \theta_2 \mid N \circ \gamma) \,.$$

(3.13)

The second factor of the right hand side extends onto S (i.e., $\theta_2 = 0$ is admissible) and is invertible, the left hand side is defined for $\theta_2 = 0$ anyway. After inverting, we send θ_2 to zero and so we have ($\Phi(\theta_1, 0) = \gamma(\theta_1)$)

$$D\,\text{ecp} \circ \gamma = (D_{\theta_1}\gamma \mid 0) \cdot (D_{\theta_1}\gamma \mid N \circ \gamma)^{-1} \,.$$

As $D_{\theta_1}\gamma$ and $N \circ \gamma$ are orthogonal, i.e., $D_{\theta_1}\gamma^T \cdot N \circ \gamma = 0$ and $N \circ \gamma^T \cdot D_{\theta_1}\gamma = 0$, we can write the inverse in terms of the pseudo inverses of the sub-matrices

$$(D_{\theta_1}\gamma \mid N \circ \gamma)^{-1} = \begin{pmatrix} D_{\theta_1}\gamma^\dagger \\ N \circ \gamma^\dagger \end{pmatrix}$$

and so

$$D\,\text{ecp} \circ \gamma = (D_{\theta_1}\gamma \mid 0) \cdot (D_{\theta_1}\gamma \mid N \circ \gamma)^{-1} = (D_{\theta_1}\gamma \mid 0) \cdot \begin{pmatrix} D_{\theta_1}\gamma^\dagger \\ N \circ \gamma^\dagger \end{pmatrix} = D_{\theta_1}\gamma \cdot D_{\theta_1}\gamma^\dagger = P \circ \gamma \,.$$

In the latter equality we have used that the outer product of a full column-rank matrix A and its pseudo inverse gives the projector onto the image of A which in our case is the tangent space. Finally we get the assertion:

$$D\,\text{ecp} \circ \gamma = P \circ \gamma \qquad \Leftrightarrow \qquad D\,\text{ecp}(y) = P(y) \,, \quad y \in S \,.$$

□

Remark. As a consequence of Theorem 3.8 we see that the function

$$x - \text{ecp}(x) = d(x) \cdot \nabla d(x) = \nabla \left(\frac{d(x)^2}{2} \right)$$

is continuously differentiable. The article [9] introduces $v(x) := x - \text{ecp}(x)$ as the *vector distance function* and refers to the article [2] for some of its features. In particular the authors of [2] prove that the squared distance function is differentiable and show that the Hessian $D^2\eta(y)$ of the function $\eta := d^2/2$ when evaluated at a surface point $y \in S$ is exactly the projector onto the normal space $\mathcal{N}_y S$. Here, we have an alternative proof that η (and thereby the squared distance function) is differentiable twice with $I - P(y) = Dv(y) = D^2\eta(y)$ on S which is the projector onto $\mathcal{N}_y S$.

3.2.1. Additional Smoothness of the Euclidean Closest Point Function. Theorem 3.8 implies only C^1-smoothness of ecp but taking a closer look at Φ as defined in (3.11) we see that Φ is as smooth as N (which typically is one order less smooth than the surface S). Note also that ecp inherits its degree of smoothness from N. For example, given a C^3-smooth surface S, we have Φ C^2-smooth. So we can differentiate (3.13) and solve for $D^2\,\text{ecp} \circ \Phi$, again by appealing to the non-singularity of $D\Phi$. The limit $\theta_2 \to 0$ exists here again which shows $D^2\,\text{ecp}$ has a continuous extension onto S, hence ecp is C^2-smooth for a C^3-smooth surface. Applying these ideas repeatedly proves that ecp is C^l-smooth for a C^{l+1}-smooth surface.

3.3. Derivatives of Higher Order. For C^l-smooth surface functions we can recover surface differential operators of higher order by applying Theorem 3.2 (or the Gradient and Divergence Principles 3.4 and 3.5) several times. For example the surface Hessian $D_S^2 u$ of a scalar surface function $u \in C^l(S)$ with $l \geq 2$ can be calculated by combining Theorem 3.2 and the Gradient Principle 3.4:

$$D_S^2 u(y) = D_S \nabla_S u(y) = D[\nabla_S u \circ \mathrm{cp}](y) = D[\nabla[u \circ \mathrm{cp}] \circ \mathrm{cp}](y) , \quad y \in S .$$

Interestingly, higher order derivatives do not require more smoothness of the closest point function; C^1 is sufficient. To see this expand $\nabla[u \circ \mathrm{cp}]$ in terms of an arbitrary extension u_E

$$\nabla[u \circ \mathrm{cp}](x) = D\,\mathrm{cp}(x)^T \cdot \nabla u_E \circ \mathrm{cp}(x) . \tag{3.14}$$

The clue here is that the extension of $D\,\mathrm{cp}$ is the extension of the projector P:

$$D\,\mathrm{cp}(y) = P(y) , \ y \in S \qquad \Rightarrow \qquad D\,\mathrm{cp} \circ \mathrm{cp}(x) = P \circ \mathrm{cp}(x),$$

and thus a second extension of (3.14) gives

$$\nabla[u \circ \mathrm{cp}] \circ \mathrm{cp}(x) = P \circ \mathrm{cp}(x) \cdot \nabla u_E \circ \mathrm{cp}(x). \tag{3.15}$$

By the assumption at the end of Section 2.1, the surface must be C^{l+1}-smooth and thus the surface identity map id_S is C^{l+1}-smooth. By (3.3) $P = D_S\,\mathrm{id}_S$ is C^l-smooth. Therefore we can handle differential operators of higher order by iterating Theorem 3.2 even though cp is only C^1-smooth because we never differentiate cp more than once.

   In the next section, we will discuss special second order differential operators where we can drop the second extension. In that case we differentiate (3.14) instead of (3.15) and hence we need a second derivative of cp. There we will require cp to be a C^2-smooth closest point function.

4. Surface Intrinsic Diffusion Operators. In this section we discuss the treatment of diffusion operators, that is, second order differential operators of the form

$$\mathrm{div}_S(A(y)\nabla_S u),$$

in terms of the closest point calculus. Of course, by combining the Gradient and Divergence Principles 3.4 and 3.5, we can set up the diffusion operator as follows

$$w(x) := A \circ \mathrm{cp}(x)\,\nabla[u \circ \mathrm{cp}](x) , \quad x \in B(S),$$
$$\Rightarrow \quad w(y) = A(y)\nabla_S u(y) , \quad y \in S$$
$$\Rightarrow \quad \mathrm{div}[w \circ \mathrm{cp}](y) = \mathrm{div}_S w(y) = \mathrm{div}_S(A(y)\nabla_S u(y)) .$$

In this set-up, we have a second extension $w \circ \mathrm{cp}$ in the last step. If the surface vector field $v = A(y)\nabla_S u$ is tangent to the surface, we call the operator a *surface intrinsic diffusion operator* (these are relevant regarding the physical modeling of surface processes). The subject of this section is that we can drop the second extension in many cases (depending on A and cp) given the tangency of v. The key to this result is the following lemma on the divergence of vector fields which are tangential on the surface while tangency is allowed to be mildly perturbed off the surface.

   LEMMA 4.1. *(Divergence of tangential fields) Let S be a smooth surface, and let $\gamma : U \subset \mathbb{R}^k \to \Omega_S$ ($k = \dim S$) be a regular parametrization of a generic surface patch $\Omega_S \subset S$. Let Ω be a corresponding open subset of the embedding space $\mathbb{R}^n$ such that $\Omega \cap S = \Omega_S$. Let $\Phi : U \times V \to \Omega$ ($V \subset \mathbb{R}^{n-k}$) be a coordinate system on Ω that satisfies*

$$\Phi(\theta_1, \theta_2) = \gamma(\theta_1) + N \circ \gamma(\theta_1) \cdot \theta_2 + \mathcal{O}(|\theta_2|^2) , \ as \ \ \theta_2 \to 0 .$$

Here the columns of the $n \times (n-k)$ matrix $N(y) := (N_1(y)| \ldots |N_{n-k}(y))$, $y \in S$, give some basis of the normal space $\mathcal{N}_y S$. Let $v : B(S) \to \mathbb{R}^n$ be a continuously differentiable vector field and let

$$\bar{v}(\theta_1, \theta_2) = v \circ \Phi(\theta_1, \theta_2) = D_{\theta_1} \gamma(\theta_1) \cdot \tilde{v}(\theta_1, \theta_2) + N \circ \gamma(\theta_1) \cdot \eta(\theta_1, \theta_2)$$

be the representation of this vector field on Ω in $\theta = (\theta_1, \theta_2)$-variables with a decomposition into the two components ($\tilde{v} \in \mathbb{R}^k$, $\eta \in \mathbb{R}^{n-k}$) which are tangential and normal to the surface S.

