# ON *W<sup>k,p</sup>*-MANIFOLDS AND *W<sup>k,p</sup>*-SURFACES FOR ANALYSIS OF THE CONVERGENCE OF MESH-BASED APPROXIMATION

KEVIN SCULLY

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To categorize the convergence properties of mesh-based approximations to manifolds and surfaces, this paper defines these approximations as " $W^{k,p}$ -manifolds" and " $W^{k,p}$ surfaces." In particular, this paper examines the importance of these classifications in the convergence in  $L^1$ -norm of interpolants, built on the approximate manifold or surface, of functions defined on the approximated manifold or surface. To provide context, the applicability of an interpolation framework established by Nédélec involving the convergence of metric determinants is examined. An extension of Nédélec's framework to  $W^{k,p}$ -surfaces is presented.

## 1. Introduction

The paper [16] presents a framework for measuring error in mesh-based approximations of functions across multiple coordinate systems of a manifold or surface. That paper also points out the need to clarify the role "weak"  $W^{k,p}$ -differentiability plays in such approximation. To fill this need, this paper defines  $W^{k,p}$ -manifolds and surfaces and discusses where they fit into mesh-based approximation. Thus, we will review the convergence measuring framework of [16]. We will then discuss the need for  $W^{k,p}$ -manifolds and  $W^{k,p}$ -surfaces within this framework and present definitions. To provide context, we will discuss the importance of Nédélec's approximation framework [14] in measuring convergence and examine when this framework applies. We then extend this framework to  $W^{k,p}$ -surfaces and present numerical results verifying this extension.

## 2. Background

While the most common error estimates for mesh-based approximation on surfaces and manifolds are local or  $L^{\infty}$ -estimates (a commonly used  $L^{\infty}$ -estimate appears in Sheng and Hirsch [17]. The work [15] provides a survey of error estimates for mesh-based approximation on surfaces and manifolds), the work [16] provides a global  $L^1$ -estimate. We now review the framework for measuring the convergence of mesh-based interpolants of functions on surfaces and manifolds from [16].

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Mesh-based approximation on a manifold or surface involves three separate approximations. The first step is the approximation of the different, local coordinate domains with triangulated sets. The second step is the approximation of the maps from the local coordinate domains to the global set (i.e., the surface or underlying manifold). The final step is the approximation of the desired function with a mesh-based interpolant (e.g., piecewise-linear finite elements). Each step produces approximation error.

The difference between a function f on a manifold M and an approximation  $f_h$  of f on a triangulated approximation  $M_h$  of M is measured via a "metric"  $d_{M,M_h}(f, f_h)$ . This metric essentially sums the  $L^1$ -norms of the differences of f and  $f_h$  (both weighted with their manifolds' respective metric determinants g and  $g_h$  and partition of unity functions  $\phi_i$  and  $\phi_{h,i}$ ) over the sets  $D_i$ , triangulated approximations of  $C_i$ , the coordinate patches of M. The following estimate governs the convergence of  $f_h$  to f in this metric:

$$d_{M,M_{h}}(f,f_{h}) \leq K \sum_{i} \left( \left| \left| \phi_{i} - \phi_{h,i} \right| \right|_{L^{1}(D_{i})} + \left| \left| f - f_{h} \right| \right|_{L^{1}(D_{i})} + \left| \left| \left| g \right| - \left| g_{h} \right| \right| \right|_{L^{1}(D_{i})} + Jh^{r} \right),$$

$$(2.1)$$

where *K* is a constant and *J* is the number of  $D_i$ , which do not exactly coincide with their respective  $C_i \cdot r$ , r = 1 or 2, refers to the piecewise,  $W^{r,1}$ -differentiability of the boundary curves of  $C_i$ , and *h* refers to the maximum length of the side of a triangle.

The  $||f - f_h||$  term reflects how well the mesh-based interpolant  $f_h$  approximates f on each triangle. The  $||\phi_i - \phi_{h,i}||$  and  $Jh^r$  terms reflect how well the triangulated sets  $D_i$  approximate  $C_i$ , which in turn reflect the differentiability of the transition functions. The metric term  $||g| - |g_h|||$  reflects the quality of approximation of the maps from the coordinate patches to the global set, which in turn reflects the differentiability of the chart-to-surface maps.

### 3. The need for $W^{k,p}$ -manifolds and $W^{k,p}$ -surfaces

The classical definitions of manifolds and surfaces and the differentiability of these quantities do not address important considerations in the approximation of these quantities via mesh-based interpolation. Further, to understand the convergence of such approximations, we must remember the often overlooked point that the differentiability of a surface and the differentiability of the same structure, viewed as a manifold, are related, but different, quantities. These issues become apparent when one examines the partition of unity and metric determinant terms of the preceding estimate.

