



Error bounds for a least squares meshless finite difference method on closed manifolds

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Abstract

We present an error bound for a least squares version of the kernel based meshless finite difference method for elliptic differential equations on smooth compact manifolds of arbitrary dimension without boundary. In particular, we obtain sufficient conditions for the convergence of this method. Numerical examples are provided for the equation $-\Delta_{\mathcal{M}}u + u = f$ on the 2- and 3-spheres, where $\Delta_{\mathcal{M}}$ is the Laplace-Beltrami operator.

Keywords RBF-FD · Kernel based methods · PDE on manifolds · Error bounds · Meshless finite difference method · Generalized finite differences

Mathematics Subject Classification 65N12 · 65N15 · 65N06

1 Introduction

Let \mathcal{M} be a smooth compact manifold of dimension d without boundary, and let L be an elliptic differential operator of order 2κ , $\kappa \in \mathbb{N}$, on \mathcal{M} with infinitely differentiable coefficients in local coordinates, and a trivial null space. Then the equation

$$Lu = f \tag{1}$$

has a unique solution u in the Sobolev space $H^t(\mathcal{M})$, $t \in \mathbb{R}$, whenever $f \in H^{t-2\kappa}(\mathcal{M})$, and there are constants $A, B > 0$, depending only on \mathcal{M}, L, t and the choice of the Sobolev norms, such that

$$A\|f\|_{H^{t-2\kappa}(\mathcal{M})} \leq \|u\|_{H^t(\mathcal{M})} \leq B\|f\|_{H^{t-2\kappa}(\mathcal{M})}, \tag{2}$$

see e.g. [3, Sect. 6].

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Meshless numerical methods are particularly attractive for solving operator equations on manifolds, in particular on the sphere [32, 33], because of the difficulties of creating and maintaining suitable meshes or grids in this setting. Error bounds for meshless methods for the approximation of functions and specifically solutions of operator equations on manifolds have been studied for example in [12, 14, 34, 36, 37, 42, 43, 45–47, 53]. However, these results do not apply to localized finite difference type methods considered below.

Meshless finite difference methods discretize a differential equation (1) (or similarly a boundary value problem) on a set of irregular nodes $X = \{x_1, \dots, x_n\} \subset \mathcal{M}$ with the help of numerical differentiation formulas

$$Lu(x_i) \approx \sum_{j \in J_i} w_{ij} u(x_j), \quad J_i \subset J := \{1, \dots, n\}, \quad i \in I, \quad (3)$$

where the coefficients $w_{ij} \in \mathbb{R}$ are obtained by requiring that the formula is exact for certain finite dimensional spaces of functions, for example polynomials or kernel sums or a combination thereof, and the size of the sets of influence $X_i = \{x_j : j \in J_i\}$ is bounded by a fixed number $\nu \ll n$. In particular, the kernel-based formulas are exact for all linear combinations $\sum_{j \in J_i} c_j K(\cdot, x_j)$, $c_j \in \mathbb{R}$, where $K : \mathcal{M} \times \mathcal{M} \rightarrow \mathbb{R}$ is a positive definite kernel [20]. The discrete approximate solution $\hat{u} \in \mathbb{R}^n$ of (1), such that $\hat{u}_i \approx u(x_i)$, $i = 1, \dots, n$, is obtained by solving the sparse linear system

$$\sum_{j \in J_i} w_{ij} \hat{u}_j = f(x_i), \quad i \in I. \quad (4)$$

Numerical performance of methods of this type has been studied e.g. in the book [32] and papers [6, 31, 40, 52, 61–64, 66], in particular for differential equations on the sphere and other manifolds. In contrast to those meshless methods that discretize the weak form of the equations (see the surveys [7, 49]), no integration of the trial functions over subdomains is needed, which is challenging in the meshless setting as the subdomains are not generated from a few reference shapes controlled by the mesh. In contrast to the global collocation methods (see e.g. [39, 54]), the linear systems are sparse. Moreover, by optimizing the selection of the sets of influence J_i , they may be made as sparse as they are in the mesh based methods, such as the finite element method, with comparable accuracy [18, 21–24, 50]. However, error bounds for meshless finite difference methods are underdeveloped.

In the classical setting $I = \{1, \dots, n\}$, and hence (4) is a square linear system. An extension of the classical error analysis that requires that the system matrix of (4) is an M -matrix has been proposed in [28], and conditions for the M -matrix property were investigated in [28, 60]. However, this approach only applies to special geometric configurations of the sets of influence with low convergence order, and no general theory exists. Moreover, except of the situations when the M -matrix property can be shown, no conditions are known to guarantee the solvability of the square system (4), even if the method performs very well in numerical experiments.

By using more than n numerical differentiation formulas (3) we arrive at an overdetermined system, and \hat{u} may be obtained by the least squares minimization. In [40,

[67] this situation arises from evaluating Lu in the left hand side of (3) on a different set of nodes, larger than X . This is similar to the “overtesting” mode that admits, for the collocation and other methods employing trial functions, an error analysis under very general conditions [56, 58], which however does not cover finite difference type methods [59]. The papers we just mentioned also discuss numerical and theoretical motivations for using overtesting instead of the classical setting of a square linear system. An error analysis of the overtesting least squares method is provided in [67] with the help of trial spaces defined by piecewise radial basis functions over the Voronoi tessalation of the domain with respect to the nodes in X . The overtesting is supposed to be dense enough, such that the discrete bilinear form that defines the least squares method inherits coercitivity from the continuous bilinear form in a continuous least squares formulation of the boundary value problem.

In this paper we derive error bounds for an overdetermined version of the meshless finite difference method for elliptic differential equations on smooth closed manifolds, solved by least squares, where the numerical differentiation formulas (3) are generated in blocks corresponding to a family of overlapping subsets $J_\ell \subset J$,

$$[Lu(x_j)]_{j \in J_\ell} \approx W_\ell[u(x_j)]_{j \in J_\ell}, \quad \ell = 1, \dots, m. \tag{5}$$

The local differentiation matrices W_ℓ are invertible since they correspond to a reproducing kernel K for a Sobolev space $H^s(\mathcal{M})$, such that L is positive and self-adjoint with respect to the inner product defined by K . This condition in particular implies that the system matrix has full rank and hence there exists a unique least squares solution of the overdetermined linear system

$$W_\ell[\hat{u}_j]_{j \in J_\ell} = [f(x_j)]_{j \in J_\ell}, \quad \ell = 1, \dots, m. \tag{6}$$

Under certain regularity assumptions that involve in particular the quasi-uniformity of X and the existence of an atlas $\mathcal{A} = \{(U_\ell, \varphi_\ell)\}_{\ell=1}^m$ with sufficiently nice $U_\ell \subset \mathcal{M}$ such that $X \cap U_\ell = X_\ell := \{x_j : j \in J_\ell\}$ and X_ℓ, X_k significantly overlap whenever $U_\ell \cap U_k \neq \emptyset$, we show in Theorem 1 that

$$\max_{j \in J} |u(x_j) - \hat{u}_j| = \mathcal{O}(h_{\mathcal{A}}^{s-2\kappa-d-r_0}), \quad r_0 := \max\{0, \lfloor \frac{d}{2} \rfloor - 2\kappa + 1\},$$

and there exists $\tilde{u} \in H^{s+2\kappa}(\mathcal{M})$ such that $\tilde{u}(x_j) = \hat{u}_j, j \in J$, and

$$\|u - \tilde{u}\|_{H^{2\kappa+r}(\mathcal{M})} = \mathcal{O}(h_{\mathcal{A}}^{s-2\kappa-d-r}), \quad 0 \leq r < s - \kappa,$$

where $h_{\mathcal{A}}$ is the maximum diameter of the sets $\varphi_\ell(U_\ell)$. This shows the pointwise convergence of the method for $h_{\mathcal{A}} \rightarrow 0$ when $s > \max\{2\kappa, \frac{d}{2} + 1\} + d$, and convergence in $H^{2\kappa}(\mathcal{M})$ when $s > 2\kappa + d$.

The results apply in particular to the operators of the form $L = (-\Delta_{\mathcal{M}} + \alpha I)^\kappa$, $\kappa \in \mathbb{N}, \alpha > 0$, where $\Delta_{\mathcal{M}}$ is the Laplace-Beltrami operator, I is the identity, and $\mathcal{M} = \mathbb{S}^d$ is the d -dimensional sphere. In this case the differentiation matrices W_ℓ may be efficiently computed by employing restrictions to \mathbb{S}^d of the Matérn or Wendland

kernels for the ambient Euclidean space \mathbb{R}^{d+1} . Numerical experiments in the case $\alpha = \kappa = 1$ and $d \in \{2, 3\}$ provided in Section 6 indicate higher convergence orders than those shown in Theorem 1.

The paper is organized as follows. Sections 2 and 4 are devoted to auxiliary statements on various topics needed in the main parts of the paper, such as equivalent norms for Sobolev spaces on manifolds, properties of reproducing kernels and self-adjoint differential operators, sampling inequalities and local differentiation matrices. Our least squares meshless finite difference method is presented in Section 3, the error bounds in Section 5, numerical examples in Section 6, and a short conclusion in Section 7.

2 Preliminaries

We denote the partial derivative of a real function u defined on a subset of \mathbb{R}^d by $\partial^\alpha u := \frac{\partial^{|\alpha|} u}{\partial x_1^{\alpha_1} \dots \partial x_d^{\alpha_d}}$, where $\alpha \in \mathbb{Z}_+^d$ and $|\alpha| := \sum_{i=1}^d \alpha_i$. We will extensively use the Leibniz product rule and the estimates that follow from the multivariate chain rule, see e.g. Sections 1.2, 1.63 and 3.41 in [1].

The cardinality of a finite set X will be denoted $\#X$, and ∂S will stand for the boundary of a set S in \mathbb{R}^d or \mathcal{M} . We will use the usual notations $C(S)$, $C^\infty(S)$, $L^\infty(S)$, $L^2(S)$ for the spaces of continuous, infinitely differentiable, essentially bounded or square integrable functions on appropriate subsets of \mathbb{R}^d or \mathcal{M} .

Apart from the usual restriction $f|_S$ for a subset S of the domain of definition of a function f , we denote by $f|_X$ the vector $[f(x)]_{x \in X}$ when X is a finite set, and by $w|_I$ the vector $[w_j]_{j \in I}$, for any $w = [w_j]_{j \in J}$ and a subset $I \subset J$.

In what follows various ‘‘constants’’ denoted C , C_1 , C_2 , etc. will be different at different occurrences and depend on the manifold \mathcal{M} (and thus on d) on default. We will explicitly list other parameters these constant may depend on in each case unless stated otherwise.