If the coefficient η of the normal part satisfies

$$\eta(\theta_1, 0) = 0 \quad and \quad \text{trace } D_{\theta_2} \eta(\theta_1, 0) = 0 \,,$$

then (as the surface patch is generic)

$$\text{div } v(y) = \text{div}_S v(y) \,, \quad y \in S \,.$$

The condition $\eta(\theta_1, 0) = 0$ means that the restriction $v|_S$ is a tangential surface vector field.

   Proof. We show $\text{div}_S v \circ \gamma = \text{div } v \circ \gamma$. For a tangential field the surface divergence in terms of a parametrization γ is given by

$$\text{div}_S v \circ \gamma = \frac{1}{\sqrt{g}} \, \text{div}_{\theta_1} (\tilde{v}(\theta_1, 0) \sqrt{g}) = \text{div}_{\theta_1} (\tilde{v}(\theta_1, 0)) + \sum_{l=1}^{k} \frac{\partial_l g}{2g} \tilde{v}_l(\theta_1, 0) \,. \tag{4.1}$$

where $g = \det G$ and $G = D_{\theta_1} \gamma^T D_{\theta_1} \gamma$ is the metric tensor induced by γ.

   Next, we turn to $\text{div } v \circ \gamma$. In a first step, we obtain

$$\text{div } v \circ \gamma = \text{trace } Dv \circ \gamma = \text{trace } Dv \circ \Phi(\theta_1, 0) = \text{trace } \left(D_\theta \tilde{v}(\theta_1, 0) \cdot D_\theta \Phi(\theta_1, 0)^{-1} \right) \,.$$

The derivative of $\tilde{v}$ is

$$D_\theta \tilde{v}(\theta_1, \theta_2) = \sum_{l=1}^{k} \partial_l \gamma \nabla_\theta \tilde{v}_l^T + \sum_{l=1}^{n-k} N_l \circ \gamma \nabla_\theta \eta_l^T + \sum_{l=1}^{k} \tilde{v}_l \, \partial_l D_\theta \gamma + \sum_{l=1}^{n-k} \eta_l \, D_\theta (N_l \circ \gamma) \,.$$

$$D_\theta \tilde{v}(\theta_1, 0) = \sum_{l=1}^{k} \partial_l \gamma \nabla_\theta \tilde{v}_l^T + \sum_{l=1}^{n-k} N_l \circ \gamma \nabla_\theta \eta_l^T + \sum_{l=1}^{k} \tilde{v}_l \, \partial_l D_\theta \gamma$$

since $\eta(\theta_1, 0) = 0$. By our assumptions on Φ we have

$$D_\theta \Phi(\theta_1, 0) = (D_{\theta_1} \gamma \mid N \circ \gamma) \,, \quad D_\theta \Phi(\theta_1, 0)^{-1} = (D_{\theta_1} \gamma \mid N \circ \gamma)^{-1} = \begin{pmatrix} D_{\theta_1} \gamma^\dagger \\ N \circ \gamma^\dagger \end{pmatrix} \,.$$

Now, we write the divergence as

$$\text{div } v \circ \gamma = \sum_{l=1}^{k} \text{trace} \left(\partial_l \gamma \nabla_\theta \tilde{v}_l^T \cdot D_\theta \Phi(\theta_1, 0)^{-1} \right) + \sum_{l=1}^{n-k} \text{trace} \left(N_l \circ \gamma \nabla_\theta \eta_l^T \cdot D_\theta \Phi(\theta_1, 0)^{-1} \right)$$

$$+ \sum_{l=1}^{k} \text{trace} \left(\partial_l D_\theta \gamma \cdot D_\theta \Phi(\theta_1, 0)^{-1} \right) \tilde{v}_l \,.$$

Using the rules of the trace operator we get

$$\text{div } v \circ \gamma = \text{trace} \left(D_\theta \begin{pmatrix} \tilde{v} \\ \eta \end{pmatrix} D_\theta \Phi(\theta_1, 0)^{-1} (D_{\theta_1} \gamma \mid N \circ \gamma) \right) + \sum_{l=1}^{k} \text{trace} \left(\partial_l D_\theta \gamma \cdot D_\theta \Phi(\theta_1, 0)^{-1} \right) \tilde{v}_l \,.$$

Next, we use $D_\theta \gamma = (D_{\theta_1} \gamma \mid 0)$ and the second assumption $\text{trace } D_{\theta_2} \eta(\theta_1, 0) = 0$ to get

$$\text{div } v \circ \gamma = \text{trace} \left(D_\theta \begin{pmatrix} \tilde{v} \\ \eta \end{pmatrix} \right) + \sum_{l=1}^{k} \text{trace} \left(\partial_l D_{\theta_1} \gamma \cdot D_{\theta_1} \gamma^\dagger \right) \tilde{v}_l$$

$$= \text{trace} \left(D_{\theta_1} \tilde{v} \right) + \sum_{l=1}^{k} \text{trace} \left(\partial_l D_{\theta_1} \gamma \cdot D_{\theta_1} \gamma^\dagger \right) \tilde{v}_l \tag{4.2}$$

$$= \text{div}_{\theta_1} (\tilde{v}(\theta_1, 0)) + \sum_{l=1}^{k} \text{trace} \left(\partial_l D_{\theta_1} \gamma \cdot D_{\theta_1} \gamma^\dagger \right) \tilde{v}_l$$

The final step is to show that trace $\left(\partial_l D_{\theta_1} \gamma \cdot D_{\theta_1} \gamma^\dagger\right) = \frac{\partial_l g}{2g}$. Partial differentiation of the definition of $G = D_{\theta_1} \gamma^T D_{\theta_1} \gamma$ and using the definition of $D_{\theta_1} \gamma^\dagger = G^{-1} D_{\theta_1} \gamma^T$ yields

$$\text{trace}\left(\partial_l D_{\theta_1} \gamma \cdot D_{\theta_1} \gamma^\dagger\right) = \frac{1}{2}\text{trace}(G^{-1}\partial_l G) \tag{4.3}$$

While partial differentiation of the equation $G^{-1}G = I$ results in the (matrix) ordinary differential equation (ODE)

$$\partial_l \left(G^{-1}\right) = -(G^{-1}\partial_l G)\, G^{-1}\,,$$

which implies $\partial_l \det G^{-1} = -\text{trace}(G^{-1}\partial_l G) \det G^{-1}$ and hence $g = \det G$ satisfies

$$-\frac{1}{g^2}\partial_l g = \partial_l \frac{1}{g} = \partial_l \det G^{-1} = -\text{trace}(G^{-1}\partial_l G) \det G^{-1} = -\text{trace}(G^{-1}\partial_l G)\frac{1}{g}\,.$$

This result combined with (4.3) completes the proof: we replace the last term in the last equality of (4.2) with

$$\text{trace}\left(\partial_l D_{\theta_1} \gamma \cdot D_{\theta_1} \gamma^\dagger\right) = \frac{1}{2}\text{trace}(G^{-1}\partial_l G) = \frac{\partial_l g}{2g}\,,$$

and compare with (4.1) to see that $\text{div}_S v \circ \gamma = \text{div}\, v \circ \gamma$.   □

4.1. Diffusion Operators using Fewer Extensions. Armed with Lemma 4.1 we obtain a closest point calculus involving fewer extensions, for all surface intrinsic diffusion operators. There are two situations depending on how much "help" we get from the diffusion tensor A. First, we look at the situation where $A(y)$ maps all vectors $\xi \in \mathbb{R}^n$ to tangent vectors.

THEOREM 4.2. *Let $A : S \to \mathbb{R}^{n \times n}$ be a tangential diffusion tensor field, that maps all vectors to tangent vectors, i.e., $\forall y \in S$ we have $\forall \xi \in \mathbb{R}^n \Rightarrow A(y)\xi \in \mathcal{T}_y S$. Then the corresponding surface diffusion operator can be written in terms of a closest point extension as*

$$\text{div}_S\left(A\nabla_S u\right)(y) = \text{div}\left(A \circ \text{cp}\, \nabla[u \circ \text{cp}]\right)(y)\,, \quad y \in S\,.$$

A re-extension of $\nabla[u \circ \text{cp}]$ is not necessary and the result is true for all C^2-smooth closest point functions.