The partition of unity term in the preceding estimate is bounded by the  $W^{k,1}$ - differentiability of the transition functions. The effects of  $W^{k,1}$ -differentiability, as opposed to  $C^k$ -differentiability, can unexpectedly appear in common approximation problems. Consider the spherical coordinates  $(\cos\theta\cos\phi, \sin\theta\cos\phi, \sin\phi)$  and  $(\sin\alpha, \sin\beta\cos\alpha, \cos\beta\cos\alpha)$  and the transition function  $\beta = \arccos(\sin\phi/\sqrt{1 - (\cos\theta\cos\phi)^2})$ . This function has the derivative  $\partial\beta/\partial\theta = \cos\theta\cos\phi\sin\phi/(1 - (\cos\theta\cos\phi)^2)$ . If we set  $\cos\theta = \cos\phi = \sqrt{1 - \epsilon^2}$ ,  $\partial\beta/\partial\theta$  will go to infinity as  $\epsilon$  goes to zero. However, since  $\beta$  is finite-valued, this derivative is finite in  $L^1$ -norm and thus,  $\beta$  lies in  $W^{1,1}$ : its derivative is not well defined classically,

but is "well behaved" under the integral sign. Similarly, infinite derivatives in the transition function occur in the two-patch example given by George and Borouchaki [8] and studied in [16]. The convergence of an integral of a mesh-based approximation spanning these respective patches will be governed by this  $W^{1,1}$ -differentiability, as demonstrated by the numerical results in [16].

To introduce  $W^{k,1}$ -differentiability to manifolds and surfaces, we examine the classical definitions of differentiability of manifolds and surfaces.

*Definition 3.1* (adapted from [19]). A *d*-dimensional,  $C^k$ -manifold M,  $k \ge 1$ , is a set, together with a collection of subsets  $\{O_\alpha\}$  satisfying the following:

- (i) the  $\{O_{\alpha}\}$  cover *M*;
- (ii) for each  $\alpha$ , there exists a one-to-one onto map  $\psi_{\alpha} : O_{\alpha} \mapsto U_{\alpha}$ , where  $U_{\alpha}$  is an open subset of  $\mathbb{R}^d$ . ( $U_{\alpha}$  and  $\psi_{\alpha}^{-1}$  are both often called "charts" or "coordinate systems");
- (iii) if  $O_{\alpha} \cap O_{\beta}$  is nonempty, then the map  $\psi_{\beta} \circ \psi_{\alpha}^{-1}$  from  $\psi_{\alpha}[O_{\alpha} \cap O_{\beta}] \subset \mathbb{R}^{d}$  to  $\psi_{\beta}[O_{\alpha} \cap O_{\beta}] \subset \mathbb{R}^{d}$  is  $\mathbb{C}^{k}$ -continuous.

*Definition 3.2* (adapted from [7]). A subset  $S \subset R^3$  is a  $C^k$ -surface if, for each  $p \in S$ , there exist a neighborhood V in  $R^3$  and a map  $\mathbf{x} : U \mapsto V \cap S$  of an open set  $U \subset R^2$  onto  $V \cap S$  such that

- (i) the components of **x** are  $C^k$ -differentiable maps from  $R^2$  to R;
- (ii) **x** has a continuous inverse;
- (iii) **x** induces a nonsingular metric on *U*, that is,  $|(\mathbf{x}_{\mathbf{u}} \cdot \mathbf{x}_{\mathbf{u}})(\mathbf{x}_{\mathbf{v}} \cdot \mathbf{x}_{\mathbf{v}}) (\mathbf{x}_{\mathbf{u}} \cdot \mathbf{x}_{\mathbf{v}})^2| > 0$ .

Note that in the definition of surface, the degree of differentiability is defined by the local-to-global coordinate maps, whereas in the definition of manifold, the degree of differentiability is defined by the local-to-local coordinate transition functions. As these quantities play important roles in the convergence measuring framework, the distinction is crucial. To examine the relationship between these two quantities, consider  $C^1$ -differentiability. The neighborhoods  $V \cap S$  form a covering of the surface and correspond to  $\{O_{\alpha}\}$  in the manifold definition. The map **x** corresponds to  $\psi_{\alpha}^{-1}$ . Now, if  $\psi_{\beta} \circ \psi_{\alpha}^{-1}$  is  $C^1$ -continuous, S will be a  $C^1$ -manifold. Via the chain rule, the derivatives of this transition function will consist of products of derivatives of  $\psi_{\beta}$  and  $\psi_{\alpha}^{-1}$ . Since  $\psi_{\alpha}^{-1}$  has continuous derivatives by assumption, we need to establish that  $\psi_{\beta}$ , the inverse of some chart map **x**, is  $C^1$ -continuous. The following claim provides a sufficient condition for a  $C^1$ -surface to be a  $C^1$ -manifold.