2.1 Sobolev spaces on manifolds

Recall that in the case of integer $s \geq 0$, Sobolev spaces $H^s(\Omega)$ are defined on any open set Ω as Hilbert spaces with the norm [1]

$$\|u\|_{H^s(\Omega)} = \left(\sum_{k=0}^s |u|_{H^k(\Omega)}^2 \right)^{1/2}, \quad |u|_{H^k(\Omega)} := \left(\sum_{|\alpha|=k} \|\partial^\alpha u\|_{L^2(\Omega)}^2 \right)^{1/2}, \quad (7)$$

in particular, $H^0(\Omega) = L^2(\Omega)$. When $s \in \mathbb{R} \setminus \mathbb{Z}_+$ and Ω is a Lipschitz domain in \mathbb{R}^d , we refer to [3] for the definition of $H^s(\Omega)$ as the restriction to Ω of the space $H^s(\mathbb{R}^d)$ defined as the Bessel potential space. The Bessel norm for $H^s(\mathbb{R}^d)$ is equivalent to $\|\cdot\|_{H^s(\mathbb{R}^d)}$ of (7) when $s \in \mathbb{Z}_+$. However, the definition via restriction, if applied to non-Lipschitz domains and integer s , leads in general to smaller spaces due to the lack of extension of some functions with a finite norm (7), see e.g. [11, p. 287]. Even for

Lipschitz domains, where extension theorems guarantee the equivalence of (7) to the restriction norm, the constants of equivalence depend on Ω and must be taken into account when they influence estimates that have to be uniform with respect to Ω .

Following the standard definition of Sobolev spaces on smooth manifolds, we pick a finite smooth atlas $\hat{\mathcal{A}} = \left\{ (\hat{U}_\ell, \hat{\varphi}_\ell) \right\}_{\ell=1}^{\hat{n}}$ and a smooth subordinate partition of unity $\hat{\Gamma} = \{ \hat{\gamma}_\ell \}_{\ell=1}^{\hat{n}}$, see e.g. [41], such that $\hat{\gamma}_\ell \in C^\infty(\mathcal{M})$, $\hat{\gamma}_\ell \geq 0$, $\text{supp } \hat{\gamma}_\ell \subset \hat{U}_\ell$, $\sum_{\ell=1}^{\hat{n}} \hat{\gamma}_\ell = 1$, and fix a norm for the Sobolev space $H^s(\mathcal{M})$, $s \in \mathbb{R}$, in the form

$$\|u\|_{H^s(\mathcal{M})} = \left(\sum_{\ell=1}^{\hat{n}} \|u \hat{\gamma}_\ell \circ \hat{\varphi}_\ell^{-1}\|_{H^s(\mathbb{R}^d)}^2 \right)^{1/2}. \tag{8}$$

Below, when we speak of a norm for $H^s(\Omega)$ or $H^s(\mathcal{M})$ we will always assume that it is generated by an inner product. We reserve the notations $\|\cdot\|_{H^s(\Omega)}$, $\Omega \subset \mathbb{R}^d$, and $\|\cdot\|_{H^s(\mathcal{M})}$, \mathcal{M} a manifold, for the specific norms defined in (7) and (8), respectively. Different norms for $H^s(\Omega)$ and $H^s(\mathcal{M})$ defined by reproducing kernels will be discussed in Section 2.2.

2.2 Reproducing kernels

We first recall some basic facts about reproducing kernels and kernel based interpolation, see [4, 10, 29, 30, 51, 69] for details, and then discuss reproducing kernels for Sobolev spaces.

Functions $K : \Omega \times \Omega \rightarrow \mathbb{R}$ will be called *kernels* on Ω , where Ω is any set. For a kernel K and two sets S, T , $K|_{S,T}$ stands for the restriction of K to $S \times T$, and for two finite sets X, Y we also denote by $K|_{X,Y}$ the matrix $[K(x, y)]_{x \in X, y \in Y}$. To simplify the notation we set $K|_S := K|_{S,S}$ and $K|_X := K|_{X,X}$. For an operator A that can be applied to one or both of the arguments of the kernel K , we write A_1K or A_2K in order to clarify whether A is applied to the first or the second argument. We will also use the notation $K_A := A_1K$.

A kernel $K : \Omega \times \Omega \rightarrow \mathbb{R}$ is said to be *symmetric* if $K(x, y) = K(y, x)$ for all $x, y \in \Omega$, and *positive (semi-)definite* if the matrix $K|_X$ is positive (semi-)definite for any finite subset X of Ω .

If K is a symmetric positive semi-definite kernel on a set Ω , then there is a unique Hilbert space $H_K = H_K(\Omega)$ of functions on Ω called *native space* of K , with the inner product denoted by $(\cdot, \cdot)_K = (\cdot, \cdot)_{K,\Omega}$ and norm by $\|\cdot\|_K = \|\cdot\|_{K,\Omega}$, such that

$$K(\cdot, y) \in H_K \quad \text{for all } y \in \Omega, \tag{9}$$

$$(f, K(\cdot, y))_K = f(y) \quad \text{for all } f \in H_K, y \in \Omega. \tag{10}$$

A Hilbert space H of functions on Ω admits a kernel K with these properties if and only if the linear functional $\delta_x f := f(x)$ of point evaluation is bounded on H for all $x \in \Omega$. Then K is a *reproducing kernel* of H , and H is said to be a *reproducing kernel Hilbert space*.

The identity (10) means that $K(\cdot, y)$ is the Riesz representer of the linear functional $\delta_y \in H_K^*$. Moreover, the kernel K delivers Riesz representers for all bounded linear functionals.

Lemma 1 [69, Theorem 16.7] *For any bounded linear functional $\gamma \in H_K^*$, the Riesz representer of γ is the function $\gamma_1 K = \gamma_2 K$ that belongs to H_K .*

Assume that K is positive definite. The *kernel sums* of the form

$$\sigma = \sum_{j=1}^n c_j K(\cdot, x_j), \quad c_j \in \mathbb{R}, \quad x_j \in \Omega, \tag{11}$$

are dense in $H_K(\Omega)$, and their kernel norm is given explicitly by

$$\|\sigma\|_K^2 = \sum_{i,j=1}^n c_i c_j K(x_i, x_j). \tag{12}$$

Given $X = \{x_1, \dots, x_n\} \subset \Omega$, and data $a_1, \dots, a_n \in \mathbb{R}$, the kernel sum (11) is uniquely determined by the interpolation conditions $\sigma(x_i) = a_i, i = 1, \dots, n$. We will call it the *kernel interpolant* of this data. In the case when $a_i = v(x_i), i = 1, \dots, n$, for some $v \in H_K$, we say that σ is the kernel interpolant of v . It satisfies

$$(v - \sigma, \sigma)_K = 0 \tag{13}$$

and hence

$$\|v - \sigma\|_K^2 + \|\sigma\|_K^2 = \|v\|_K^2. \tag{14}$$

The restriction $K|_G$ on a subset $G \subset \Omega$ is obviously also a symmetric positive semi-definite kernel. Thanks to (12), any kernel sum (11) satisfies

$$\|\sigma\|_{K,G} = \|\sigma\|_K \quad \text{whenever } X \subset G. \tag{15}$$

The native space of $K|_G$ can be described as follows.

Lemma 2 [4] *If K is a reproducing kernel on Ω and $G \subset \Omega$, then $K|_G$ is a reproducing kernel on G with native space $H_K(G) := \{u|_G : u \in H_K(\Omega)\}$, and*

$$\|u\|_{K,G} = \min\{\|\tilde{u}\|_{K,\Omega} : \tilde{u} \in H_K(\Omega), \tilde{u}|_G = u\}.$$

If Ω is an open set in \mathbb{R}^d , then by Sobolev embedding $H^s(\Omega)$ is a reproducing kernel Hilbert space as long as $s > d/2$. Every (equivalent) norm for $H^s(\Omega)$ corresponds to a positive definite kernel on Ω .

For $G \subset \Omega \subset \mathbb{R}^d$, the space $H^s(G)$ may be larger than the restriction of $H^s(\Omega)$ to G . Indeed, the existence of an extension of every $u \in H^s(G)$ to Ω with a finite H^s -norm is known to be possible only under additional assumptions on the open set G . Even if this extension is available for all $u \in H^s(G)$, we may need to know how

much the H^s -norm may be increased as a result, and hence how much the kernel norm $\|u\|_{K,G}$ may differ from the Sobolev norm $\|u\|_{H^s(G)}$. To quantify this, for any pair of open sets $G \subset \Omega \subset \mathbb{R}^d$, we denote by $\mathcal{E}_s(G, \Omega)$ the *extension constant*

$$\mathcal{E}_s(G, \Omega) = \sup_{u \in H^s(G) \setminus \{0\}} \inf\{\|\tilde{u}\|_{H^s(\Omega)} / \|u\|_{H^s(G)} : \tilde{u} \in H^s(\Omega), \tilde{u}|_G = u\}.$$

In the case $\Omega = \mathbb{R}^d$ we write $\mathcal{E}_s(G) := \mathcal{E}_s(G, \mathbb{R}^d)$. The extension constant $\mathcal{E}_s(G)$ is finite for Lipschitz domains due to well known extension theorems.

The next statement follows immediately from Lemma 2.

Lemma 3 *Let Ω, G be two open sets in \mathbb{R}^d with $G \subset \Omega$, and let K be a reproducing kernel for $H^s(\Omega)$, where $s > d/2$. Then $H_K(G) \subset H^s(G)$ and*

$$\|u\|_{H^s(G)} \leq C_1 \|u\|_{K,G}, \quad u \in H_K(G).$$

Moreover, if the extension constant $\mathcal{E}_s(G, \Omega)$ is finite, then $H_K(G) = H^s(G)$ and

$$\|u\|_{K,G} \leq C_2 \mathcal{E}_s(G, \Omega) \|u\|_{H^s(G)}, \quad u \in H_K(G).$$

The constants C_1, C_2 depend only on the constants of equivalence between $\|\cdot\|_{K,\Omega}$ and $\|\cdot\|_{H^s(\Omega)}$.

Any reproducing kernel for $H^s(\Omega)$ satisfies $K(x, \cdot) \in H^s(\Omega)$ for all $x \in \Omega$ because of (9). However, with the help of Lemma 1 we see that also derivatives $\partial_1^\beta K(x, \cdot)$, with $|\beta| < s - d/2$, belong to $H^s(\Omega)$.