Proof. As A maps all vectors to tangent vectors the field $v := A \circ \text{cp}\, \nabla[u \circ \text{cp}]$ is tangential to S for all x. Now, we want to apply Lemma 4.1, that means we have to define the coordinate system Φ and the field $\bar{v}(\theta_1, \theta_2)$. We reuse the parametrization γ of a generic surface patch from Lemma 4.1. For a fixed value of θ_1 and the corresponding surface point $\gamma(\theta_1)$ we simply parametrize (with θ_2) the pre-image $\text{cp}^{-1}(\gamma(\theta_1))$ in order to get $\Phi(\theta_1, \theta_2)$. Since by Theorem 3.7 the pre-image $\text{cp}^{-1}(\gamma(\theta_1))$ intersects S orthogonally, we can organize its parametrization in such a way that Φ satisfies

$$\Phi(\theta_1, \theta_2) = \gamma(\theta_1) + N \circ \gamma(\theta_1) \cdot \theta_2 + \mathcal{O}(|\theta_2|^2)\,, \quad \text{as} \quad \theta_2 \to 0\,.$$

As our particular vector field v is tangential to S for all x in a band $B(S)$ around S, the corresponding $\bar{v}$ from Lemma 4.1 takes the form

$$\bar{v}(\theta_1, \theta_2) = v \circ \Phi(\theta_1, \theta_2) = D_{\theta_1}\gamma(\theta_1) \cdot \tilde{v}(\theta_1, \theta_2)$$

with η equal to zero. Hence, by Lemma 4.1 we conclude the first equality of

$$\text{div}(A \circ \text{cp}\, \nabla[u \circ \text{cp}])(y) = \text{div}_S(A \circ \text{cp}\, \nabla[u \circ \text{cp}])(y) = \text{div}_S(A\nabla_S u)(y)\,, \quad y \in S\,,$$

while the second equality is because we have $\text{cp}\,|_S = \text{id}_S$ and $\nabla[u \circ \text{cp}]|_S = \nabla_S u$.   □

Next, we look at the situation where $A(y)$ maps only tangent vectors $\xi \in \mathcal{T}_y S$ to tangent vectors. This case is particularly interesting since—by considering diffusion tensors of the form

$$A(y) = a(y) \cdot I\,, \tag{4.4}$$

where $I \in \mathbb{R}^{n \times n}$ is the identity matrix on the embedding space—it covers the special case where we are given a scalar diffusion coefficient $a(y) \in \mathbb{R}$. It is clear that the diffusion tensor in (4.4) can only map tangent vectors to tangent vectors (this is weaker than the requirement in Theorem 4.2).

THEOREM 4.3. *Let $A : S \to \mathbb{R}^{n \times n}$ be a tangential diffusion tensor field, that maps only tangent vectors to tangent vectors, i.e., $\forall y \in S$ we have $\forall \xi \in \mathcal{T}_y S \Rightarrow A(y)\xi \in \mathcal{T}_y S$. If cp is a C^2-smooth closest point function such that the transpose of its Jacobian maps tangent vectors to tangent vectors, i.e.,*

$$\forall x \in B(S) \quad \text{we have:} \quad \forall \xi \in \mathcal{T}_{\mathrm{cp}(x)} S \Rightarrow D\,\mathrm{cp}(x)^T \xi \in \mathcal{T}_{\mathrm{cp}(x)} S \,.$$

then the corresponding surface diffusion operator can be written in terms of a closest point extension as

$$\mathrm{div}_S \left(A \nabla_S u \right)(y) = \mathrm{div}(A \circ \mathrm{cp}\, \nabla[u \circ \mathrm{cp}])(y)\,, \quad y \in S\,.$$

A re-extension of $\nabla[u \circ \mathrm{cp}]$ is not necessary.

Proof. As A maps only tangent vectors to tangent vectors the field $v := A \circ \mathrm{cp}\, \nabla[u \circ \mathrm{cp}]$ will be tangential to S only if $\nabla[u \circ \mathrm{cp}]$ is tangential to S. Since cp is a retraction its Jacobian satisfies (compare to (3.6))

$$D\,\mathrm{cp} = P \circ \mathrm{cp}\, D\,\mathrm{cp}\,. \tag{4.5}$$

Now, we expand $\nabla[u \circ \mathrm{cp}]$ by referring to an arbitrary extension u_E of u as of Definition 2.1:

$$\nabla[u \circ \mathrm{cp}] = D\,\mathrm{cp}^T \nabla u_E \circ \mathrm{cp} = D\,\mathrm{cp}^T P \circ \mathrm{cp}\, \nabla u_E \circ \mathrm{cp} = D\,\mathrm{cp}^T \nabla_S u \circ \mathrm{cp}\,.$$

Since $\xi := \nabla_S u \circ \mathrm{cp}(x)$ belongs to $\mathcal{T}_{\mathrm{cp}(x)} S$, $\nabla[u \circ \mathrm{cp}](x)$ also belongs to $\mathcal{T}_{\mathrm{cp}(x)} S$ by our requirement on $D\,\mathrm{cp}(x)^T$. Now, we are sure that $v := A \circ \mathrm{cp}\, \nabla[u \circ \mathrm{cp}]$ is tangential to S for all x, and so the same arguments used in the proof of Theorem 4.2 apply. □

PROPOSITION 4.4. *If cp is a C^2-smooth closest point function with a symmetric Jacobian $D\,\mathrm{cp} = D\,\mathrm{cp}^T$ then cp satisfies the requirements of Theorem 4.3. The Euclidean closest point function ecp is one such closest point function with symmetric Jacobian*

$$D\,\mathrm{ecp}(x) = \begin{cases} I - \nabla d(x) \cdot \nabla d(x)^T - d(x)D^2 d(x) & x \in B(S) \setminus S, \\ P(x) & x \in S. \end{cases}$$

Proof. Equation (4.5) combined with symmetry of the Jacobian yields

$$P \circ \mathrm{cp}\, D\,\mathrm{cp} = D\,\mathrm{cp} = D\,\mathrm{cp}^T$$

which shows that $D\,\mathrm{cp}^T$ in this case maps all vectors ξ to tangent vectors. For the derivation of $D\,\mathrm{ecp}$ see the proof of Theorem 3.8. For further smoothness properties of ecp see Section 3.2.1. □

4.1.1. More General Diffusion Coefficients. In both Theorems 4.2 and 4.3 the crucial bit is that $A(y)$ for fixed y maps certain vectors ξ to the tangent space, i.e., $A(y)\xi \in \mathcal{T}_y S$. The theorems are still true if we let A also depend on the function u, for example this dependence could be of the form $A(y, u(y), \nabla_S u(y))$.

4.2. The Laplace–Beltrami operator. As an example we discuss the surface Laplacian (the Laplace–Beltrami operator) in terms of the closest point calculus:
1. We may write the Laplace–Beltrami operator as

$$\Delta_S u = \mathrm{div}_S(\nabla_S u)\,.$$

Given a closest point function that satisfies the requirement of Theorem 4.3, e.g., the Euclidean closest point function ecp, we have

$$\Delta[u \circ \mathrm{cp}](y) = \Delta_S u(y)\,, \quad y \in S\,.$$

2. Alternatively, we may rewrite the Laplace–Beltrami operator by using a diffusion tensor as

$$\Delta_S u = \mathrm{div}_S(P\nabla_S u)\,.$$

The diffusion tensor here is the projector onto the tangent space. So we have replaced the identity matrix with the surface intrinsic identity matrix. Now Theorem 4.2 allows us to compute the Laplace–Beltrami operator like

$$\mathrm{div}(P \circ \mathrm{cp}\, \nabla[u \circ \mathrm{cp}])(y) = \Delta_S u(y)\,, \quad y \in S\,,$$

without any further requirements on $D\,\mathrm{cp}$.

3. If P is not known a priori and cp does not satisfy the requirement of Theorem 4.3, we can always work with re-extensions (directly applying the Gradient and Divergence Principles 3.4 and 3.5)

$$\mathrm{div}(\nabla[u \circ \mathrm{cp}] \circ \mathrm{cp})(y) = \Delta_S u(y)\,, \quad y \in S.$$

Note by expanding the expression $\nabla[u \circ \mathrm{cp}] \circ \mathrm{cp}$ as in (3.15)

$$\nabla[u \circ \mathrm{cp}] \circ \mathrm{cp} = P \circ \mathrm{cp}\, \nabla u_E \circ \mathrm{cp},$$

we can see that re-extension in fact means an implicit version of approach 2.

4.3. Proof of a Principle of Ruuth & Merriman. For the original Closest Point Method (with ecp) Ruuth & Merriman in [19] also reasoned that a re-extension is not necessary for some diffusion operators based on the fact that the Euclidean closest point extension satisfies the PDE

$$\langle\, \nabla d(x), \nabla[u \circ \mathrm{ecp}]\,\rangle = 0\,, \quad x \in B(S) \setminus S$$

and the special principle:

> "Let v be any vector field on $\mathbb{R}^n$ that is tangent at S and also tangent at all surfaces displaced by a fixed distance from S (i.e., all surfaces defined as level sets of the distance function d to S). Then at points y on the surface $\mathrm{div}_S v(y) = \mathrm{div}\, v(y)$."

We give a proof of this below as a consequence of Lemma 4.1 but with the additional assumption of C^2-regularity of the vector field v if codim $S \geq 2$.

Ruuth & Merriman [19] also use this principle to establish a divergence principle. This requires that the surface vector field w be tangent to the surface and it also requires the use of the Euclidean closest point function to extend the surface vector field to the embedding space as $v = w \circ \mathrm{ecp}$. In contrast, the more general Divergence Principle 3.5 works for any (possibly non-tangential) surface vector field with extensions using any closest point function.