CLAIM 3.3. A  $C^1$ -surface S defines a  $C^1$ -manifold if whenever a chart set  $U \subset R^2$ , where  $S = (f_1(u,v), f_2(u,v), f_3(u,v))$  on U, overlaps another chart set, the functions  $f_i$  satisfy the following condition: for all pairs  $i, j \in \{1,2,3\}, i \neq j, \partial(f_i, f_j)/\partial(u,v) \neq 0$ , where  $\partial(f_i, f_j)/\partial(u,v) = (\partial f_i/\partial u)(\partial f_j/\partial v) - (\partial f_i/\partial v)(\partial f_j/\partial u)$ .

*Proof.* The inverse of the chart map will have bounded, continuous first derivatives if the implicit function theorem is satisfied for all three equations  $F_1 = x - f_1(u, v) = 0$ ,  $F_2 = y - f_2(u, v) = 0$ , and  $F_3 = z - f_3(u, v) = 0$ . Requiring these three functions to be zero produces an overdetermined system. Thus, the implicit function theorem must be satisfied for all pairs  $F_i$ ,  $F_j$ ,  $i, j \in \{1, 2, 3\}$ ,  $i \neq j$ . If  $\partial(f_i, f_j)/\partial(u, v) \neq 0$ , the implicit function theorem will apply.

This claim emphasizes the important point that a  $C^1$ -surface is not necessarily a  $C^1$ -manifold. As we have seen, the spherical coordinates  $(\cos\theta\cos\phi,\sin\theta\cos\phi,\sin\phi)$  and  $(\sin\alpha,\sin\beta\cos\alpha,\cos\beta\cos\alpha)$  can form a  $C^{\infty}$ -surface which is not a  $C^1$ -manifold. The infinite derivatives of the transition functions prevent the surface from being a  $C^1$ -manifold. The following claim helps set a context for when such an infinite derivative can occur.

CLAIM 3.4. Let U be a chart set with a chart map  $f(u,v) = (f_1(u,v), f_2(u,v), f_3(u,v))$ , where the derivatives of f are continuous on U. Suppose that there exist points  $n_z$  and z in the parameter set (u,v) such that  $(\partial(f_i, f_j)/\partial(u,v))(n_z) \neq 0$  and  $(\partial(f_i, f_j)/\partial(u,v))(z) =$ 0. Suppose further that  $\partial(f_i, f_j)/\partial(u,v)$  is not constant in a neighborhood of z, and that  $(\partial f_j/\partial u)(z) \neq 0$  or  $(\partial f_j/\partial v)(z) \neq 0$ . Assume that f has continuous, well-defined inverse functions  $h = (h_1, h_2)$ , where  $u = h_1(x_1, x_2, x_3)$  and  $v = h_2(x_1, x_2, x_3)$ . Then,

$$\lim_{n_p \to f(z), n_p \in U} \left| \frac{\partial h_k}{\partial x_i}(n_p) \right| = \infty$$
(3.1)

holds for k = 1 if  $(\partial f_i / \partial v)(z) \neq 0$ , and for k = 2 if  $(\partial f_i / \partial u)(z) \neq 0$ .

*Proof.* We suppose that  $|(\partial f_j/\partial v)(z)| = K \neq 0$  and note that the proof will work similarly in the other case. By the continuity of the derivatives of f,  $\partial(f_i, f_j)/\partial(u, v)$  is continuous. So, as  $n_p \to f(z)$ ,  $(\partial(f_i, f_j)/\partial(u, v))(h(n_p)) \to 0$  and  $|(\partial f_j/\partial v)(h(n_p))| \to K$ . Further, by assumption, we may choose  $n_p$  so that  $(\partial(f_i, f_j)/\partial(u, v))(h(n_p)) \neq 0$ ,  $n_p \neq z$ . Now, fix  $n_p$  close enough to f(z) that  $|(\partial(f_i, f_j)/\partial(u, v))(h(n_p))| < \epsilon$  and  $|(\partial f_j/\partial v)(h(n_p))| > K/2$ . Now, apply the implicit function theorem to a small neighborhood of  $n_p$ . We then have a well-defined inverse function, which, by uniqueness, must be  $h_1$ . Further,  $h_1$  has a continuous derivative which satisfies

$$\left|\frac{\partial h_1}{\partial x_i}(n_p)\right| = \left|\frac{\partial f_j}{\partial v}(h(n_p))/\frac{\partial (f_i, f_j)}{\partial (u, v)}(h(n_p))\right| > \frac{K}{2\epsilon}.$$
(3.2)

Thus, as  $n_p \to f(z)$ ,  $\epsilon \to 0$  and  $|(\partial h_1 / \partial x_i)(n_p)| \to \infty$ .

From this claim, we see, if we apply this inverse function  $h_1$  to an overlapping chart  $(r_1(a_1, a_2), r_2(a_1, a_2), r_3(a_1, a_2))$ , the potential for a transition function with an infinite derivative. In fact, unless the derivatives  $\{\partial r_i/\partial a_k\}$  cancel out the unboundedness of  $|\partial h_1/\partial x_i|$ , a transition function will have an infinite derivative.