Lemma 4 *Let $K : \Omega \times \Omega \rightarrow \mathbb{R}$ be a reproducing kernel for $H^s(\Omega)$, $s > d/2$. Then $\partial_1^\beta K(x, \cdot) \in H^s(\Omega)$ for all $x \in \Omega$ and all $\beta \in \mathbb{Z}_+^d$ satisfying $|\beta| < s - d/2$.*

Proof By Sobolev embedding (applied to a ball centered at x and contained in Ω) the linear functionals γ of the form $\gamma v = \partial^\beta v(x)$, $v \in H^s(\Omega)$, are bounded on $H^s(\Omega) = H_K$ for all $x \in \Omega$ and $\beta \in \mathbb{Z}_+^d$ with $|\beta| < s - d/2$. Hence the statement follows by Lemma 1. □

If \mathcal{M} is a smooth closed manifold of dimension d , then $H^s(\mathcal{M})$ is a reproducing kernel Hilbert space when $s > d/2$. It may however be difficult to compute the reproducing kernel such that its native space coincides with a given norm of $H^s(\mathcal{M})$. If an orthonormal basis is known for a Sobolev space, for example for $L^2(\mathcal{M}) = H^0(\mathcal{M})$, then reproducing kernels can be constructed via infinite series, see e.g. [43, 46] and [69, Section 17.4]. We discuss this in somewhat more detail in Section 2.3.

If \mathcal{M} is embedded into \mathbb{R}^m , $m > d$, then in view of the trace theorems (see e.g. [3, Theorem 2.3.7]) reproducing kernels K for $H^s(\mathcal{M})$, $s > d/2$, can be obtained by restricting to \mathcal{M} one of explicitly known positive definite kernels defined on \mathbb{R}^m with the native space norm equivalent to $H^{s+(m-d)/2}(\mathbb{R}^m)$. The best known examples are Matérn and Wendland kernels.

The Matérn kernel is given by

$$M_{s,d}(x, y) = \Phi_{s,d}(x - y), \quad \Phi_{s,d}(x) := \frac{1}{2^{s-1}\Gamma(s)} \mathcal{K}_{s-d/2}(\|x\|_2) \|x\|_2^{s-d/2}, \quad x \in \mathbb{R}^m, \tag{16}$$

where \mathcal{K}_ν denotes the modified Bessel function of second kind. The native space norm $\|\cdot\|_{\Phi_{s,d}}$ coincides with the Bessel potential norm of $H^{s+(m-d)/2}(\mathbb{R}^m)$ since the m -dimensional Fourier transform of $\Phi_{s,d}$ is $(1 + \|\omega\|_2^2)^{-s-(m-d)/2}$. By scaling $M_{s,d}$ with a *shape parameter* $\varepsilon > 0$, we obtain the kernel $M_{s,d}^\varepsilon(x, y) = M_{s,d}(\varepsilon x, \varepsilon y)$ whose native space also coincides with $H^{s+(m-d)/2}(\mathbb{R}^m)$, with a different but equivalent norm.

The native space of the Wendland compactly supported kernel $W_{m,\ell}(x, y) = \phi_{m,\ell}(\|x - y\|_2)$, $\ell \in \mathbb{Z}_+$, see [69], is norm equivalent to $H^{s+(m-d)/2}(\mathbb{R}^m)$ for $s = (d + 1)/2 + \ell$ (where $m \geq 3$ if $\ell = 0$). Hence, in the case when $s - d/2 \in \mathbb{Z}_+ + \frac{1}{2}$, the restriction of $W_{m,r}$, $m > d$, $r = \lfloor s - d/2 \rfloor = \lceil s - d/2 \rceil - 1$, is a reproducing kernel for $H^s(\mathcal{M})$.

2.3 Differential operators

Assuming that \mathcal{M} is a smooth compact manifold of dimension d without boundary, we say that a differential operator L on \mathcal{M} has *smooth coefficients* if its coefficients $a_{\ell,\alpha}$ in local coordinates,

$$Lu \circ \hat{\phi}_\ell^{-1} = \sum_{|\alpha| \leq m} a_{\ell,\alpha} \partial^\alpha (u \circ \hat{\phi}_\ell^{-1}), \quad u : \hat{U}_\ell \rightarrow \mathbb{R}, \quad a_{\ell,\alpha} : \hat{\phi}_\ell(\hat{U}_\ell) \rightarrow \mathbb{R},$$

are infinitely differentiable and uniformly bounded, such that for some constants $C_{\alpha\beta}$,

$$\|\partial^\beta a_{\ell,\alpha}\|_{L^\infty(\hat{\phi}_\ell(\hat{U}_\ell))} \leq C_{\alpha\beta}, \quad \alpha, \beta \in \mathbb{Z}_+^d, \quad |\alpha| \leq m, \quad \ell = 1, \dots, \hat{n}. \tag{17}$$

Consider an elliptic operator L with smooth coefficients and even order $m = 2\kappa$. In fact, all elliptic operators have even order if $d > 2$ [3]. For all $t \in \mathbb{R}$, L is a bounded linear operator from $H^t(\mathcal{M})$ to $H^{t-2\kappa}(\mathcal{M})$. Moreover, its inverse is a bounded linear operator from $H^{t-2\kappa}(\mathcal{M})$ to $H^t(\mathcal{M})$ as soon as the null space $N(L) = \{u : Lu = 0\}$ of L is trivial [3, Theorem 6.2.1], which implies (2).

Since $H^{t_2}(\mathcal{M})$ is compactly embedded in $H^{t_1}(\mathcal{M})$ for $t_1 < t_2$ [3, Theorem 2.3.1], the operator $L^{-1} : H^t(\mathcal{M}) \rightarrow H^t(\mathcal{M})$ is compact for any $t \in \mathbb{R}$. Hence the spectrum of L consists of isolated eigenvalues of finite multiplicity with no finite accumulation points. Assume that L , as an unbounded operator on $H^s(\mathcal{M})$ with domain $H^{s+2\kappa}(\mathcal{M})$, is positive and self-adjoint with respect to an inner product $(\cdot, \cdot)_s$ in $H^s(\mathcal{M})$, that is, $(Lv, v)_s > 0$ for all $v \in H^{s+2\kappa}(\mathcal{M}) \setminus \{0\}$ and $(Lv, w)_s = (v, Lw)_s$ for all $v, w \in H^{s+2\kappa}(\mathcal{M})$. Then it follows from the spectral theorem (see e.g. [68, Theorem 7.17], where real valued Hilbert spaces are considered) that there exists an orthonormal

basis of $H^s(\mathcal{M})$ consisting of eigenfunctions $e_j, j \in \mathbb{N}$, of L , such that

$$Lv = \sum_{j=1}^{\infty} \lambda_j c_j e_j, \quad L^{-1}v = \sum_{j=1}^{\infty} \lambda_j^{-1} c_j e_j \quad \text{for any } v = \sum_{j=1}^{\infty} c_j e_j \in H^s(\mathcal{M}),$$

where $\lambda_j > 0$ are the eigenvalues of L and $c_j \in \mathbb{R}$. This implies for all $k \in \mathbb{N}$,

$$H^{s-km} = \left\{ \sum_{j=1}^{\infty} \lambda_j^k c_j e_j : \|c\|_2 < \infty \right\}, \quad H^{s+km}(\mathcal{M}) = \left\{ \sum_{j=1}^{\infty} \lambda_j^{-k} c_j e_j : \|c\|_2 < \infty \right\},$$

where $\|c\|_2^2 := \sum_{j=1}^{\infty} c_j^2$, and by interpolation (see e.g. [3, Section 13]),

$$H^t(\mathcal{M}) = \left\{ \sum_{j=1}^{\infty} \lambda_j^{(s-t)/m} c_j e_j : \|c\|_2 < \infty \right\}, \quad t \in \mathbb{R}.$$

The norm in $H^t(\mathcal{M})$ defined by $\| \sum_{j=1}^{\infty} \lambda_j^{(s-t)/m} c_j e_j \|_t := \|c\|_2$ is equivalent to the standard Sobolev norms, and $\lambda_j^{(s-t)/m} e_j, j = 1, 2, \dots$, is an orthonormal basis with respect to this norm. It is easy to see that L is positive and self-adjoint with respect to the corresponding inner products $(\cdot, \cdot)_t, t \in \mathbb{R}$. Note that eigenfunctions e_j belong to $H^t(\mathcal{M})$ for all $t \in \mathbb{R}$, and thus to $C^\infty(\mathcal{M})$ since the eigenspaces of L are independent of the choice of s and inner product in $H^s(\mathcal{M})$. The eigenvalues λ_j , numbered in nondecreasing order with multiplicities taken into account satisfy $\lambda_j = j^{2\kappa/d}(C + o(1)), j \rightarrow \infty$, where C is a positive constant independent of j , see [2, Theorem 6.1.1].

If $s > d/2$, then $H^s(\mathcal{M})$ is embedded into $C(\mathcal{M})$, and hence $H^s(\mathcal{M})$ is a reproducing kernel Hilbert space. It is easy to see that its kernel corresponding to the inner product $(\cdot, \cdot)_s$ is given by

$$K(x, y) = \sum_{j=1}^{\infty} e_j(x)e_j(y), \tag{18}$$

where the series is a well defined real function on $\mathcal{M} \times \mathcal{M}$ since for each fixed $x \in \mathcal{M}$ the sequence $e_j(x) = (v_x, e_j), j = 1, 2, \dots$, where $v_x \in H^s(\mathcal{M})$ is the Riesz representer of the point evaluation functional at x , is square summable. If $t > d/2$, then the kernel of $H^t(\mathcal{M})$ for the norm $\| \cdot \|_t$ is given by

$$L_1^{2(s-t)/m} K(x, y) = \sum_{j=1}^{\infty} \lambda_j^{2(s-t)/m} e_j(x)e_j(y), \tag{19}$$

where the powers of L are defined by

$$L^\theta v = \sum_{j=1}^\infty \lambda_j^\theta c_j e_j, \quad v = \sum_{j=1}^\infty c_j e_j, \quad \theta \in \mathbb{R},$$

such that

$$\|L^\theta v\|_t = \|v\|_{t+m\theta}, \quad t, \theta \in \mathbb{R}, \quad v \in H^{t+m\theta}(\mathcal{M}).$$

Since $\lambda_j > 0$ for all j , the kernels $K_{L^\theta} = L_1^\theta K$ are positive definite whenever $s - \theta\kappa > d/2$.

We summarize in the following lemma the main findings of this section.

Lemma 5 *Let L be an elliptic differential operator of order 2κ with smooth coefficients and trivial null space, and let K be a reproducing kernel for $H^s(\mathcal{M})$, where $s > d/2$. Assume that L is positive and self-adjoint with respect to the inner product of $H^s(\mathcal{M})$ defined by K . Then $K_{L^\theta} = L_1^\theta K$ is a positive definite reproducing kernel for $H^{s-\theta\kappa}(\mathcal{M})$ for any $\theta \in \mathbb{R}$ such that $s - \theta\kappa > d/2$. In particular, $K_{L^{-1}}$ is a reproducing kernel for $H^{s+\kappa}(\mathcal{M})$. If $s > \kappa + d/2$, then K_L is a reproducing kernel for $H^{s-\kappa}(\mathcal{M})$ and*

$$\|Lv\|_{K_L} = \|v\|_{K_{L^{-1}}}, \quad v \in H^{s+\kappa}(\mathcal{M}). \tag{20}$$

Note that Lemma 5 also holds for certain classes of pseudodifferential operators on \mathcal{M} , see [2, 3].