As said, their principle can also be used with the Euclidean closest point function to allow fewer extensions in certain surface diffusion operators. Theorem 4.3 generalizes this, allowing for a larger class of closest point functions.

Proof. Given the parametrization γ of a generic surface patch, the map

$$\Phi(\theta_1, \theta_2) = \gamma(\theta_1) + N \circ \gamma(\theta_1) \cdot \theta_2$$

parametrizes $\mathrm{ecp}^{-1}(\gamma(\theta_1))$ for fixed θ_1 and gives us the required coordinate system. For points x off the surface the normal ∇d to the level-sets of the distance map is given by

$$\nabla d(x) = \frac{x - \mathrm{ecp}(x)}{|x - \mathrm{ecp}(x)|} \quad \Rightarrow \quad \nabla d \circ \Phi(\theta_1, \theta_2) = \frac{N \circ \gamma(\theta_1) \cdot \theta_2}{|N \circ \gamma(\theta_1) \cdot \theta_2|}.$$

Then the image of the following projection matrix

$$Q(x) = I - \nabla d(x)\nabla d(x)^T \quad \Rightarrow \quad \bar{Q}(\theta_1, \theta_2) = Q \circ \Phi(\theta_1, \theta_2) = I - \frac{N\theta_2\theta_2^T N^T}{|N \cdot \theta_2|^2}$$

is tangent to level lines of the Euclidean distance map d. Since v is itself tangent to the latter level lines, we have $Q \cdot v = v$ or in θ-variables $\bar{Q}\bar{v} = \bar{v}$ with

$$\bar{v}(\theta_1, \theta_2) = v \circ \Phi(\theta_1, \theta_2) = D_{\theta_1}\gamma(\theta_1) \cdot \tilde{v}(\theta_1, \theta_2) + N \circ \gamma(\theta_1) \cdot \eta(\theta_1, \theta_2)$$

as in Lemma 4.1. Since ∇d is also normal to the surface S, the product $\bar{Q}\bar{v}$ is

$$\bar{Q}\bar{v} = D_{\theta_1}\gamma \cdot \tilde{v} + \bar{Q}N\eta .$$

If the codimension is one, the matrix N is an $n \times 1$ matrix and $\nabla d = \pm N$, hence, the summand $\bar{Q}N\eta$ cancels out, and this product reduces to $\bar{Q}\bar{v} = D_{\theta_1}\gamma \cdot \tilde{v}$. Consequently, in order for $\bar{Q}\bar{v} = \bar{v}$ to hold, $\eta \equiv 0$ must vanish, and Lemma 4.1 yields the result. If the codimension is higher, we rewrite the product as

$$\bar{Q}\bar{v} = D_{\theta_1}\gamma \cdot \tilde{v} + N \cdot \left(I - \frac{\theta_2 \theta_2^T N^T N}{|N \cdot \theta_2|^2} \right) \eta .$$

The coefficient must satisfy $\eta(\theta_1, 0) = 0$ so that $v(x)$ is tangent to the surface if $x \in S$. In order to have additionally $\bar{Q}\bar{v} = \bar{v}$, η must also satisfy

$$\theta_2^T A\eta = 0 \quad \text{where} \quad A = A(\theta_1) := (N \circ \gamma(\theta_1))^T \cdot N \circ \gamma(\theta_1) .$$

We differentiate the new condition $\theta_2^T A\eta = 0$ with respect to θ_2 and obtain

$$\eta^T A + \theta_2^T A D_{\theta_2}\eta = 0 \qquad \Rightarrow \qquad \eta = -A^{-1}D_{\theta_2}\eta^T A\theta_2$$

Since in higher codimension v is assumed to be C^2, we can differentiate again which yields

$$D_{\theta_2}\eta = -A^{-1}D_{\theta_2}\eta^T A - A^{-1}D_{\theta_2}^2\eta^T A\theta_2 .$$

We apply the trace-operator and get

$$\text{trace } D_{\theta_2}\eta = -\text{trace } D_{\theta_2}\eta^T - \text{trace } \left(A^{-1}D_{\theta_2}^2\eta^T A\theta_2 \right) .$$

Finally, since the second derivative $D_{\theta_2}^2\eta$ is bounded on a small compact neighborhood of $(\theta_1, 0)$ we have

$$\text{trace } D_{\theta_2}\eta = \mathcal{O}(|\theta_2|) , \quad \theta_2 \to 0 .$$

So the second requirement on η is satisfied and Lemma 4.1 yields the result. □

5. Construction of Closest Point Functions from Level-Set Descriptions. Beginning with the case of codim $S = 1$, we present a general construction of closest point functions in the special case when the surface is given by a level set (or as an intersection of several level sets.)

5.1. Codimension One. Let $\varphi : B(S) \to S$ denote a C^2-smooth scalar level-set function. The surface S is the zero-level of φ, which we assume is a proper implicit description of S, i.e.,

$$\nabla\varphi(x) \neq 0 \quad \text{for all} \quad x \in B(S) . \tag{5.1}$$

Thus the normals to level-sets are given by $N : B(S) \to \mathbb{R}^n$, $N = \nabla\varphi/|\nabla\varphi|$ and the normal field of S is $N|_S : S \to \mathbb{R}^n$. Again $B(S) \subset \mathbb{R}^n$ denotes a band around S and condition (5.1) will determine a reasonable band $B(S)$ when starting out with a φ defined on all of $\mathbb{R}^n$.

Now closely following [16], we construct a retraction by solving the following initial value problem (IVP):

$$\xi' = -\nabla\varphi \circ \xi , \qquad \xi(0, x) = x . \tag{5.2}$$

We denote the corresponding family of trajectories by $\xi(\tau, x)$, where τ is the ODE-time, while the parameter x refers to the initial point. If we start at a point x with $\varphi(x) > 0$ and solve forward in ODE-time, ξ is a steepest descent trajectory, while if we start at a point x with $\varphi(x) < 0$ and solve backward in ODE-time, we will obtain a steepest ascent trajectory heading for the surface. The unique intersection of the trajectory $\xi(\,\cdot\,, x)$ with the surface S defines a retraction that maps the initial point x to some point on S. The next step is to find the point of intersection which we achieve by a suitable transformation of ODE (5.2). We consider the descent case ($\varphi(x) > 0$), and relate the ODE-time τ and the level label λ by

$$\varphi(\xi(\tau(\lambda), x)) = \varphi(x) - \lambda \,. \tag{5.3}$$

The implicit function $\tau : [0, \varphi(x)] \to \mathbb{R}_+, \lambda \to \tau(\lambda)$ takes the value $\tau(0) = 0$ and has the derivative $\tau' = 1/|\nabla \varphi|^2 \circ \xi$. The transformation that we want is $\eta(\lambda, x) := \xi(\tau(\lambda), x)$ because (5.3) can be rewritten as $\varphi(\eta(\lambda, x)) = \varphi(x) - \lambda$, and thus evaluating η at $\lambda = \varphi(x)$ returns the corresponding point on the surface S:

$$\varphi(\eta(\varphi(x), x)) = 0 \quad \Leftrightarrow \quad \eta(\varphi(x), x) \in S.$$

We obtain η as the solution of the new initial value problem (see also [16])

$$\eta'(\lambda, x) = -\frac{\nabla \varphi}{|\nabla \varphi|^2} \circ \eta(\lambda, x) \,, \qquad \eta(0, x) = x \,. \tag{5.4}$$

So far we have considered the descent case but for ascent we end up with the same IVP. Finally, we obtain the desired closest point function cp by

$$\mathrm{cp} : B(S) \to S \,, \qquad \mathrm{cp}(x) := \eta(\varphi(x), x) \,.$$

By construction, this function is a C^1-retraction (because the right-hand side of ODE (5.4) is C^1-smooth the differentiability of $\eta(\tau, x)$ with respect to x follows from ODE-theory, see e.g., [12, Chapter 4.6]). And that it is in fact a closest point function is a direct consequence of Theorem 3.7: because of our construction the pre-image $\mathrm{cp}^{-1}(y)$ is exactly a trajectory of the ODE (5.4) and this trajectory intersects S orthogonally.