Transition functions with infinite derivatives should integrate to finite values. Since we know their antiderivatives, the transition functions are finite. Thus, the transition functions are in  $W^{1,1}$ . This fact leads us to consider  $W^{k,p}$ -manifolds and  $W^{k,p}$ -surfaces.

A further problem with the classical definitions appears in the reliance on open covers and the resultant reliance on partitions of unity with measurable overlap. This problem is more a headache of implementation than a theoretical obstacle. In practice, the difficulty in implementing separate, overlapping triangulations across different chart sets has led most researchers to ignore overlap (see Lin [12] for a discussion of these difficulties). Manifolds are treated as though they have been decomposed into polygonal, nonoverlapping (overlap occurs only on the boundaries of the polygons) chart sets and the overlap, which still occurs if the chart sets are not exactly polygonal, is ignored. While Munkres [13] has shown that all manifolds may be exactly partitioned into measurably disjoint, polygonal charts sets, others have observed that such chart sets are often difficult to find or give rise to complicated chart maps [12, 15]. Thus, mesh-based surface modeling techniques in engineering and computer graphics generally partition manifolds and surfaces into chart sets "disjointly," via boundary curves, often called "trimming curves." Examples of this approach appear in Shimada et al. [18], Anglada et al. [1], Cho et al. [4, 5], Klein [11], George and Borouchaki [8], and Borouchaki et al. [2]. The disjoint coverings used in this approach are insufficient to define a  $C^k$ -manifold or surface. This type of partitioning corresponds to discontinuous, characteristic functions as partition of unity functions and as such fits more naturally with  $W^{k,p}$ -differentiability.

In summary, we extend these definitions of surfaces and manifolds to the spaces  $W^{k,p}$  for the following reasons:

- (i) many PDEs and finite element approximations to PDEs are naturally posed on these spaces;
- (ii) surfaces implemented in existing applications often have transition functions with unbounded derivatives;
- (iii) finite element methods and surface modeling techniques in engineering and computer graphics generally favor measurably disjoint partitions which fit better with  $W^{k,p}$ -differentiability.

## 4. $W^{k,p}$ -manifolds and $W^{k,p}$ -surfaces

*Definition 4.1.* A *d*-dimensional,  $W^{k,p}$ -manifold *M* is a set, together with a collection of subsets  $\{O_{\alpha}\}$  satisfying the following:

- (i) the  $\{O_{\alpha}\}$  cover M;
- (ii) for each  $\alpha$ , there exists a one-to-one onto map  $\psi_{\alpha} : O_{\alpha} \mapsto U_{\alpha}$ , where  $U_{\alpha}$  is a closed, connected subset of  $\mathbb{R}^d$  with piecewise  $W^{k,p}$ -boundary;
- (iii) if  $O_{\alpha} \cap O_{\beta}$  is nonempty, then the map  $\psi_{\beta} \circ \psi_{\alpha}^{-1}$  from  $\psi_{\alpha}[O_{\alpha} \cap O_{\beta}] \subset \mathbb{R}^{d}$  to  $\psi_{\beta}[O_{\alpha} \cap O_{\beta}] \subset \mathbb{R}^{d}$  is in  $W^{k,p}$ .

Definition 4.2. A subset  $S \subset \mathbb{R}^3$  is a  $W^{k,p}$ -surface if, for each  $p \in S$ , there exist a set V in  $\mathbb{R}^3$  and a map  $\mathbf{x} : U \mapsto V \cap S$  of a set  $U \subset \mathbb{R}^2$  (U is a closed connected set with piecewise  $W^{k_2,p}$ -boundary) onto  $V \cap S$  such that

- (i) the components of **x** are  $W^{k,p}$ -differentiable maps from  $R^2$  to R;
- (ii) **x** has a continuous inverse;
- (iii) **x** induces a nonsingular metric on *U*, that is,  $|(\mathbf{x}_{\mathbf{u}} \cdot \mathbf{x}_{\mathbf{u}})(\mathbf{x}_{\mathbf{v}} \cdot \mathbf{x}_{\mathbf{v}}) (\mathbf{x}_{\mathbf{u}} \cdot \mathbf{x}_{\mathbf{v}})^2| > 0$ .