Lemma 6 *Under the hypotheses of Lemma 5, $K(\cdot, x) \in H^{s+2\kappa r}(\Omega)$ for all $x \in \Omega$, where r is any integer satisfying $2\kappa r < s - d/2$. In particular, $K(\cdot, x) \in H^{s+2\kappa}(\Omega)$ for all $x \in \Omega$ if $s > 2\kappa + d/2$.*

Proof By Lemma 4, $L_1^r K(x, \cdot) \in H^s(\Omega)$ for all $x \in \Omega$ as soon as $2\kappa r < s - d/2$. Since the kernel $L_1^r K$ is symmetric, it follows that $L_1^r K(\cdot, x) \in H^s(\Omega)$ for all $x \in \Omega$, and the statement is obtained by applying (2) to $u = K(\cdot, x)$ and the operator L^r of order $2\kappa r$. □

In the case of the d -dimensional sphere $\mathcal{M} = \mathbb{S}^d$ of particular interest is a class of elliptic pseudodifferential operators [33] that can be represented in the form

$$Lv = \sum_{j=1}^\infty \lambda_j c_j e_j, \quad v = \sum_{j=1}^\infty c_j e_j, \quad \lambda_j > 0, \quad j \in \mathbb{N}, \tag{21}$$

where e_j are the spherical harmonics, that is the eigenfunctions of the Laplace-Beltrami operator $\Delta_{\mathcal{M}}$, normalized with respect to the standard inner product of $L^2(\mathbb{S}^d)$. For $d = 2$ these operators have important applications in physical geodesy.

In particular, operators of the form

$$L = (-\Delta_{\mathcal{M}} + \alpha I)^\kappa, \quad \kappa \in \mathbb{N}, \quad \alpha > 0, \tag{22}$$

where I is the identity operator, are elliptic differential operators of order 2κ on \mathbb{S}^d with smooth coefficients and trivial null spaces. These operators satisfy (21) and are positive and self-adjoint with respect to the inner products for Sobolev spaces $H^s(\mathbb{S}^d)$, $s > d/2$, generated by reproducing kernels of the type

$$K(x, y) = \sum_{j=1}^{\infty} \mu_j e_j(x) e_j(y), \tag{23}$$

with appropriately decaying positive real sequences $\{\mu_j\}_{j=1}^{\infty}$. Explicit *zonal* kernels $K(x, y) = \psi(x^T y)$ with this property are obtained as restrictions to \mathbb{S}^d of radially symmetric kernels (radial basis functions) $K(x, y) = \phi(\|x - y\|_2)$, $x, y \in \mathbb{R}^{d+1}$ since $\|x - y\|_2 = \sqrt{2 - 2x^T y}$ if $\|x\|_2 = \|y\|_2 = 1$, see e.g. [69, Section 17.2]. In particular, the hypotheses of Lemma 5 are satisfied for the differential operators (22) and kernels for $H^s(\mathbb{S}^d)$ obtained by restricting to \mathbb{S}^d the Matérn and Wendland kernels for \mathbb{R}^{d+1} , as well as their scaled versions.

If \mathcal{M} is a Cartesian product of multiple spheres, possibly of different dimensions, then appropriate kernels, with respect to which the corresponding tensor products of the operators (22) are positive and self-adjoint, are obtained for $H^s(\mathcal{M})$ by taking tensor products of the spherical restrictions of the Matérn and Wendland kernels. This follows from the fact that tensor products of kernels may be identified with the kernels of the tensor products of the respective reproducing kernel Hilbert spaces, see e.g. [51]. This applies in particular to the d -dimensional torus $\mathcal{M} = \mathbb{T}^d$ [46].

Differential operators (22) on arbitrary Riemannian manifolds also satisfy the assumptions of Lemma 5, see [3]. However, closed form formulas for the kernels of the form (23), where e_j are the eigenfunctions of $\Delta_{\mathcal{M}}$, are not available in general. By considering the flat torus $\mathcal{M} = \mathbb{R}^d / \mathbb{Z}^d$ we may find appropriate kernels for the periodic boundary value problems for the operators $L = (-\Delta + \alpha I)^\kappa$ on the unit cube, where Δ is the d -dimensional Laplace operator. In the univariate case $d = 1$ this kernel is known in terms of Bernoulli polynomials, see e.g. [30, Section 3.2].

3 A meshless finite difference method

Assume that L is an elliptic differential operator on \mathcal{M} of order 2κ with smooth coefficients and trivial null space, and K is a reproducing kernel for $H^s(\mathcal{M})$, where $s > \kappa + d/2$, such that L is positive and self-adjoint with respect to the inner product $(\cdot, \cdot)_K$ of $H^s(\mathcal{M})$ defined by K .

We consider the equation $Lu = f$, with continuous f , and look for a discrete solution $\hat{u} \in \mathbb{R}^n$ to approximate $u|_X$ on a given set of *nodes* $X = \{x_1, \dots, x_n\} \subset \mathcal{M}$.

We choose a system $\mathcal{X} = \{X_\ell : \ell = 1, \dots, m\}$ of subsets $X_\ell = \{x_j : j \in J_\ell\} \neq \emptyset$, with $J_\ell \subset J := \{1, \dots, n\}$, such that $\bigcup_{\ell=1}^m X_\ell = X$. Let $n_\ell := \#X_\ell$. Consider the local differentiation matrices $W_\ell := W_{X_\ell} \in \mathbb{R}^{n_\ell \times n_\ell}$ of (40), that is

$$W_\ell = K_L|_{X_\ell} (K|_{X_\ell})^{-1} \quad \ell = 1, \dots, m. \tag{24}$$

The kernel K_L is well defined and positive definite by Lemma 5, and hence the matrices W_ℓ are non-singular.

We now set up an overdetermined linear system

$$WMv = Mf|_X \tag{25}$$

with unknown vector $v \in \mathbb{R}^N$, the block diagonal matrix

$$W = \text{diag}(W_1, \dots, W_m) := \begin{bmatrix} W_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & W_m \end{bmatrix} \in \mathbb{R}^{N \times N}, \quad N := n_1 + \cdots + n_m,$$

and the incidence matrix

$$M = \begin{bmatrix} M_1 \\ \vdots \\ M_m \end{bmatrix} \in \mathbb{R}^{N \times n}, \quad M_\ell = [\delta_{ij}]_{i \in J_\ell, j \in J} \in \mathbb{R}^{n_\ell \times n}, \quad \delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

The matrix WM has the full rank n since W is non-singular and $\text{rank } M = n$. We determine the discrete solution $\hat{u} \in \mathbb{R}^n$ as the unique least squares solution of (25), such that

$$\|WM\hat{u} - Mf|_X\|_2 = \min_{v \in \mathbb{R}^n} \|WMv - Mf|_X\|_2. \tag{26}$$

Note that (25) can be more explicitly written as

$$W_\ell v|_{J_\ell} = f|_{X_\ell}, \quad \ell = 1, \dots, m, \tag{27}$$

and hence, in line with the main idea of meshless generalized finite differences, each linear equation in (25) is derived from a numerical differentiation formula

$$Lu(x_i) \approx \sum_{j \in J_\ell} w_{i,j}^{(\ell)} u(x_j), \quad i \in J_\ell,$$

where the weight vector $[w_{i,j}^{(\ell)}]_{j \in J_\ell}$ is the row of W_ℓ corresponding to the node x_i . Since

$$\|WMv - Mf|_X\|_2^2 = \sum_{\ell=1}^m \|W_\ell v|_{J_\ell} - f|_{X_\ell}\|_2^2, \tag{28}$$

we in fact minimize in (26) the sum of squared residuals of the numerical differentiation on the subsets X_ℓ .

Even if this method is well defined for any arbitrarily chosen nodes $X \subset \mathcal{M}$ and any system \mathcal{X} of their subsets satisfying $\bigcup_{\ell=1}^m X_\ell = X$, we have in mind X_ℓ being clusters of neighboring nodes, with a significant overlap between neighboring clusters. In Section 5 we present an error bound for $\|u|_X - \hat{u}\|_\infty$ under certain assumptions on X and \mathcal{X} , that in particular quantify the overlaps in terms of certain determining

properties of the images of the non-empty intersections $X_\ell \cap X_p$ in the charts of an atlas for \mathcal{M} .

For a practical realization of the method we suggest to choose a set $Y = \{y_1, \dots, y_m\} \subset \mathcal{M}$, possibly $Y \subset X$, and select each X_ℓ as the set of n_ℓ nearest nodes to y_ℓ , either in the sense of a properly defined distance on \mathcal{M} , or by the distance in an ambient Euclidian space. The latter approach with $Y = X$ is used in numerical examples of Section 6 for $\mathcal{M} = \mathbb{S}^d$, $d \in \{2, 3\}$, with \mathbb{R}^{d+1} as ambient space.

Remark 1 Instead of (26) we may in principle define $\hat{u} \in \mathbb{R}^n$ by minimizing a different p -norm,

$$\|WM\hat{u} - Mf|_X\|_p = \min_{v \in \mathbb{R}^n} \|WMv - Mf|_X\|_p, \quad 1 \leq p \leq \infty, \quad (29)$$

see also Remark 4 below. The 2-norm is preferable from the point of view of computational efficiency. In particular, for large n and m and small n_ℓ we may use existing efficient methods for sparse linear least squares, see [8]. Both cases $p = 1$ and ∞ have the interesting property that the solution \hat{u} of (29) satisfies certain linear systems with a matrix A consisting of relatively few rows of WM , and vector b of corresponding components of $Mf|_X$. Namely, A is an $n \times n$ -matrix with $A\hat{u} = b$ when $p = 1$ [16], and an $(n + 1) \times n$ -matrix with all components of the residual $A\hat{u} - b$ equal in absolute value when $p = \infty$ [13, p. 36]. In both cases this means that \hat{u} may be obtained by minimizing $\|Av - b\|_p$ as soon as A has full rank. This size reduction of the system (25) is however computationally demanding.

4 Auxiliary results

Before formulating and proving in Section 5 the error bounds for the above method we provide several technical results needed in the proof.