5.1.1. Remarks.
- If one is only interested in the construction of a retraction map it suffices to replace $\nabla \varphi$ in (5.4) with a transversal field c, i.e., $|c| = 1$ and $\langle c, N \rangle \geq \beta > 0$. After a similar transformation the retraction is given by $r(x) = \eta(\varphi(x), x)$. This approach to retractions is actually the method of backward characteristics (see e.g., [16]): the solution of the PDE

$$\langle c(x), \nabla v \rangle = 0 \,, \quad v|_S = u \,, \tag{5.5}$$

  is $v = u \circ r$. So, in a neighborhood of S, v defines an extension of the surface function u and is as smooth as u (see the method of characteristics in e.g., [8]). The idea of extending surface functions by solving (5.5) with $c = \nabla \varphi$ has been used in other earlier works, see e.g., [4].
- Note that the same ODE as in (5.4) is used in [11] for the construction of diffeomorphisms.
- If $f : \mathbb{R} \to \mathbb{R}$ is a smooth function with $f' \neq 0$ then the closest point function obtained from using $\hat{\varphi} := f \circ \varphi$ in IVP (5.4) is the same as that obtained from the original φ because the corresponding ODEs parametrize the same curve through the initial point x.
- The Euclidean closest point function is a special case our construction: let $\varphi = \mathrm{sd}$ be the signed Euclidean distance function. In this case, the IVP for η reduces to $\eta'(\lambda, x) = -\nabla \mathrm{sd}(x)$, $\eta(0, x) = x$, with a right-hand side independent of λ. This has the solution $\eta(\lambda, x) = x - \lambda \nabla \mathrm{sd}(x)$ and the corresponding closest point function is the Euclidean one

$$\eta(\mathrm{sd}(x), x) = x - \mathrm{sd}(x) \nabla \mathrm{sd}(x) = \mathrm{ecp}(x) \,.$$

5.2. Higher Codimension. In the case of higher codimension, $\operatorname{codim} S = m \geq 2$, we assume that S is the proper intersection of m surfaces of codimension one. Given this, we construct the closest point function $\operatorname{cp} = \operatorname{cp}_m \circ \cdots \circ \operatorname{cp}_2 \circ \operatorname{cp}_1$ as the composition of m closest point functions, where cp_1 retracts onto S_1, cp_2 retracts S_1-intrinsically onto $S_1 \cap S_2$, cp_3 retracts $S_1 \cap S_2$-intrinsically onto $S_1 \cap S_2 \cap S_3$, and so on. We demonstrate only the situation where $\operatorname{codim} S = 2$, since this is essentially the inductive step for the general case.

Let again $B(S) \subset \mathbb{R}^n$ be a band around S and let $\varphi_j : B(S) \to S$, $j \in \{1,2\}$, be C^2-smooth level-set functions. Each level-set function φ_j shall yield a proper implicit description of a codimension-one surface S_j as its zero-level, thus we require:

$$\nabla \varphi_j(x) \neq 0 , \quad \text{for all} \quad x \in B(S) .$$

The two surfaces S_1 and S_2 are orientable with normal vector fields given by $N_j : S_j \to \mathbb{R}^n$, $N_j = \nabla \varphi_j / |\nabla \varphi_j|$. We assume their intersection $S = S_1 \cap S_2$ to be proper, that is, the normal vectors have to be linearly independent on S. In fact we assume the linear independence to hold on all of $B(S)$ (possibly we have to narrow $B(S)$). This implies that any two level-sets $S_1^{\mu_1} := \{x : \varphi_1(x) = \mu_1\}$, $S_2^{\mu_2} := \{x : \varphi_2(x) = \mu_2\}$ intersect properly (as long as the intersection is non-empty).

Now, we set up a closest point function $\operatorname{cp} = \operatorname{cp}_2 \circ \operatorname{cp}_1$ in two steps. The first step is the same as in the previous section: $\operatorname{cp}_1 : B(S) \to B(S) \cap S_1$ maps onto the subset $B(S) \cap S_1$ of the first surface S_1 by $\operatorname{cp}_1 = \eta_1(\varphi_1(x), x)$ where η_1 solves (5.4) with φ_1 in place of φ.

The second step is more interesting: we construct an S_1-intrinsic retraction $\operatorname{cp}_2 : B(S) \cap S_1 \to S$. The idea is essentially the same as that of the previous set-up, but now it is S_1-intrinsic: we consider the IVP

$$\eta_2'(\lambda, x) = -\frac{\nabla_{S_1} \varphi_2}{|\nabla_{S_1} \varphi_2|^2} \circ \eta_2(\lambda, x) , \qquad \eta_2(0, x) = x , \tag{5.6}$$

by transforming analogously to the codimension-one case (c.f., (5.4)). Note that $\nabla_{S_1} \varphi_2$ is given by $\nabla_{S_1} \varphi_2 = P_1 \nabla \varphi_2$ with $P_1 = I - N_1 N_1^T$ and that the assumption of a proper intersection guarantees that $\nabla_{S_1} \varphi_2$ does not vanish since N_1 and $\nabla \varphi_2$ are linearly independent. Because we start in S_1 and $\nabla_{S_1} \varphi_2$ is tangential to S_1, the curve $\eta_2(\cdot, x)$ is contained in S_1. Hence, we obtain an S_1-intrinsic closest point function cp_2 by

$$\operatorname{cp}_2 : B(S) \cap S_1 \to S , \qquad \operatorname{cp}_2(x) := \eta_2(\varphi_2(x), x) .$$

The composition $\operatorname{cp} = \operatorname{cp}_2 \circ \operatorname{cp}_1$ defines certainly a C^1-retraction $\operatorname{cp} : B(S) \to S$, and, as all the intersections are orthogonal, Theorem 3.7 guarantees cp to be a closest point function.

5.3. Example 1. We construct a closest point function for a circle S of radius $\sqrt{3}/2$ embedded in $\mathbb{R}^3$ as the intersection of a sphere and a plane (Figure 5.1 left). The two level set functions are

$$\varphi_1(x_1, x_2, x_3) = x_1^2 + x_2^2 + x_3^2 - 1 , \qquad\qquad \varphi_2(x_1, x_2, x_3) = x_3 - \tfrac{1}{2} .$$

The equation $\varphi_1 = 0$ yields the unit sphere as the codimension-one surface S_1, equation $\varphi_2 = 0$ specifies the second codimension-one surface S_2 which is a plane parallel to the $x_1 x_2$-plane at $x_3 = 1/2$, and the circle $S = S_1 \cap S_2$ is the intersection.

First step: we set up a closest point map cp_1 onto the sphere S_1. Let $c_1 = \nabla \varphi_1$, the IVP for η_1 is

$$\eta_1' = -\frac{\nabla \varphi_1}{|\nabla \varphi_1|^2} \circ \eta_1 = -\frac{\eta_1}{2 \cdot |\eta_1|^2} , \quad \eta_1(0, x) = x \in \mathbb{R}^3 \setminus \{0\} . \tag{5.7}$$

The maximal band around the sphere where $\nabla \varphi_1 \neq 0$ does not vanish is $\mathbb{R}^3 \setminus \{0\}$. The solution η_1 of IVP (5.7) and the corresponding closest point function $\operatorname{cp}_1 : \mathbb{R}^3 \setminus \{0\} \to S_1$ are

$$\eta_1(\lambda, x) = \sqrt{|x|^2 - \lambda} \cdot \frac{x}{|x|} \quad \Rightarrow \quad \operatorname{cp}_1(x) = \eta_1(\varphi_1(x), x) = \frac{x}{|x|} .$$
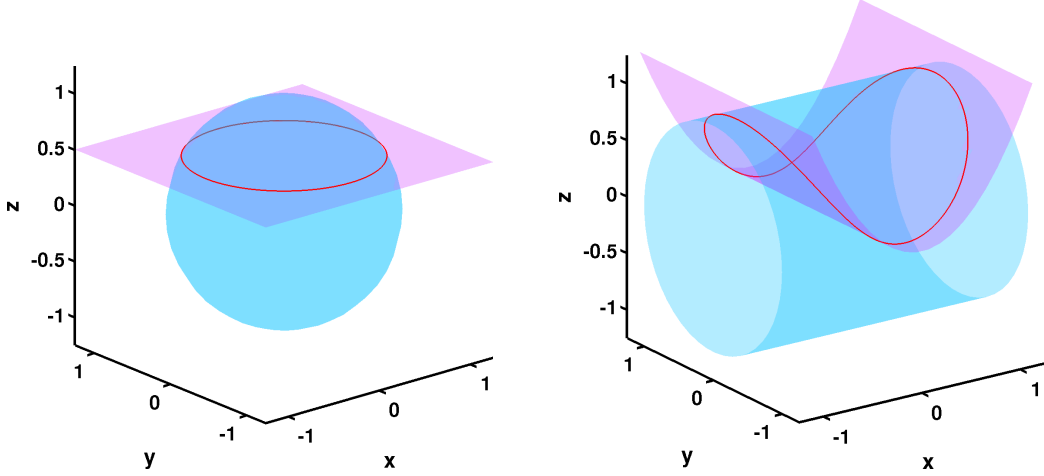
FIG. 5.1. *Example 1 (left): a circle (red) embedded in $\mathbb{R}^3$, given as the intersection of a sphere and a plane. Example 2 (right): a curve (red) embedded in $\mathbb{R}^3$, given as the intersection of a cylinder and a parabola.*

(Note that φ_1 is of the form $\varphi_1 = f \circ \mathrm{sd}$ with f strictly monotone. Hence cp_1 is the Euclidean closest point function, see the remarks 5.1.1.)