Note that these definitions use closed chart sets rather than the traditional open sets. In surface triangulation, we commonly see decompositions of surfaces into sets of charts which intersect only at their boundaries. The use of closed chart sets accommodates these triangulations. Further, some surfaces of interest cannot easily be represented with open chart sets. For example, surfaces formed by the stitching together of two surfaces such as the outer surface formed by the joining of two spheres have closed chart sets. The curves of intersection of the two distinct surfaces will be boundary curves of the corresponding charts. An open covering would require a chart containing a neighborhood of points on the boundary curves, which would require one surface's coordinate system to be defined on the other surface. The relaxation of the open set requirement is a natural development from the substitution of  $W^{k,p}$  with  $C^k$ , as boundary curves are sets of measure zero, which do not affect the  $W^{k,p}$ -differentiability of a function (e.g.,  $|x| \in C^1((0,1))$  but  $|x| \notin C^1([0,1])$ ; however,  $W^{1,1}((0,1))$  and  $W^{1,1}([0,1])$  are the same space). We also note that the change to the conventional definition of a surface may allow for surfaces with self-intersections and cusps (curves where the tangent plane is discontinuous), provided their metric determinants are still bounded away from zero at these points.

We require the chart sets to have piecewise  $W^{k',p}$ -boundaries. The boundaries of these chart sets will generally come from applying transition functions to piecewise smooth boundaries of other chart sets. Thus, the differentiability of the boundaries should reflect the differentiability of the transition functions. Thus, in the  $W^{k,p}$ -manifold definition, k' = k. In the  $W^{k,p}$ -surface definition,  $k' = k_2$ , where  $k_2$  may be different from k, as the chart-to-surface maps and the transition functions need not have the same level of differentiability.

The functions used to define the manifolds and surfaces determine the values of k and  $k_2$ . However, the value of p is arbitrary, depending on the norm in which one wishes to measure functions on the surface. Because we use the global  $L^1$ -estimate of [16], we use p = 1 in this paper.

Earlier in this paper, we discuss cases, detailed in [16], where the  $W^{1,1}$ -differentiability, of the transition functions and thus the manifold, limits the convergence of mesh-based interpolants. The  $W^{k,p}$ -manifold differentiability governs the convergence in the partition of unity term and the  $Jh^r$  term of the convergence estimate.  $W^{k,p}$ -surface differentiability, on the other hand, governs the convergence of the metric determinant term. To see how surface differentiability affects the metric determinant term  $||g| - |g_h||$  of the convergence estimate, we examine the applicability of the approximation framework of Nédélec.

#### 5. Approximation in the Nédélec framework

Nédélec [14] provides a framework for analyzing the convergence of the metric determinant of an approximate surface to the metric determinant of the desired, "true" surface. Provided the true surface is "sufficiently differentiable," Nédélec demonstrates a rate of convergence one degree higher than would be expected from standard interpolation theory (such a lower order estimate, using standard interpolation theory, of the convergence of the metric determinant appears in [6]). More specifically, if we build the approximate metric determinant  $|g_h|$  from the derivatives of piecewise, degree l polynomial approximations of the chart-to-surface maps  $\Phi_i$ , standard interpolation theory predicts  $O(h^l)$ convergence in the  $L^{\infty}$ -norm (and by extension, the  $L^p$ -norm,  $1 \le p < \infty$ , since we restrict ourselves to finite measure chart sets),

$$\left\| |g| - |g_h| \right\|_{L^{\infty}} \le Ch^l \left\| D^{l+1} \Phi_i \right\|_{L^{\infty}}.$$
(5.1)

Nédélec proves  $O(h^{l+1})$  convergence

$$|||g| - |g_h|||_{L^{\infty}} \le Ch^{l+1} ||D^{l+1}\Phi_i||_{L^{\infty}}.$$
(5.2)

Using degree *l* polynomials to approximate both the maps  $\Phi_i$  and the function *f*, we would obtain  $O(h^{l+1})$  convergence in both the  $||f - f_h||$  term and the metric term in our estimate. Given an exact, disjoint partition of the manifold *M* into polygonal chart sets, the partition of unity term and *Jh*<sup>*r*</sup> term vanish, allowing the approximate integral of *f* to converge at  $O(h^{l+1})$ .

This framework depends on the properties of a map (the map  $\Psi$  discussed below in the sketch of the proof of Claim 5.1) between the approximate surface and the true surface that allows us to identify points on the approximate surface with points on the true surface in a one-to-one, well-behaved manner. Subsequent authors, for example, Kalik and Wendland [10], Kalik et al. [9], and Brodzik [3] have recognized and exploited the faster convergence granted by this correspondence to build surface triangulation algorithms with good convergence properties. These authors, like Nédélec, rely upon the true surface being sufficiently smooth to give this correspondence without investigating just what the smoothness requirements on the true surface are. Because the role of surface differentiability in the convergence of mesh-based approximation lies at the heart of this paper, we will examine these requirements. To understand more fully the smoothness requirements on M which give this faster convergence, we present the following claim.