4.1 Admissible atlases

Recall that we have chosen and fixed a finite smooth atlas $\hat{\mathcal{A}} = \left\{ \left(\hat{U}_\ell, \hat{\varphi}_\ell \right) \right\}_{\ell=1}^{\hat{n}}$ of \mathcal{M} and a smooth subordinate partition of unity $\hat{\Gamma} = \{ \hat{\gamma}_\ell \}_{\ell=1}^{\hat{n}}$, and consider the norms for the Sobolev spaces $H^s(\mathcal{M})$ in the form (8) dependent on this choice.

It follows from the properties of $\hat{\gamma}_\ell$ that the sets $\hat{U}_\ell^c := \{x \in \mathcal{M} : \hat{\gamma}_\ell(x) > c\} \subset \hat{U}_\ell$, $\ell = 1, \dots, \hat{n}$, form an open cover of \mathcal{M} when $c = 0$, and hence also for all sufficiently small $c > 0$. We say that a finite smooth atlas $\mathcal{A} = \{ (U_\ell, \varphi_\ell) \}_{\ell=1}^m$ for \mathcal{M} is *c-admissible*, where $c > 0$, if for each $\ell = 1, \dots, m$ there exists $k = k(\ell)$ such that $U_\ell \subset \hat{U}_k^c$ and $\varphi_\ell = \hat{\varphi}_k|_{U_\ell}$. An atlas \mathcal{A} is *admissible* if it is *c-admissible* for some $c > 0$. The *covering number* of \mathcal{A} is defined as

$$\mu_{\mathcal{A}} := \max_{1 \leq \ell \leq m} \#\{j : U_j \cap U_\ell \neq \emptyset\}. \quad (30)$$

We show that the Sobolev norm of a function u on \mathcal{M} may be characterized in terms of Sobolev norms of the compositions $u \circ \varphi_\ell^{-1}$ for any c -admissible atlas, without multiplying u by the partition of unity function $\hat{\gamma}_\ell$ as in (8).

Lemma 7 *Let $\mathcal{A} = \{(U_\ell, \varphi_\ell)\}_{\ell=1}^m$ be a c -admissible atlas for \mathcal{M} for some $c > 0$. Then for all integer $s \geq 0$,*

$$C_1 \|u\|_{H^s(\mathcal{M})} \leq \left(\sum_{\ell=1}^m \|u \circ \varphi_\ell^{-1}\|_{H^s(\varphi_\ell(U_\ell))}^2 \right)^{1/2} \leq C_2 \sqrt{\mu_{\mathcal{A}}} \|u\|_{H^s(\mathcal{M})}, \quad u \in H^s(\mathcal{M}), \tag{31}$$

where $C_1 > 0$ depends only on s , the choice of the atlas $\hat{\mathcal{A}}$ and the partition of unity $\hat{\Gamma}$, and C_2 depends in addition on c .

Proof Let $L_k := \{\ell : U_\ell \cap \hat{U}_k \neq \emptyset\}$. Then $\hat{U}_k \subset \bigcup_{\ell \in L_k} U_\ell$ and hence

$$\|u \hat{\gamma}_k \circ \hat{\varphi}_k^{-1}\|_{H^s(\mathbb{R}^d)}^2 = \|u \hat{\gamma}_k \circ \hat{\varphi}_k^{-1}\|_{H^s(\hat{\varphi}_k(\hat{U}_k))}^2 \leq \sum_{\ell \in L_k} \|u \hat{\gamma}_k \circ \hat{\varphi}_k^{-1}\|_{H^s(\hat{\varphi}_k(U_\ell \cap \hat{U}_k))}^2.$$

Since $\hat{\varphi}_k^{-1} = \varphi_\ell^{-1} \circ \hat{\varphi}_k(\ell) \circ \hat{\varphi}_k^{-1}$ on $\hat{\varphi}_k(U_\ell \cap \hat{U}_k)$, we have by the Leibniz and the chain rules,

$$\|u \hat{\gamma}_k \circ \hat{\varphi}_k^{-1}\|_{H^s(\hat{\varphi}_k(U_\ell \cap \hat{U}_k))}^2 \leq C \|u \circ \varphi_\ell^{-1}\|_{H^s(\varphi_\ell(U_\ell \cap \hat{U}_k))}^2,$$

where C depends only on the size of derivatives of order up to s of the functions $\hat{\gamma}_k \circ \hat{\varphi}_k^{-1}$ and the transition maps $\hat{\varphi}_j \circ \varphi_k^{-1}$ of $\hat{\mathcal{A}}$, and the (nonzero) determinants of their Jacobi matrices. Finally,

$$\sum_{\ell=1}^m \sum_{\substack{k=1 \\ \ell \in L_k}}^{\hat{n}} \|u \circ \varphi_\ell^{-1}\|_{H^s(\varphi_\ell(U_\ell \cap \hat{U}_k))}^2 \leq \hat{n} \sum_{\ell=1}^m \|u \circ \varphi_\ell^{-1}\|_{H^s(\varphi_\ell(U_\ell))}^2,$$

and we deduce the first inequality in (31).

On the other hand, for each $k = 1, \dots, \hat{n}$,

$$\sum_{\substack{\ell=1 \\ k(\ell)=k}}^m \|u \circ \varphi_\ell^{-1}\|_{H^s(\varphi_\ell(U_\ell))}^2 \leq \mu_{\mathcal{A}} \|u \circ \hat{\varphi}_k^{-1}\|_{H^s(\hat{\varphi}_k(\hat{U}_k^c))}^2.$$

By applying the Leibniz product rule to $\frac{1}{\hat{\gamma}_k} \cdot (u \hat{\gamma}_k)$ and estimating the L^2 -norm of the products of (bounded) derivatives of $\frac{1}{\hat{\gamma}_k \circ \hat{\varphi}_k^{-1}}$ with derivatives of $u \circ \hat{\varphi}_k^{-1}$, we obtain

$$\|u \circ \hat{\varphi}_k^{-1}\|_{H^s(\hat{\varphi}_k(\hat{U}_k^c))} \leq C \|u \hat{\gamma}_k \circ \hat{\varphi}_k^{-1}\|_{H^s(\mathbb{R}^d)}, \tag{32}$$

where C depends only on $\hat{\mathcal{A}}, \hat{\Gamma}, c$ and s . This completes the proof of the second inequality in (31). □

Note that (31) holds without any assumptions about the boundaries of the sets $\varphi_\ell(U_\ell)$. In particular, they do not need to be Lipschitz domains. If they are, then we can extend the functions $u|_{U_\ell}$ to \mathcal{M} , which will be useful for establishing double estimates for $\|u\|_{H^s(\mathcal{M})}$ in terms of the native space norms of a reproducing kernel in charts, see (34) below.

Lemma 8 *Let $U \subset \mathcal{M}$ be a domain such that $U \subset \hat{U}_k^c$ for some $c > 0$ and k , and the extension constant $\mathcal{E}_s(\hat{\varphi}_k(U))$ is finite for an integer $s \geq 0$. Then for any $u : U \rightarrow \mathbb{R}$ such that $u \circ \hat{\varphi}_k^{-1} \in H^s(\hat{\varphi}_k(U))$ there exists a function $\tilde{u} \in H^s(\mathcal{M})$ such that $\tilde{u}|_U = u$ and*

$$\|\tilde{u}\|_{H^s(\mathcal{M})} \leq C\mathcal{E}_s(\hat{\varphi}_k(U))\|u \circ \hat{\varphi}_k^{-1}\|_{H^s(\hat{\varphi}_k(U))},$$

where C depends only on $\hat{\mathcal{A}}, \hat{\Gamma}, s, c$.

Proof Let $w \in H^s(\mathbb{R}^d)$ be an extension of $u \circ \hat{\varphi}_k^{-1}$ such that

$$\|w\|_{H^s(\mathbb{R}^d)} \leq 2\mathcal{E}_s(\hat{\varphi}_k(U))\|u \circ \hat{\varphi}_k^{-1}\|_{H^s(\hat{\varphi}_k(U))}.$$

We define \tilde{u} as follows,

$$\tilde{u}(x) = \begin{cases} (\chi_{k,c} w \circ \hat{\varphi}_k)(x), & \text{if } x \in \hat{U}_k, \\ 0, & \text{otherwise,} \end{cases}$$

where $\chi_{k,c} \in C^\infty(\mathbb{R}^d)$ is a cutoff function, see e.g. [41], that satisfies

$$\chi_{k,c}(x) = 1, \quad x \in \hat{\varphi}_k(\hat{U}_k^c), \quad \text{and} \quad \chi_{k,c}(x) = 0, \quad x \notin \hat{\varphi}_k(\hat{U}_k).$$

Then $\tilde{u}|_U = u$, and for any ℓ by the Leibniz and the chain rules,

$$\begin{aligned} \|\tilde{u}\hat{\gamma}_\ell \circ \hat{\varphi}_\ell^{-1}\|_{H^s(\mathbb{R}^d)} &= \|(\hat{\gamma}_\ell \circ \hat{\varphi}_\ell^{-1})(\chi w \circ \hat{\varphi}_k \circ \hat{\varphi}_\ell^{-1})\|_{H^s(\hat{\varphi}_\ell(\hat{U}_k \cap \hat{U}_\ell))} \\ &\leq C_1 \|w\|_{H^s(\hat{\varphi}_k(\hat{U}_k \cap \hat{U}_\ell))}, \end{aligned}$$

where C_1 depends only on c, s and the choice of $\hat{\mathcal{A}}, \hat{\Gamma}$ and the cutoff function $\chi_{k,c}$. Clearly, cutoff functions $\chi_{k,c}, k = 1, \dots, \hat{n}$, may be chosen once and for all as soon as other parameters are fixed. Hence

$$\|\tilde{u}\|_{H^s(\mathcal{M})}^2 = \sum_{\ell=1}^{\hat{n}} \|\tilde{u}\hat{\gamma}_\ell \circ \hat{\varphi}_\ell^{-1}\|_{H^s(\mathbb{R}^d)}^2 \leq 4\hat{n}C_1^2\mathcal{E}_s^2(\hat{\varphi}_k(U))\|u \circ \hat{\varphi}_k^{-1}\|_{H^s(\hat{\varphi}_k(U))}^2.$$

□

If K is a reproducing kernel on \mathcal{M} , U an open set in \mathcal{M} , and $\varphi : U \rightarrow \mathbb{R}^d$ a homeomorphism from U to $\varphi(U) \subset \mathbb{R}^d$, then $K^\varphi(x, y) := K(\varphi^{-1}(x), \varphi^{-1}(y)), x, y \in \varphi(U)$, is obviously the reproducing kernel for the Hilbert space

$$H_K(\varphi(U)) = \{u \circ \varphi^{-1} : u \in H_K(U)\} \tag{33}$$

isometric to $H_K(U)$, with the norm given by

$$\|u \circ \varphi^{-1}\|_{K^\varphi, \varphi(U)} = \|u\|_{K,U},$$

where we use the notation introduced in Lemma 2. We show an analogue of Lemma 3, relating the native space norm on U to the Sobolev norm on its chart image in \mathbb{R}^d in the case when K is a reproducing kernel for a Sobolev space.