Second step: we set up an S_1-intrinsic closest point map cp_2 onto the circle S. Let $c_2 = \nabla_{S_1} \varphi_2 = P_1 \cdot \nabla \varphi_2$. The projector P_1 is given by

$$P_1(x) = I - \frac{\nabla \varphi_1(x) \cdot \nabla \varphi_1(x)^T}{|\nabla \varphi_1(x)|^2} = \frac{1}{x_1^2 + x_2^2 + x_3^2} \cdot \begin{pmatrix} x_2^2 + x_3^2 & -x_1 x_2 & -x_1 x_3 \\ -x_1 x_2 & x_1^2 + x_3^2 & -x_2 x_3 \\ -x_1 x_3 & -x_2 x_3 & x_1^2 + x_2^2 \end{pmatrix}.$$

For $x \in S_1$, i.e., $|x| = 1$, we get then

$$\nabla_{S_1} \varphi_2(x) = P_1(x) \cdot \nabla \varphi_2(x) = \left(-x_1 x_3, \ -x_2 x_3, \ x_1^2 + x_2^2 \right)^T = \left(-x_1 x_3, \ -x_2 x_3, \ 1 - x_3^2 \right)^T,$$

$$|\nabla_{S_1} \varphi_2(x)|^2 = 1 - x_3^2.$$

The largest subset of S_1 where $\nabla_{S_1} \varphi_2$ does not vanish is the sphere without the poles $S_1 \setminus \{\pm e_3\}$, and so the IVP for η_2 is

$$\eta_2' = -\frac{\nabla_{S_1} \varphi_2}{|\nabla_{S_1} \varphi_2|^2} \circ \eta_2 = \left(\frac{\eta_{2,3}}{1 - \eta_{2,3}^2} \cdot \eta_{2,1}, \ \frac{\eta_{2,3}}{1 - \eta_{2,3}^2} \cdot \eta_{2,2}, \ -1 \right)^T, \quad \eta_2(0, x) = x \in S_1 \setminus \{\pm e_3\}, \quad (5.8)$$

where $\eta_{2,j}$ is the j-th component of η_2. The solution η_2 of IVP (5.8) and the corresponding closest point function $\mathrm{cp}_2 : S_1 \setminus \{\pm e_3\} \to S$ are

$$\eta_2(\lambda, x) = \left(\sqrt{\frac{1 - (x_3 - \lambda)^2}{1 - x_3^2}} \cdot x_1, \ \sqrt{\frac{1 - (x_3 - \lambda)^2}{1 - x_3^2}} \cdot x_2, \ x_3 - \lambda \right)^T$$

$$\Rightarrow \quad \mathrm{cp}_2(x) = \eta_2(\varphi_2(x), x) = \frac{1}{2} \cdot \left(\frac{\sqrt{3}}{\sqrt{1 - x_3^2}} \cdot x_1, \ \frac{\sqrt{3}}{\sqrt{1 - x_3^2}} \cdot x_2, \ 1 \right)^T.$$

Finally, we compose the closest point function $\mathrm{cp} : B(S) = \mathbb{R}^3 \setminus \{x : x_1 = x_2 = 0\} \to S$ by

$$\mathrm{cp}(x) = \mathrm{cp}_2 \circ \mathrm{cp}_1(x) = \frac{1}{2} \cdot \left(\frac{\sqrt{3} x_1}{\sqrt{x_1^2 + x_2^2}}, \ \frac{\sqrt{3} x_2}{\sqrt{x_1^2 + x_2^2}}, \ 1 \right)^T.$$

Figure 5.2 shows this construction of cp schematically. The maximal band $B(S)$ around S— where cp is defined—is $\mathbb{R}^3$ without the x_3-axis, since the x_3-axis gets retracted by cp_1 to the north-/south-pole of the sphere S_1 where cp_2 is not defined.
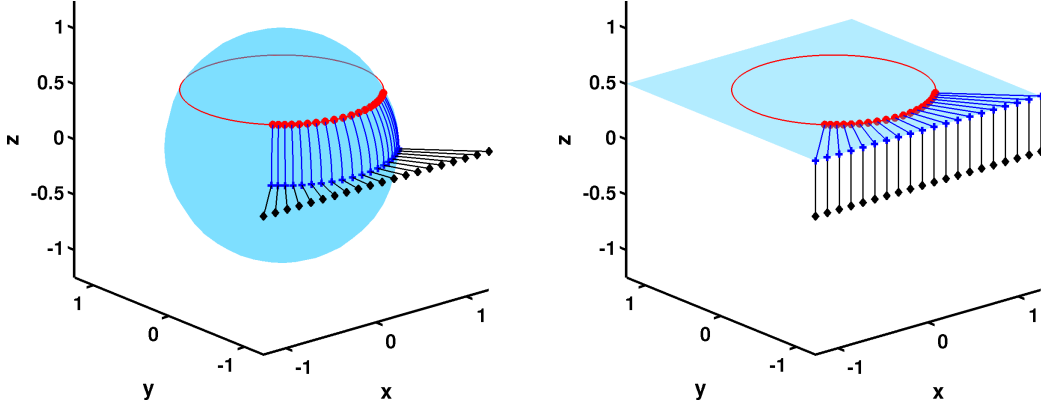
FIG. 5.2. *A circle (red) embedded in $\mathbb{R}^3$, given as the intersection of a sphere and a plane. Left: the closest point function* $\mathrm{cp} = \mathrm{cp}_2 \circ \mathrm{cp}_1$ *maps the black diamonds to the red dots by a two-stage retraction: first* cp_1 *maps the black diamonds onto the blue crosses on the light blue sphere, and second* cp_2 *maps blue crosses onto the red dots on the red circle by following trajectories on the sphere. Right: the closest point function* $\hat{\mathrm{cp}}(x) = \hat{\mathrm{cp}}_1 \circ \hat{\mathrm{cp}}_2(x)$ *first maps the black diamonds onto the blue crosses in the light blue plane, then maps the blue crosses onto the red dots on the red circle by following trajectories contained in the plane.*

This first example is intended to highlight the concept of our approach. In fact, in this particular case, it is much simpler to first project onto S_2 by $\hat{\mathrm{cp}}_2(x) = (x_1, x_2, 1/2)^T$, and then retract S_2-intrinsically (i.e., in the plane) onto S by $\hat{\mathrm{cp}}_1 : S_2 \setminus \{0\} \to S$, to obtain $\hat{\mathrm{cp}}(x) = \hat{\mathrm{cp}}_1 \circ \hat{\mathrm{cp}}_2(x)$ This approach is also illustrated in Figure 5.2 and, in this particular case, yields the same closest point function (and in fact they are both equal to ecp).

5.4. Example 2. We consider a curve embedded in $\mathbb{R}^3$ given as the intersection of a cylinder with a parabola (see Figure 5.1 right). The two level set functions are

$$\varphi_1(x_1, x_2, x_3) = 1 - x_2^2 - x_3^2 , \quad \varphi_2(x_1, x_2, x_3) = x_3 - x_1^2 . \tag{5.9}$$

This time we find the closest point functions numerically using the ODE solver `ode45` in MATLAB. The first closest point function cp—which first maps onto the cylinder—is obtained by solving the two ODEs below

$$\eta_1 = -\frac{\nabla \varphi_1}{|\nabla \varphi_1|^2} \circ \eta_1 , \quad \eta_1(0, x) = x , \qquad \Rightarrow \quad z := \eta_1(\varphi_1(x), x) ,$$

$$\eta_2 = -\frac{P_1 \nabla \varphi_2}{|P_1 \nabla \varphi_2|^2} \circ \eta_2 , \quad \eta_2(0, z) = z , \qquad \Rightarrow \quad \mathrm{cp}(x) := \eta_2(\varphi_2(z), z) ,$$

in the given order. In the same way we obtain the second function $\hat{\mathrm{cp}}$—which maps first onto the parabola—by interchanging the roles of φ_1 and φ_2 and numerically solving the ODEs

$$\eta_2 = -\frac{\nabla \varphi_2}{|\nabla \varphi_2|^2} \circ \eta_2 , \quad \eta_2(0, x) = x , \qquad \Rightarrow \quad z := \eta_2(\varphi_1(x), x) ,$$

$$\eta_1 = -\frac{P_2 \nabla \varphi_1}{|P_2 \nabla \varphi_1|^2} \circ \eta_1 , \quad \eta_1(0, y) = z , \qquad \Rightarrow \quad \hat{\mathrm{cp}}(x) := \eta_1(\varphi_1(z), z).$$

The retraction stages of the resulting closest point functions cp and $\hat{\mathrm{cp}}$ are visualized in Figure 5.3.