CLAIM 5.1. Consider a surface M, consisting of chart maps  $\Phi_i : T_i \mapsto M$ ,  $T_i \subset R^2$ ,  $M \subset R^3$ . Consider also a series of triangulated surfaces  $M_h$ , built from  $T_i$  and polynomial interpolants of  $\Phi_i$ , converging to M as h goes to 0. The accelerated convergence of the metric determinant of  $M_h$  to the metric determinant of M in Nédélec's framework holds when M is a  $G^1$ -surface (i.e., tangent plane continuous) with the maps  $\Phi_i$  having  $L^{\infty}$ -bounded second derivatives and the chart sets  $T_i$  are polygonal.

Sketch of proof. In [14] where Nédélec presents his proof of the accelerated convergence, he invokes the map  $\Psi$  from  $M_h$  to M such that for each x on M,  $\Psi^{-1}(x)$  is the point of  $M_h$  intersecting the unit normal to M at x. The correspondence of  $M_h$  to M under  $\Psi$  represents the key to Nédélec's proof. More specifically, Nédélec's proof depends on the following key assumptions:

(i)  $\Psi$  as a well-defined bijection;

(ii) the map  $V = \Phi_i^{-1} \cdot \Psi$  and its first derivatives are Lipschitz-continuous.

To ensure that  $\Psi$  is a well-defined bijection, we require the surface to have polygonal chart sets and a continuous normal vector across chart boundaries (i.e., M must be  $G^1$ continuous). A discontinuity in the normal vector would either omit points of M from the range of  $\Psi$  or cause  $\Psi$  to be ambiguous (i.e., a distribution rather than a function). Similarly, if the sets  $T_i$  are not polygonal, then these sets must be approximated with polygonal sets to construct  $M_h$  and in this approximation, the one-to-one correspondence between points of M and points of  $M_h$  will likely be lost.

We prove that the second requirement holds. Consider the function  $U(\hat{r}, \hat{x}): M_h \times T_i \mapsto R^2$ , where  $(U(\hat{r}, \hat{x}))_i = (\hat{r} - \Phi(\hat{x})) \cdot \partial \Phi / \partial x_i$ . The set  $\{(\hat{r}, \hat{x}): U(\hat{r}, \hat{x}) = 0\}$  defines the  $\hat{r}$  and  $\hat{x}$  such that  $V(\hat{r}) = \hat{x}$ . Through the implicit function theorem, our understanding of U

will give rise to our understanding of V. Thus, we now examine the derivatives of U to show that U satisfies the requirements of the implicit function theorem.

Note that as a degree-one polynomial, U is differentiable with respect to  $\hat{r}$ . And because  $\Phi$  is twice differentiable with respect to  $\hat{x}$ , U is differentiable with respect to  $\hat{x}$ . For fixed  $\hat{r}$ , consider the 2-by-2 differential  $D(\hat{r}, \hat{x})$  with respect to the components  $x_i$  of  $\hat{x}$ . Observe that

$$D_{ij} = \frac{\partial (U(\hat{r}, \hat{x}))_i}{\partial x_j} = -\frac{\partial \Phi}{\partial x_i} \cdot \frac{\partial \Phi}{\partial x_j} + (\hat{r} - \Phi(\hat{x})) \cdot \frac{\partial^2 \Phi}{\partial x_i \partial x_j}.$$
(5.3)

Thus,

$$D_{ij} = -g_{ij} + \left(\hat{r} - \Phi(\hat{x})\right) \cdot \frac{\partial^2 \Phi}{\partial x_i \partial x_j}.$$
(5.4)

So,

$$det(D) = D_{11}D_{22} - D_{12}^2$$

$$= g_{11}g_{22} - g_{12}^2 - g_{11}(\hat{r} - \Phi(\hat{x})) \cdot \frac{\partial^2 \Phi}{\partial x_2^2} - g_{22}(\hat{r} - \Phi(\hat{x})) \cdot \frac{\partial^2 \Phi}{\partial x_1^2}$$

$$+ \left( (\hat{r} - \Phi(\hat{x})) \cdot \frac{\partial^2 \Phi}{\partial x_2^2} \right) \left( (\hat{r} - \Phi(\hat{x})) \cdot \frac{\partial^2 \Phi}{\partial x_1^2} \right) + 2g_{12}(\hat{r} - \Phi(\hat{x})) \cdot \frac{\partial^2 \Phi}{\partial x_1 \partial x_2}$$

$$- \left( (\hat{r} - \Phi(\hat{x})) \cdot \frac{\partial^2 \Phi}{\partial x_1 \partial x_2} \right)^2.$$
(5.5)

Therefore, if the first and second derivatives of  $\Phi$  are bounded, we have

$$\det(D) \ge \det(g) - C_1 |\hat{r} - \Phi| - C_2 |\hat{r} - \Phi|^2$$
(5.6)

(and a comparable inequality if det(g) < 0). Thus, if the metric is nonsingular and  $M_h$  is close to M (i.e.,  $|\hat{r} - \Phi|$  is small), D will be nonsingular.