Lemma 9 *Let K be a reproducing kernel for $H^s(\mathcal{M})$, with an integer $s > d/2$, and let $U \subset \mathcal{M}$ be a domain such that $U \subset \hat{U}_k^c$ for some $c > 0$ and k . Then $H_K(\hat{\varphi}_k(U)) \subset H^s(\hat{\varphi}_k(U))$ and*

$$\|u \circ \hat{\varphi}_k^{-1}\|_{H^s(\hat{\varphi}_k(U))} \leq C_1 \|u\|_{K,U}, \quad u \in H_K(U).$$

Moreover, if the extension constant $\mathcal{E}_s(\hat{\varphi}_k(U))$ is finite, then $H_K(\hat{\varphi}_k(U)) = H^s(\hat{\varphi}_k(U))$ and

$$\|u\|_{K,U} \leq C_2 \mathcal{E}_s(\hat{\varphi}_k(U)) \|u \circ \hat{\varphi}_k^{-1}\|_{H^s(\hat{\varphi}_k(U))}, \quad u \in H_K(U).$$

The constants C_1, C_2 depend only on $K, \hat{\mathcal{A}}, \hat{\Gamma}, c$ and s .

Proof Let $v \in H_K(\hat{\varphi}_k(U))$, that is $v = u \circ \hat{\varphi}_k^{-1}$ for some $u \in H_K(U)$. Then u is the restriction to U of a function in $H_K(\mathcal{M})$, denoted u again. By Lemma 2 we assume without loss of generality that $\|u\|_{K,U} = \|u\|_{K,\mathcal{M}}$. As in the proof of Lemma 7, we obtain by (32),

$$\|u \circ \hat{\varphi}_k^{-1}\|_{H^s(\hat{\varphi}_k(U))} \leq \|u \circ \hat{\varphi}_k^{-1}\|_{H^s(\hat{\varphi}_k(\hat{U}_k^c))} \leq C \|u \hat{\gamma}_k \circ \hat{\varphi}_k^{-1}\|_{H^s(\mathbb{R}^d)} \leq C \|u\|_{H^s(\mathcal{M})},$$

where C depends only on $\hat{\mathcal{A}}, \hat{\Gamma}, c$ and s . Since the norms $\|\cdot\|_{K,\mathcal{M}}$ and $\|\cdot\|_{H^s(\mathcal{M})}$ are equivalent, the first assertion of the lemma follows.

We now assume that $\mathcal{E}_s(\hat{\varphi}_k(U)) < \infty$. For any $v \in H^s(\hat{\varphi}_k(U))$, the function $u = v \circ \hat{\varphi}_k$ is by Lemma 8 the restriction to U of a function $\tilde{u} \in H^s(\mathcal{M})$ such that

$$\|\tilde{u}\|_{H^s(\mathcal{M})} \leq C \mathcal{E}_s(\hat{\varphi}_k(U)) \|v\|_{H^s(\hat{\varphi}_k(U))},$$

where C depends only on $c, s, \hat{\mathcal{A}}, \hat{\Gamma}$. Since $H^s(\mathcal{M}) = H_K(\mathcal{M})$ with equivalent norms, it follows from Lemma 2 that $\|u\|_{K,U} \leq C \|\tilde{u}\|_{H^s(\mathcal{M})}$, where C depends only on $K, \hat{\mathcal{A}}, \hat{\Gamma}$. Hence $v \in H_K(\hat{\varphi}_k(U))$, and the second assertion follows. \square

Given a c -admissible atlas $\mathcal{A} = \{(U_\ell, \varphi_\ell)\}_{\ell=1}^m$ for \mathcal{M} , with $c > 0$, we obtain from Lemma 9, for any $u \in H^s(\mathcal{M})$ and $\ell = 1, \dots, m$,

$$C_1^{-1} \|u \circ \varphi_\ell^{-1}\|_{H^s(\varphi_\ell(U_\ell))} \leq \|u|_{U_\ell}\|_{K,U_\ell} \leq C_2 \mathcal{E}_s(\varphi_\ell(U_\ell)) \|u \circ \varphi_\ell^{-1}\|_{H^s(\varphi_\ell(U_\ell))},$$

with constants C_1, C_2 of Lemma 9. Hence, it follows by Lemma 7 that

$$C_1 \|u\|_{H^s(\mathcal{M})} \leq \left(\sum_{\ell=1}^m \|u|_{U_\ell}\|_{K,U_\ell}^2 \right)^{1/2} \leq C_2 \sqrt{\mu_{\mathcal{A}}} \max_{\ell=1,\dots,m} \mathcal{E}_s(\varphi_\ell(U_\ell)) \|u\|_{H^s(\mathcal{M})}, \tag{34}$$

for all $u \in H^s(\mathcal{M})$, with constants C_1, C_2 depending only on $K, \widehat{\mathcal{A}}, \widehat{\Gamma}, c$ and s .

Since $\|u\|_{H^s(\mathcal{M})}$ and the native space norm $\|u\|_K$ are equivalent, we also get the same double estimate with $\|u\|_{H^s(\mathcal{M})}$ replaced by $\|u\|_K$. Thus, a detour via Sobolev spaces delivers a relation between $\|u\|_K$ and $\|u|_{U_\ell}\|_{K,U_\ell}, \ell = 1, \dots, m$.

4.2 Extension constants

Since we will need to bound the extension constants $\mathcal{E}_s(\widehat{\varphi}_k(U))$ uniformly for families of local subdomains $U \subset \mathcal{M}$, compare (34), we consider the question of estimating $\mathcal{E}_s(\Omega)$ for Lipschitz domains $\Omega \subset \mathbb{R}^d$.

A bounded domain Ω satisfies the Lipschitz condition if it has a locally Lipschitz boundary, that is, each point on the boundary of Ω has a neighborhood whose intersection with $\partial\Omega$ is the graph of a function satisfying the Lipschitz condition, with uniformly bounded Lipschitz constants.

For any bounded domain $\Omega \subset \mathbb{R}^d$, we denote by $\chi(\Omega)$ its *chunkiness parameter* [9], the quotient of the diameter of Ω to the maximum radius of a ball $B \subset \Omega$ such that Ω is star-shaped with respect to B . Clearly, $\chi(\Omega) < \infty$ if and only if Ω is bounded and star-shaped with respect to a ball. It is known that such domains satisfy the Lipschitz condition, see [11, Section 4.3] or [44, Section 1.3.2].

Since $\partial\Omega$ is compact, there is a finite system \mathcal{L} consisting of $P_{\mathcal{L}}$ open sets in \mathbb{R}^d that cover $\partial\Omega$ such that their intersections with $\partial\Omega$ are the graphs of continuous functions with Lipschitz constants not exceeding some number $M_{\mathcal{L}}$. Such a system is not unique, and a smaller $M_{\mathcal{L}}$ may be obtained at the expense of increasing $P_{\mathcal{L}}$. We will call any such system \mathcal{L} a *Lipschitz cover* of $\partial\Omega$. Apart from $P_{\mathcal{L}}$ and $M_{\mathcal{L}}$, another parameter of \mathcal{L} important for the extension constant is a number $r_{\mathcal{L}} > 0$ such that for each $x \in \partial\Omega$ the ball with radius $r_{\mathcal{L}}$ centered at x is contained in one of the sets of \mathcal{L} . It is easy to see that a positive $r_{\mathcal{L}}$ exists for any Lipschitz cover.

The Stein Extension Theorem [65] shows that $\mathcal{E}_s(\Omega)$ is bounded from the above by a constant depending only on $d, s, P_{\mathcal{L}}, M_{\mathcal{L}}$ and $r_{\mathcal{L}}$.

Since we will need bounds for $\mathcal{E}_s(\Omega)$ for domains with diameter tending to zero, we will use the parameter $\tau_{\mathcal{L}} := r_{\mathcal{L}}/\text{diam}(\Omega)$ in place of $r_{\mathcal{L}}$. The following estimate follows immediately from the results in [44, Section 3.1.5].

Lemma 10 *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain star-shaped with respect to a ball, and let \mathcal{L} be a Lipschitz cover of its boundary. If $\chi(\Omega) \leq \chi, P_{\mathcal{L}} \leq P, M_{\mathcal{L}} \leq M$ and $\tau_{\mathcal{L}} \geq \tau > 0$, then for any integer $s \geq 0$,*

$$\mathcal{E}_s(\Omega) \leq Ch^{-d/2}, \quad h = \text{diam}(\Omega),$$

where C depends only on d, s, χ, P, M and τ .

4.3 Sampling inequalities

Sampling inequalities bound a weaker Sobolev norm of a function f in terms of its values on a finite set $X \subset \Omega$ and a stronger Sobolev norm of f , see the survey [55] and references therein. In Lemma 11 we follow a standard way of proving sampling inequalities, as e.g. in [48, 70], but obtain a local version that makes use of the diameter of the domain Ω as the discretization parameter h instead of the fill distance of X . Therefore our estimates (35), (36) depend on a polynomial Lebesgue constant, which is usually avoided in global estimates by requiring that X is sufficiently dense in Ω . We refer to [25, Section 4] for a demonstration that this requirement is too restrictive for the setting of local error bounds to which we will apply the sampling inequalities in Section 4.4. A different local sampling inequality in terms of a growth function is given in [25, Corollary 13].

For any finite $Y \subset \mathbb{R}^d$ we consider the *Lebesgue function*

$$\lambda_r(y, Y) = \sup\{|p(y)| : \|p|_Y\|_\infty \leq 1 \text{ for all } p \in \Pi_r^d\}, \quad y \in \mathbb{R}^d, \quad r \in \mathbb{N},$$

where $\Pi_r^d, r \in \mathbb{N}$, denotes the space of d -variate polynomials of total order at most r (or degree less than r). Note that $\lambda_r(y, Y) < \infty$ for all $y \in \mathbb{R}^d$ if and only if Y is a r -determining set, that is $p \in \Pi_r^d$ and $p|_Y = 0$ imply $p \equiv 0$. For any set $\Omega \subset \mathbb{R}^d$, the *Lebesgue constant* is given by

$$\lambda_r(\Omega, Y) = \sup_{y \in \Omega} \lambda_r(y, Y).$$

Note that the *Lebesgue constant* is the reciprocal of the *norming constant* [38]. On the other hand, the Lebesgue function is a special case of a *growth function* [17, 26], and we rely in the proof on a general duality theory for growth functions [26, Theorem 9] that replaces the “local polynomial reproduction” arguments, compare [69, Chapter 3].