In contrast with our first example, here the two closest point functions cp and $\hat{\mathrm{cp}}$ are different. We define a $50 \times 50 \times 50$ Cartesian grid G on a reference box $R = [-1.25, 1.25] \times [-1.25, 1.25] \times [-0.25, 1.25]$ containing S. We use a subset of these points as a narrow band of grid points sur-
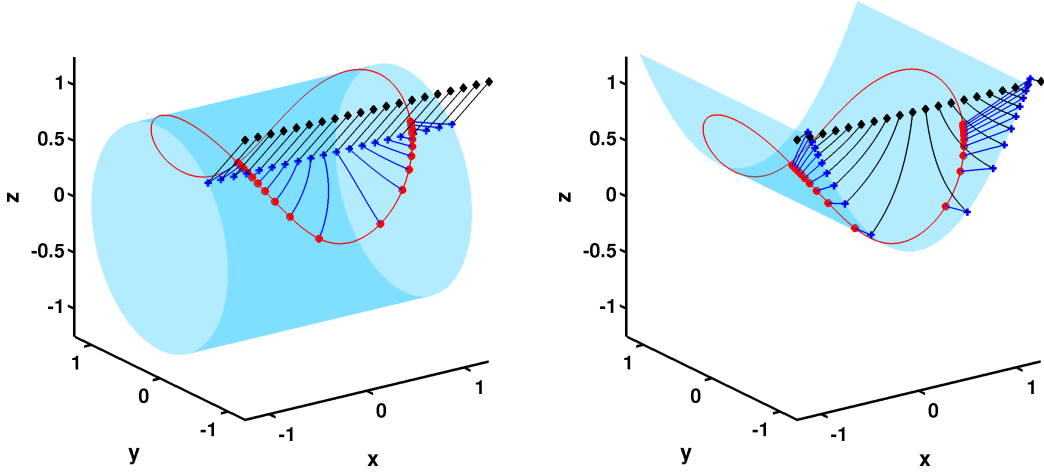
FIG. 5.3. *A curve (red) embedded in* $\mathbb{R}^3$*, given as illustrated in Figure 5.1 (right). Left: the closest point function* $\mathrm{cp} = \mathrm{cp}_2 \circ \mathrm{cp}_1$ *maps the black diamonds to the red dots by a two-stage retraction: first* cp_1 *maps the black diamonds onto the blue crosses on the light blue cylinder, and second* cp_2 *maps the blue crosses onto the red dots on the red curve by following trajectories on the cylinder surface. Right: the closest point function* $\hat{\mathrm{cp}} = \hat{\mathrm{cp}}_1 \circ \hat{\mathrm{cp}}_2$ *first maps the black diamonds onto the blue crosses on the light blue parabola by* $\hat{\mathrm{cp}}_2$*, then* $\hat{\mathrm{cp}}_1$ *maps the blue crosses onto the red dots on the red curve by following trajectories on the parabola.*

rounding S.[3] Comparing the values of the distance function $\varphi = (\varphi_1^2 + \varphi_2^2)^{\frac{1}{2}}$ at the closest points

$$\max_{x \in G \cap B(S)} \varphi(\, \mathrm{cp}(x)\,) = 4.4893 \cdot 10^{-15},$$

$$\max_{x \in G \cap B(S)} \varphi(\, \hat{\mathrm{cp}}(x)\,) = 4.4758 \cdot 10^{-15}$$

we can see that both numerical functions cp and $\hat{\mathrm{cp}}$ are very accurate. We also note they are indeed different mappings because $\max_{x \in G \cap B(S)} |\, \mathrm{cp}(x) - \hat{\mathrm{cp}}(x)\,| = 1.7095 \cdot 10^{-03}$ (see also Table 6.2 where they are clearly distinct from ecp).

6. The Closest Point Method with Non-Euclidean Closest Point Functions. In this section we demonstrate that the explicit Closest Point Method based on Euler time-stepping still works when replacing the Euclidean closest point function with non-Euclidean ones.

Given an evolution equation on a smooth closed surface S as

$$\partial_t u - A_S(t, y, u) = 0 , \qquad\qquad u(0, y) = u_0(y) , \quad y \in S$$

where A_S is a linear or nonlinear surface-spatial differential operator on S, following [19], the semi-discrete explicit Closest Point Method based on Euler time-stepping with time step τ is

Initialization:	$v_0 = u_0 \circ \mathrm{cp}$
Evolve step:	$w_{n+1} = v_n + \tau A(t_n, x, v_n) , \quad x \in B(S)$
Extension step:	$v_{n+1} = w_{n+1} \circ \mathrm{cp}$

where A is a spatial operator on $B(S)$ which is defined from A_S via the closest point calculus and hence

$$A(t, x, u \circ \mathrm{cp})|_{x=y} = A_S(t, y, u) , \quad y \in S .$$

For the fully discrete Closest Point Method which is also discrete with respect to the spatial variable $x \in B(S)$ we replace A with a discretization of it, while the extension $w_{n+1} \circ \mathrm{cp}(x)$ is replaced with interpolation of the discrete w_{n+1} in a neighborhood of $\mathrm{cp}(x)$ because the point $\mathrm{cp}(x)$ is not a grid point in general [19].

---

[3]For this particular example we define a band by $B(S) = \{(x_1, x_2, x_3) : \varphi \leq 0.125\}$ where we use $\varphi = (\varphi_1^2 + \varphi_2^2)^{\frac{1}{2}}$ in lieu of Euclidean distance. Our banded grid is $G \cap B(S)$ and contains 1660 grid points. It contains more points than are strictly necessary: see [15, Appendix A] for an approach to banded grids for the Closest Point Method.

TABLE 6.1
Errors measured in l_∞-norm at stop time $t = 1$ for Closest Point Method approximation of the advection problem (6.1) on the curve shown in Figure 5.1 (right) using various closest point functions. There is no significant difference regarding the choice of the closest point function.

h	cp	cp̂	ecp
0.0125	9.1630e-03	9.1592e-03	9.0615e-03
0.00625	4.6182e-03	4.6172e-03	4.5544e-03
0.003125	2.3262e-03	2.3260e-03	2.2908e-03

6.1. Advection Equation. We consider an advection problem with a constant unit speed on the curve S shown in Figure 5.1 (right):

$$\partial_t u + \operatorname{div}_S (u \cdot T(y)) = 0 \,, \qquad u(0,y) = y_3 \,, \quad y \in S \,,$$

$$\text{with} \quad T(y) = -\frac{\nabla \varphi_1(y) \times \nabla \varphi_2(y)}{|\nabla \varphi_1(y) \times \nabla \varphi_2(y)|} \,. \tag{6.1}$$

The surface-spatial operator is $A_S(y, u) = -\operatorname{div}_S (u \cdot T(y))$, while the operator used in the Closest Point Method is

$$A(x, v) = -\operatorname{div}(v \cdot T \circ \mathrm{cp}(x)) \,, \quad v = u \circ \mathrm{cp} \,, \quad x \in B(S)$$

according to the Divergence Principle 3.5.

We solved this advection problem with three different closest point functions—namely cp, cp̂ from Example 2, and the Euclidean closest point function ecp—and with three different mesh sizes h on the reference box $R = [-1.25, 1.25] \times [-1.25, 1.25] \times [-0.25, 1.25]$. The ecp was computed with a numerical optimization procedure using Newton's method. The evolve step uses the first order accurate Lax–Friedrichs scheme (time step $\tau = 0.95h$ in accordance with the CFL-condition) and the extension step is performed with WENO interpolation [14] (based on tri-quadratic interpolation). The solution is advected until time $t = 1$.

We compare to a highly accurate solution obtained from parametrizing the problem. By using the parametrization $\gamma : [0, 2\pi) \to S$, $\gamma(\theta) = (\cos(\theta), \sin(\theta)\sqrt{1 + \cos(\theta)^2}, \cos(\theta)^2)^T$ the advection problem (6.1) is equivalent to

$$|\gamma'(\theta)|\partial_t \bar{u} - \partial_\theta \bar{u} = 0 \,, \qquad \bar{u}(0, \theta) = \cos(\theta)^2 \,, \quad \bar{u}(t, 2\pi) = \bar{u}(t, 0) \,, \tag{6.2}$$

where $\bar{u}(t, \theta) = u(t, \gamma(\theta))$. The formal solution of the latter is

$$\bar{u}(t, \theta) = \cos\left(s^{-1}(t + s(\theta))\right)^2 \,, \quad \text{where} \quad s(\theta) = \int_0^\theta |\gamma'(\alpha)| \, d\alpha \tag{6.3}$$

is the arc-length function. We used Chebfun [20] within MATLAB to find a highly accurate approximation to $s(\theta)$ and thereafter a Newton iteration to approximate the value $s^{-1}(t + s(\theta))$.

Table 6.1 shows the error in the results measured in l_∞-norm at $t = 1$. We see there is no significant difference regarding the choice of the closest point function and that the error is of order $O(h)$ as expected from the Lax–Friedrichs scheme.