Thus, in the neighborhood of a point  $(\hat{r}_0, \hat{x}_0)$  such that  $U(\hat{r}_0, \hat{x}_0) = 0$ , the requirements of the implicit function theorem are satisfied. We know that V exists and that V is continuously differentiable. We will examine the derivatives of V to determine when V and its derivatives are Lipschitz.

For the points  $(\hat{r}, V(\hat{r}))$ , U = 0. Differentiating this equation produces  $\partial U/\partial r_i + (\partial U/\partial x_1)(\partial V_1/\partial r_i) + (\partial U/\partial x_2)(\partial V_2/\partial r_i) = 0$  (here,  $\partial U/\partial r_i$  refers only to the derivative of U with respect to its components in  $\hat{r}$ , not to the appearance of  $r_i$  in  $V(\hat{r})$ ). Solving for  $\partial V/\partial r_i$  produces  $(\partial V/\partial r_i)(\hat{r}) = -D(\hat{r}, V(\hat{r}))^{-1}(\partial U/\partial r_i)(\hat{r}, V(\hat{r}))$ . We may conclude that the first derivatives of V are bounded from the boundedness of the derivatives of  $\Phi$  and, therefore, V is Lipschitz. Further, if  $-D(\hat{r}, V(\hat{r}))^{-1}(\partial U/\partial r_i)(\hat{r}, V(\hat{r}))$  is Lipschitz, then the derivatives of V will be Lipschitz. The lower bound on det(D) produces an upper bound on det( $D^{-1}$ ). Thus, since the entries of D are bounded and det( $D^{-1}$ ) is bounded,  $D^{-1}$  is

bounded. And since  $\partial U/\partial r_i$  is linear in  $\hat{r}$ , it is Lipschitz. Thus, the derivatives of V are Lipschitz.

We now have a clearer picture of when the accelerated convergence of Nédélec's framework occurs. We can now ask if a weakened version of this convergence holds when the second derivatives of the chart maps do not lie in  $L^{\infty}$ .

### 6. The extension of Nédélec's framework to W<sup>k,1</sup>-surfaces

To start, we consider surfaces whose chart maps have bounded first derivatives, and second derivatives which have singularities but are bounded in  $L^1$ -norm.

THEOREM 6.1. Let  $\alpha : C \mapsto R^3$ , let  $\alpha \in W^{2,1}(C)$  be a chart map on a polygonal set C. Suppose that in C,  $D^2 \alpha$  has a singularity given by the curve  $\varphi(x, y) = 0$ , where  $\varphi$  is an affine function of x and y. Now, suppose that there exists b, 0 < b < 1, such that  $\varphi^b D^2 \alpha \in L^{\infty}(C)$ , but for  $\epsilon >$ 0,  $\varphi^{b-\epsilon}D^2 \alpha \notin L^{\infty}(C)$ . Then, using the standard piecewise linear interpolation framework, the approximate metric determinant will converge to the true metric determinant at rate of at least  $O(h^{2-b})$ .

*Proof.* We consider the set *N* of all triangles which share a point with the set  $\{|\varphi| \le h/2\}$ ,

$$\int_{C} |g - g_{h}| = \int_{N} |g - g_{h}| + \int_{N^{c}} |g - g_{h}|.$$
(6.1)

On *N*, we do not have the Nédélec framework. We do, however, have the estimate which comes from viewing the components of *g* as dot products of first derivatives of  $\alpha$ . Thus,

$$\int_{N} |g - g_{h}| dy dx \le Kh \int_{N} |D^{2}\alpha| dy dx.$$
(6.2)

Since  $|D^2\alpha| \le K/|\varphi|^b$  almost everywhere, we have

$$\int_{N} \left| g - g_h \right| dy \, dx \le Kh \int_{N} \frac{1}{|\varphi|^b} dy \, dx.$$
(6.3)

Recall that the values which  $\varphi$  may take in *N* are of O(h), and the maximum length of the level curves of  $\varphi$  is independent of *h*. Therefore, mN = O(h). Additionally, we may parametrize *N* by  $\varphi$  and a variable *z* along the normal line  $\varphi = 0$ ,

$$\int_{N} \left| g - g_h \right| dy \, dx \le Kh \int_{z} \left( \int_{0}^{h} \frac{1}{|\varphi|^b} d\varphi \right) dz \le KO(h^{2-b}). \tag{6.4}$$

We now turn to  $N^c$ . Since, by definition, all points in this set lie a distance of at least O(h) away from any singular point, we know that  $|\varphi|^b \ge ch^b$ . Thus,  $|D^2\alpha| \le K/h^b$ . Hence, on  $N^c$ , we have  $L^{\infty}$ -bounded, second derivatives of the chart map and we may use the Nédélec framework. Thus,

$$\int_{N^{c}} |g - g_{h}| \le Kh^{2} \int_{N^{c}} |D^{2}\alpha|.$$
(6.5)

Using the bound on  $|D^2\alpha|$ , we have

$$\int_{N^c} \left| g - g_h \right| \le K h^2 \left( \frac{1}{h^b} \right) (mN^c) \le K h^{2-b} (mC).$$
(6.6)

 $\square$ 

Combining our estimates for N and  $N^c$  completes the proof.