Lemma 11 *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with chunkiness parameter $\chi(\Omega) \leq \chi$ for some constant $\chi < \infty$, let $X = \{x_1, \dots, x_n\} \subset \Omega$ be an r -determining set for some integer $r > d/2$, and let $v \in H^r(\Omega)$. We set $h = \text{diam}(\Omega)$. Then for any integer k with $0 \leq k < r$,*

$$|v|_{H^k(\Omega)} \leq Ch^{-k} \lambda_r(\Omega, X) (h^{d/2} \|v|_X\|_\infty + h^r |v|_{H^r(\Omega)}), \tag{35}$$

where C depends only on r, d and χ . Moreover, for any $\beta \in \mathbb{Z}_+^d$ with $|\beta| < r - d/2$,

$$|\partial^\beta v(x)| \leq Ch^{-|\beta|} \lambda_r(\Omega, X) (\|v|_X\|_\infty + h^{r-d/2} |v|_{H^r(\Omega)}), \quad x \in \Omega, \tag{36}$$

where C depends only on r, d and χ .

Proof By Sobolev embedding we identify v with an m times continuously differentiable function in Ω , where m is the largest integer such that $m < r - d/2$. By

Proposition 4.3.2, equation (4.1.18) and Lemma 4.3.8 in [9] there is a polynomial $p \in \Pi_r^d$ such that

$$|\partial^\beta v(x) - \partial^\beta p(x)| \leq C_1 h^{r-|\beta|-d/2} |v|_{H^r(\Omega)}, \quad x \in \Omega, \quad |\beta| < r - d/2, \quad (37)$$

$$|v - p|_{H^k(\Omega)} \leq C_2 h^{r-k} |v|_{H^r(\Omega)}, \quad k \leq r, \quad (38)$$

where both C_1 and C_2 depend only on r, d and χ .

Let $\alpha \in \mathbb{Z}_+^d$ with $|\alpha| = k$. Since X is r -determining, for any $x \in \Omega$ there exist weights $w_j \in \mathbb{R}$ such that

$$\partial^\alpha p(x) = \sum_{j=1}^n w_j p(x_j) \quad \text{and} \quad \sum_{j=1}^n |w_j| = \sup \{ \partial^\alpha q(x) : q \in \Pi_r^d, \|q|_X\| \leq 1 \},$$

see [26, Theorem 9]. By Markov inequality (see e.g. [48, Proposition 2.2]),

$$|\partial^\alpha q(x)| \leq C_3 h^{-k} \|q\|_{L^\infty(\Omega)}, \quad q \in \Pi_r^d,$$

where C_3 depends only on r, d and χ . Hence

$$\sum_{j=1}^n |w_j| \leq C_3 h^{-k} \lambda_r(\Omega, X).$$

By (37),

$$|v(x_j) - p(x_j)| \leq C_1 h^{r-d/2} |v|_{H^r(\Omega)}, \quad j = 1, \dots, n.$$

Hence

$$\begin{aligned} |\partial^\alpha p(x)| &= \left| \sum_{j=1}^n w_j v(x_j) + \sum_{j=1}^n w_j (p(x_j) - v(x_j)) \right| \\ &\leq C_3 h^{-k} \lambda_r(\Omega, X) (\|v|_X\|_\infty + C_1 h^{r-d/2} |v|_{H^r(\Omega)}), \end{aligned} \quad (39)$$

which implies

$$\|\partial^\alpha p\|_{L^2(\Omega)} \leq C_4 C_3 h^{-k+d/2} \lambda_r(\Omega, X) (\|v|_X\|_\infty + C_1 h^{r-d/2} |v|_{H^r(\Omega)}),$$

where C_4 depends only on d . By (38),

$$\|\partial^\alpha v - \partial^\alpha p\|_{L^2(\Omega)} \leq C_2 h^{r-k} |v|_{H^r(\Omega)},$$

and (35) follows since $\|\partial^\alpha v\|_{L^2(\Omega)} \leq \|\partial^\alpha v - \partial^\alpha p\|_{L^2(\Omega)} + \|\partial^\alpha p\|_{L^2(\Omega)}$ and $\lambda_r(\Omega, X) \geq 1$. Similarly, (36) follows directly from (37) and (39). \square

4.4 Local differentiation matrices

Let L be a differential operator of order m on \mathcal{M} , K the reproducing kernel of a Hilbert space $H_K(\mathcal{M})$ embedded into $C^m(\mathcal{M})$, and $X = \{x_1, \dots, x_n\} \subset \mathcal{M}$. For any $u \in C^m(\mathcal{M})$, an approximation of Lu can be obtained by applying L to the kernel interpolant (11),

$$\sigma = \sum_{j=1}^n c_j K(\cdot, x_j), \quad \sigma(x_j) = u(x_j), \quad j = 1, \dots, n,$$

$$Lu \approx L\sigma = \sum_{j=1}^n c_j K_L(\cdot, x_j).$$

In particular, the approximation $L\sigma|_X$ of $Lu|_X$ can be computed with the help of the differentiation matrix W_X ,

$$L\sigma|_X = W_X u|_X, \quad \text{where } W_X := K_L|_X (K|_X)^{-1}. \tag{40}$$

If U is an open set in \mathcal{M} and $\varphi : U \rightarrow \mathbb{R}^d$ is a homeomorphism from U to $U^\varphi := \varphi(U) \subset \mathbb{R}^d$, then we denote by L^φ the differential operator L in the local coordinates defined by φ , that is

$$L^\varphi v := L(v \circ \varphi) \circ \varphi^{-1}$$

for any sufficiently smooth function v on U^φ . Then the kernel $K^\varphi(x, y) = K(\varphi^{-1}(x), \varphi^{-1}(y))$ of the space $H_K(U^\varphi)$ defined in (33) obviously satisfies

$$L_i^\varphi K^\varphi = (L_i K)^\varphi, \quad i = 1, 2, \tag{41}$$

where $L_1 K$ and $L_2 K$ denote the result of applying the operator L to the first, respectively, second argument of K , according to the notation introduced in Section 2.2. In particular,

$$W_X = K_L^\varphi|_{X^\varphi} (K^\varphi|_{X^\varphi})^{-1},$$

where $K_L^\varphi := L_1^\varphi K^\varphi$ and $X^\varphi := \varphi(X)$.

Lemma 12 *Let L be a differential operator on \mathcal{M} of order m with smooth coefficients, and let K be a reproducing kernel for $H^s(\mathcal{M})$, with an integer $s > m + d/2$. Furthermore, let $X = \{x_1, \dots, x_n\} \subset U$ for an open set $U \subset \hat{U}_k^c \subset \mathcal{M}$ for some $k \in \{1, \dots, \hat{n}\}$ and $c > 0$. For $\varphi = \hat{\varphi}_k$, assume that U^φ is star-shaped with respect to a ball, with $\chi(U^\varphi) \leq \chi < \infty$, and X^φ is an r -determining set for some $r > m + d/2$ such that $K(\cdot, x) \in H^r(\mathcal{M})$ for all $x \in \mathcal{M}$. Then for any $u \in H^r(\mathcal{M})$,*

$$\|Lu|_X - W_X u|_X\|_\infty \leq C_1 \lambda_r(U^\varphi, X^\varphi) h^{r-m-d/2} |u^\varphi - \sigma^\varphi|_{H^r(U^\varphi)}, \tag{42}$$

where $h = \text{diam}(U^\varphi)$, $u^\varphi := u \circ \varphi^{-1}$, $\sigma^\varphi := \sigma \circ \varphi^{-1}$ and C_1 depends only on r, d, χ and L . Moreover, if X^φ is an s -determining set and $u \in H^s(\mathcal{M})$, then

$$\|Lu|_X - W_X u|_X\|_\infty \leq C_2 \lambda_s(U^\varphi, X^\varphi) h^{s-m-d/2} \|u\|_{K,U} \tag{43}$$

$$\leq C_3 \lambda_s(U^\varphi, X^\varphi) \mathcal{E}_s(U^\varphi) h^{s-m-d/2} \|u^\varphi\|_{H^s(U^\varphi)}, \tag{44}$$

where C_2, C_3 depend in addition on $K, \widehat{\mathcal{A}}, \widehat{\Gamma}$ and c .

Proof By Sobolev embedding, the condition $r > m + d/2$ ensures that $u \in C^m(\mathcal{M})$, hence Lu is well defined as a continuous function on \mathcal{M} as soon as $u \in H^r(\mathcal{M})$. Since U^φ is a Lipschitz domain, it follows that $\mathcal{E}_s(U^\varphi) < \infty$, and Lemma 9 shows that K^φ is a reproducing kernel for $H^s(U^\varphi)$. Since $s > m + d/2$, $H^s(U^\varphi)$ is embedded into $C^m(\mathcal{M})$. Moreover, $\sigma^\varphi \in H^r(U^\varphi)$ as a linear combination of the functions $K^\varphi(\cdot, x_j)$, $j = 1, \dots, n$.

In view of (40) and (41), the i -th component of the vector $Lu|_X - W_X u|_X$ has the form

$$Lu(x_i) - L\sigma(x_i) = L^\varphi u^\varphi(x_i^\varphi) - L^\varphi \sigma^\varphi(x_i^\varphi),$$

where $x_i^\varphi = \varphi(x_i)$. Since $(u^\varphi - \sigma^\varphi)|_{X^\varphi} = 0$, the sampling inequality (36) implies

$$|L^\varphi u^\varphi(x_i^\varphi) - L^\varphi \sigma^\varphi(x_i^\varphi)| \leq C \lambda_r(U^\varphi, X^\varphi) h^{r-m-d/2} |u^\varphi - \sigma^\varphi|_{H^r(U^\varphi)},$$

where C depends only on r, d, χ and the constants in (17), which implies (42).

In the case $r = s$ the condition that $K(\cdot, x) \in H^s(\mathcal{M})$ for all $x \in \mathcal{M}$ is satisfied since K is a reproducing kernel for $H^s(\mathcal{M})$, and we have by Lemma 9,

$$|u^\varphi - \sigma^\varphi|_{H^s(U^\varphi)} \leq \|u^\varphi - \sigma^\varphi\|_{H^s(U^\varphi)} \leq C \|u - \sigma\|_{K,U},$$

where C depends only on $K, \widehat{\mathcal{A}}, \widehat{\Gamma}$ and c . Then the minimum norm property (14) of the kernel interpolant implies $\|u - \sigma\|_{K,U} \leq \|u\|_{K,U}$, and (43) follows.

Finally, by Lemma 9, $\|u\|_{K,U} \leq C \mathcal{E}_s(U^\varphi) \|u^\varphi\|_{H^s(U^\varphi)}$, where C depends only on $K, \widehat{\mathcal{A}}, \widehat{\Gamma}, c$ and s , which implies (44). □

Different types of local error bounds for kernel based numerical differentiation can be found in [25, 27].