6.2. Diffusion Equation. Here, we consider the diffusion equation on the curve S shown in Figure 5.1 (right):

$$\partial_t u - \Delta_S u = 0 \,, \qquad u(0, y) = \frac{\exp(4y_3)}{50} \,, \quad y \in S \,. \tag{6.4}$$

The surface-spatial operator is now $A_S(y, u) = \Delta_S u$.

<center>TABLE 6.2</center>

Errors measured in l_∞-norm at stop time $t = 0.1$ for Closest Point Method approximation of the diffusion equation (6.4) on the curve shown in Figure 5.1 (right) using various closest point functions. The spatial operator on the embedding space is $A(v) = \Delta v$ as in (6.5). We observe convergence when using ecp as expected. But, here, cp and ĉp do not yield a convergent method as they (with hindsight) do not satisfy the requirement of Theorem 4.3.

h	cp	ĉp	ecp
0.0125	0.017394	0.017394	4.717879e-04
0.00625	0.017499	0.017499	1.173944e-04
0.003125	0.017526	0.017526	2.927441e-05

Here again, we compare to a highly accurate solution obtained from parametrizing the problem. By $\bar{u}(t, \theta) = u(t, \gamma(\theta))$, where γ is the same parametrization that we used in (6.2), the diffusion equation (6.4) transforms to

$$\partial_t \bar{u} - \frac{1}{|\gamma'(\theta)|} \partial_\theta \left(\frac{1}{|\gamma'(\theta)|} \partial_\theta \bar{u} \right) = 0, \quad \bar{u}(0, \theta) = \frac{\exp(4\cos(\theta)^2)}{50}, \quad \bar{u}(t, 2\pi) = \bar{u}(t, 0).$$

The formal solution of the latter (with frequency parameter $\omega = 2\pi/s(2\pi)$ and arc-length function $s(\theta)$) is given by

$$\bar{u}(t, \theta) = \sum_{m=-\infty}^{\infty} c_m \, e^{-\omega^2 m^2 t} \, e^{i\omega m s(\theta)}, \quad c_m = \frac{1}{s(2\pi)} \int_0^{2\pi} \frac{\exp(4\cos(\theta)^2)}{50} \, e^{-i\omega m s(\theta)} \, |\gamma'(\theta)| \, d\theta.$$

We again used Chebfun [20] to obtain highly accurate approximations to c_m and $s(\theta)$. Moreover, we restrict the summation to $-M \le m \le M$ where M is chosen such that the bound $e^{-\omega^2 M^2 t} c_0$ is lower than machine accuracy.

In Section 4, we have discussed three different ways to deal with the Laplace–Beltrami operator by the closest point calculus which in turn give rise to three different operators A. Now, we solve the diffusion equation (6.4) using the Closest Point Method with each of these (in the evolve step) and with each of our three different closest point functions ecp, and cp, ĉp from Example 2. The extension step is performed with tri-cubic interpolation. The time step is chosen as $\tau = 0.2h^2$ for numerical stability. The errors are measured at time $t = 0.1$ in the l_∞-norm.

1. Writing the Laplace–Beltrami operator as $\Delta_S u = \text{div}_S(\nabla_S u)$, the simplest possibility is

$$A(v) = \text{div}(\nabla v) = \Delta v. \tag{6.5}$$

But, recall that this need not work if the closest point function does not satisfy the requirement of Theorem 4.3. A is discretized by the usual $\mathcal{O}(h^2)$-accurate 7-point stencil. Table 6.2 shows the errors. We observe convergence at the expected rate $\mathcal{O}(h^2)$ when using the Euclidean closest point function ecp, while cp and ĉp do not yield a convergent method. With ecp, as opposed to cp and ĉp, we can be sure that $A|_S = A_S$ since ecp satisfies the requirement of Theorem 4.3.

2. Now, we rewrite the Laplace–Beltrami operator as $\Delta_S u = \text{div}_S(P\nabla_S u)$, where the projector P is given by the outer product $P(y) = T(y) \cdot T(y)^T$ and T is the tangent field as in (6.1). Based on this formulation we obtain the following operator

$$A(x, v) = \text{div}(P \circ \text{cp}(x) \cdot \nabla v) = \sum_{l=1}^3 \partial_{x_l} \left(\sum_{m=1}^3 P_{lm} \circ \text{cp}(x) \, \partial_{x_m} v \right), \tag{6.6}$$

and Theorem 4.2 ensures that the operators coincide on the surface, i.e., $A|_S = A_S$ for all closest point functions in accordance with Definition 3.1. A is discretized by replacing the partial differential operators ∂_{x_l} with corresponding $\mathcal{O}(h^2)$-accurate central difference operators. Table 6.3 shows the errors. We observe convergence at the expected rate $\mathcal{O}(h^2)$ for all three closest point functions and there is no significant difference regarding the choice of the closest point function. Note that this approach does require that we know the tangent field.

TABLE 6.3

Errors measured in l_∞-norm at stop time $t = 0.1$ for Closest Point Method approximation of the diffusion equation (6.4) on the curve shown in Figure 5.1 (right) using various closest point functions. The spatial operator on the embedding space is $A(x, v) = \text{div}(P \circ \text{cp}(x) \cdot \nabla v)$ as in (6.6). There is no significant difference regarding the choice of the closest point function.

h	cp	c$\hat{\text{p}}$	ecp
0.0125	4.805473e-05	4.856909e-05	4.793135e-05
0.00625	1.198697e-05	1.211579e-05	1.195396e-05
0.003125	2.975015e-06	3.008249e-06	2.968171e-06

TABLE 6.4

Errors measured in l_∞-norm at stop time $t = 0.1$ for Closest Point Method approximation of the diffusion equation (6.4) on the curve shown in Figure 5.1 (right) using various closest point functions. The spatial operator on the embedding space is $A(v) = \text{div}(\nabla v \circ \text{cp})$ as in (6.7). There is no significant difference regarding the choice of the closest point function.

h	cp	c$\hat{\text{p}}$	ecp
0.0125	1.508222e-04	1.503411e-04	1.492513e-04
0.00625	3.754836e-05	3.743075e-05	3.715598e-05
0.003125	9.347565e-06	9.319686e-06	9.251365e-06

3. Finally, we work with re-extensions and appeal to the Gradient and Divergence Principles 3.4 and 3.5:

$$A(v) = \text{div}(\nabla v \circ \text{cp}) = \sum_{l=1}^{3} \partial_{x_l}[(\partial_{x_l} v) \circ \text{cp}] . \qquad (6.7)$$

The discretization of A involves two steps: the partial differential operators ∂_{x_l} are replaced with corresponding central difference operators, the re-extensions $(\partial_{x_l} v) \circ \text{cp}$ are replaced with tri-cubic interpolation. Table 6.4 shows the errors. We observe convergence at the expected rate $\mathcal{O}(h^2)$ for all three closest point functions. There is no significant difference regarding the choice of the closest point function.

In the three experiments above we solved the same surface problem (6.4). In experiment 1 we confirm that when using a special closest point function satisfying the requirements of Theorem 4.3—namely ecp—we can drop the second extension. This reduces the computational costs (fewer interpolation operations) compared to experiment 3 where we explicitly use the re-extension. But comparing the right-most column of Table 6.2 with Tables 6.3 and 6.4 we can see that either using more knowledge about the surface (the explicit use of P) as in experiment 2 or doing more work (re-extensions) as in experiment 3 pays off—at least in this particular problem—with better error constants.

Moreover, experiment 3 (as well as the advection experiment above) provides some evidence that when using re-extensions after each differential operator (that is, using the framework of Section 3) all closest point functions work equally well, both in theory and in practice. The choice of the closest point function in practice might depend, for example, on which closest point function is easiest to construct.

7. Conclusions. We presented a closest point calculus which makes use of closest point functions. This calculus forms the basis of a general Closest Point Method along the lines of [19]. The original Closest Point Method of [19] inspired the present work: after becoming aware of the key property $D \text{ecp}(y) = P(y)$ which accounts for the gradient principle of the original method, we turned it into a definition of a general class of closest point functions namely Definition 3.1. Here, we characterize such closest point functions (see Theorems 3.3 and 3.7) and prove that this class of closest point functions yields the desired closest point calculus (see Theorem 3.2 and the Gradient and Divergence Principles 3.4 and 3.5 which follow). The closest point calculus is also sufficient to tackle higher order surface differential operators by appropriate combinations of the principles, however for all surface-intrinsic diffusion operators the calculus can be simplified to

use fewer closest point extensions (see Theorems 4.2 and 4.3). Finally, the basic principles of the original Closest Point Method are now contained and proven in our general framework.

In addition to the framework, we describe a construction of closest point functions given a level-set description of the surface and show examples. This demonstrates that there are interesting closest point functions besides the Euclidean one. Furthermore, we demonstrate on two examples (the advection equation and the diffusion equation on a closed space curve) that the Closest Point Method combined with non-Euclidean closest point functions works as expected.

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