The above theorem generalizes to the following.

THEOREM 6.2. In the statement of the previous theorem, let  $\alpha \in W^{k,1}(C)$  and replace  $D^2 \alpha$ with  $D^k \alpha$ . Use piecewise polynomials of degree l to approximate  $\alpha$ . Then, the approximate metric determinant will converge at a rate of at least  $O(h^{l+1-b})$ , where  $l+1 \leq k$ . (Set a maximum of k-1 for l because surface differentiability limits the effectiveness of quadrature precision. If  $\alpha \notin W^{r,1}(C)$ , r > k, using polynomials of degree higher than k-1 will not accelerate convergence.)

#### 7. Numerical results

This section provides numerical results from experiments to verify the predictions of the foregoing theorems. Consider an approximation of  $\int 1 \operatorname{across} a$  two-chart surface. Each chart set is the square  $[0,1] \times [0,1]$ . The first chart map is  $\sigma_1(x, y) = (x^s + x, y, x^s + x)$ . The second chart map is  $\sigma_2(x, y) = ((x^s + x)(e^{y-1}), y - 1, (x^s + x)(e^{y-1}))$ . This surface does not have continuous first derivatives across the mutual edge y = 0 in chart 1, and y = 1 in chart 2, but does have a continuous tangent plane (i.e., the surface is  $G^1$ -smooth). For a positive integer *s*, the chart maps have bounded second derivatives. For 1 < s < 2, the chart maps lie in  $W^{2,1}$ , as the chart maps have unbounded second derivatives. Likewise, for 2 < s < 3, the chart maps lie in  $W^{3,1}$ , as the chart maps have unbounded third derivatives. The singularities of these derivatives behave like  $x^{s-2}$  for 1 < s < 2, and  $x^{s-3}$  for 2 < s < 3, and occur on the line x = 0 in each chart.

Since the chart sets will be triangulated exactly, only one term in the convergence estimate from [16] will form an obstacle to convergence: the metric determinant term. For  $s \ge 3$ , because the surface is  $G^1$ -continuous and has bounded second derivatives, Nédélec's framework applies and we expect  $O(h^{l+1})$  convergence where piecewise polynomials of degree *l* approximate the chart maps. For 1 < s < 2, the modified Nédélec framework for  $W^{2,1}$ -functions applies and we expect  $O(h^{l-1+s})$  convergence where  $l \le 1$ . For 2 < s < 3, the modified Nédélec framework for  $W^{3,1}$ -functions applies and we expect  $O(h^s)$  convergence of  $l \ge 2$ , and  $O(h^2)$  convergence if l = 1.

Table 7.1 lists the error ratios for different values of *s*, obtained on uniform triangulations of  $[0,1] \times [0,1]$ , along with the relevant prediction of the error ratio. Here, the degree *l* of the approximating polynomials is reflected in the quadrature precision, which will be *l* + 1. The ratios compare the error at *h* = 0.031250 to the error at *h* = 0.015625.

#### 8. Conclusion

In defining  $W^{k,p}$ -manifolds and  $W^{k,p}$ -surfaces and examining the role of these definitions in approximation, this paper, like [16], seeks to provide a unifying formalism to the many ad hoc approaches employed in mesh-based approximation on manifolds and surfaces.

\$	Error ratio	Predicted ratio	Quadrature precision
1.1	2.1399	2.1435	2
1.2	2.2908	2.2974	2
1.3	2.4502	2.4623	2
1.5	2.7904	2.8284	2
2.2	3.8063	4.0	2
2.6	3.9749	4.0	2
3.0	4.0001	4.0	2
1.1	2.1435	2.1435	3
1.2	2.2974	2.2974	3
1.3	2.4622	2.4623	3
1.5	2.8283	2.8284	3
2.2	4.5934	4.5948	3
2.6	6.0477	6.0629	3
3.0	15.9992	8.0	3
1.1	2.1449	2.1435	4
1.2	2.2990	2.2974	4
1.3	2.4642	2.4623	4
1.5	2.8312	2.8284	4
2.2	4.6048	4.5948	4
2.6	6.0899	6.0629	4
3.0	16.0031	16.0	4

Table 7.1. Approximation of  $\int 1$  on  $G^1$ -surfaces.

The hope is that this formalism will prove useful to biological and physical applications, where approximating solutions to evolution equations may require modeling functions on highly curved surfaces.

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Kevin Scully: The Aerospace Corporation, M4-960, P.O. Box 92957, Los Angeles, CA 90009–2957, USA

E-mail address: kevin.j.scully@aero.org



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