Note that for an operator L and kernel K satisfying the hypotheses of Lemma 5, the estimate (42) holds, thanks to Lemma 6, for all r satisfying $2\kappa + d/2 < r < 2s - d/2$ such that $r - s$ is a multiple of 2κ . Hence, it holds in this case for all integer r with $2\kappa + d/2 < r \leq s + 2\kappa$.

5 Error bounds

The discrete solution \hat{u} is well-defined by (26) for any node set X with subsets X_ℓ such that $\bigcup_{\ell=1}^m X_\ell = X$ as soon as L is positive and self-adjoint with respect to the

inner product defined by the reproducing kernel K for $H^s(\mathcal{M})$ with $s > \kappa + d/2$. However, in order to provide an estimate of the error of \hat{u} ,

$$\|\hat{u} - u\|_X \leq \dots \tag{45}$$

we will make a number of additional assumptions. In particular, we will need to assume that

$$s \text{ is an integer satisfying } s > 2\kappa + d/2, \tag{46}$$

rather than allowing any real $s > \kappa + d/2$. This restriction comes from an application of Lemma 12 in the proof of Theorem 1.

As in Section 2.1, we denote by $\|\cdot\|_{H^s(\mathcal{M})}$ the norm of $H^s(\mathcal{M})$ associated with a fixed finite smooth atlas $\hat{\mathcal{A}} = \{(\hat{U}_k, \hat{\varphi}_k)\}_{k=1}^{\hat{n}}$ and a smooth partition of unity $\hat{\Gamma} = \{\hat{\gamma}_k\}_{k=1}^{\hat{n}}$ subordinate to it.

We assume that the sets X_ℓ of the system \mathcal{X} satisfy

$$X_\ell = X \cap U_\ell, \quad \ell = 1, \dots, m, \tag{47}$$

for a finite smooth atlas $\mathcal{A} = \{(U_\ell, \varphi_\ell)\}_{\ell=1}^m$ of \mathcal{M} , such that:

- (A1) \mathcal{A} is c -admissible with respect to $\hat{\mathcal{A}}$ and $\hat{\Gamma}$, for some $c = c_{\mathcal{A}} > 0$.
- (A2) Each $U_\ell^\varphi := \varphi_\ell(U_\ell)$ is bounded and star-shaped with respect to a ball $B_\ell \subset \mathbb{R}^d$. Thus, the following quantity is finite:

$$\chi_{\mathcal{A}} := \max_{\ell=1, \dots, m} \chi(U_\ell^\varphi),$$

where $\chi(\Omega)$ denotes the chunkiness parameter of Ω , as defined in Section 4.2.

- (A3) For all ℓ and p such that $U_p \cap U_\ell \neq \emptyset$, the set $\varphi_\ell(X_p \cap X_\ell)$ is an $(s + \kappa)$ -determining set. In other words, $\lambda_{s+\kappa}(\mathcal{A}, X) < \infty$, where

$$\lambda_r(\mathcal{A}, X) := \max_{1 \leq \ell \leq m} \max_{i \in I_\ell} \lambda_r(U_\ell^\varphi, \varphi_\ell(X_i \cap X_\ell)), \quad I_\ell := \{i : U_i \cap U_\ell \neq \emptyset\}, \quad r \in \mathbb{Z}_+.$$

Condition (A3) may be weakened, see Remark 3 below.

Note that these conditions can be taken into account when selecting the sets X_ℓ . For example, we may choose $U_\ell = \hat{\varphi}_k^{-1}(B_\ell)$ for suitable balls $B_\ell \subset \hat{\varphi}_k(\hat{U}_k^c)$ and $1 \leq k \leq \hat{n}$, such that U_ℓ and U_p overlap significantly if $U_\ell \cap U_p \neq \emptyset$, and define the subsets X_ℓ of X as $X_\ell = X \cap U_\ell$. If we first select the system \mathcal{X} , then we need to make sure that the intersections $X_\ell \cap X_p$ are sufficiently big when non-empty to ensure the existence of a suitable atlas \mathcal{A} . In this case Condition (A3') of Remark 3 is significantly easier to fulfill than (A3).

In addition to the parameters $c_{\mathcal{A}} > 0$, $\chi_{\mathcal{A}} < \infty$ and $\lambda_{s+\kappa}(\mathcal{A}, X) < \infty$ of the assumptions (A1)–(A3), we now define several further quantities needed in the estimate. Since by (47) the sets X_ℓ are determined by X and \mathcal{A} , we do not indicate in the notation when these quantities depend on $\{X_\ell\}_{\ell=1}^m$.

- As the main parameter, against which the error will be measured, we will use

$$h_{\mathcal{A}} = \max_{1 \leq \ell \leq m} h_{\ell},$$

where h_{ℓ} is the diameter of the smallest open ball in \mathbb{R}^d containing U_{ℓ}^{φ} .

- Furthermore, we set

$$\nu_{X, \mathcal{A}} := \max_{1 \leq \ell \leq m} n_{\ell},$$

where $n_{\ell} = \#X_{\ell}$ as in Section 3.

- We denote by δ_{ℓ} the *separation distance* of the set X_{ℓ} in U_{ℓ} , that is, the largest $\delta > 0$ such that the open balls of radius δ centered at $\varphi_{\ell}(x_j)$ for all $j \in J_{\ell}$ are pairwise disjoint and contained in U_{ℓ}^{φ} ,

$$\delta_{\ell} := \min \left\{ \text{dist}(X_{\ell}^{\varphi}, \partial U_{\ell}^{\varphi}), \frac{1}{2} \min_{j \in J_{\ell}} \text{dist}(\varphi_{\ell}(x_j), X_{\ell}^{\varphi} \setminus \{\varphi_{\ell}(x_j)\}) \right\}, \quad \ell = 1, \dots, n, \tag{48}$$

where $X_{\ell}^{\varphi} := \varphi_{\ell}(X_{\ell})$.

- To measure the *quasi-uniformity* of \mathcal{A} and X , we define

$$q_{\mathcal{A}} := \max_{1 \leq i, j \leq m} \frac{h_i}{h_j} = \max_{1 \leq \ell \leq m} \frac{h_{\mathcal{A}}}{h_{\ell}}, \quad q_{X, \mathcal{A}} := \max_{1 \leq \ell \leq m} \frac{h_{\mathcal{A}}}{2n_{\ell}^{1/d} \delta_{\ell}}.$$

Note that

$$q_{\mathcal{A}} < q_{X, \mathcal{A}} \tag{49}$$

since $n_{\ell} \delta_{\ell}^d < (\frac{h_{\ell}}{2})^d$ for all ℓ , which is clear from the comparison of the volume of the union of the balls in the definition of δ_{ℓ} with the volume of a ball of diameter h_{ℓ} containing U_{ℓ}^{φ} .

- It follows from (A2) that the domains U_{ℓ}^{φ} satisfy the Lipschitz condition. For each ℓ , we choose a Lipschitz cover \mathcal{L} of $\partial U_{\ell}^{\varphi}$ and consider $P_{\ell} = P_{\mathcal{L}}$, $M_{\ell} = M_{\mathcal{L}}$, $\tau_{\ell} = \tau_{\mathcal{L}}$, as defined in Section 4.2. Let

$$P_{\mathcal{A}} := \max_{\ell=1, \dots, n} P_{\ell}, \quad M_{\mathcal{A}} := \max_{\ell=1, \dots, n} M_{\ell}, \quad \tau_{\mathcal{A}} := \min_{\ell=1, \dots, n} \tau_{\ell},$$

and

$$\mathcal{E}_r(\mathcal{A}) := \max_{\ell=1, \dots, n} \mathcal{E}_r(U_{\ell}^{\varphi}), \quad r \in \mathbb{Z}_+.$$

- Finally, we choose a smooth partition of unity $\Gamma = \{\gamma_{\ell}\}_{\ell=1}^n$ subordinate to \mathcal{A} such that

$$\gamma_{\ell} \in C^{\infty}(\mathcal{M}), \quad \gamma_{\ell} \geq 0, \quad \text{supp } \gamma_{\ell} \subset U_{\ell}, \quad \sum_{\ell=1}^n \gamma_{\ell} = 1, \tag{50}$$

and set

$$\eta_r(\mathcal{A}) := \max_{1 \leq \ell \leq m} \max_{|\alpha| \leq r} \|\partial^{\alpha} g_{\ell}\|_{L^{\infty}(\mathbb{R}^d)}, \quad r \in \mathbb{Z}_+, \tag{51}$$

where $g_\ell : \mathbb{R}^d \rightarrow \mathbb{R}$ is defined by

$$g_\ell(y) := \begin{cases} (\gamma_\ell \circ \varphi_\ell^{-1})(y_\ell + h_\ell y), & \text{if } y_\ell + h_\ell y \in U_\ell^\varphi, \\ 0, & \text{otherwise,} \end{cases}$$

with $y_\ell \in \mathbb{R}^d$ being the center of the ball B_ℓ in (A2).

Although a subordinate partition of unity Γ always exists and corresponding $\eta_r(\mathcal{A})$ is finite, we provide an example of how a suitable Γ may be constructed and $\eta_r(\mathcal{A})$ estimated under an easy to check condition on \mathcal{A} .

Example 1 According to (A2), each U_ℓ^φ contains a ball B_ℓ with radius ρ_ℓ and center y_ℓ , such that $h_\ell \leq \chi_{\mathcal{A}} \rho_\ell$. We assume that there exists a positive $\alpha < 1$, such that

$$\text{for each } x \in \mathcal{M} \text{ There is an } \ell \text{ with } x \in U_\ell \text{ and } \|\varphi_\ell(x) - y_\ell\|_2 \leq \alpha \rho_\ell. \quad (52)$$

Let $\Psi : \mathbb{R}^d \rightarrow \mathbb{R}$ be an infinitely differentiable bump function supported on the unit ball of \mathbb{R}^d , for example $\Psi(y) = \psi(\|y\|_2^2)$ for some $\psi \in C^\infty[0, \infty)$, with $\psi(0) = 1$, $\psi^{(k)}(0) = 0$, $k \in \mathbb{N}$, $\psi(t) > 0$ and $\psi'(t) \leq 0$ for $0 \leq t < 1$, and $\psi(t) = 0$ for $t \geq 1$. We set

$$\tilde{\gamma}_\ell(x) := \begin{cases} \Psi\left(\frac{\varphi_\ell(x) - y_\ell}{\rho_\ell}\right), & x \in U_\ell, \\ 0, & x \in \mathcal{M} \setminus U_\ell, \end{cases}$$

and

$$\gamma_\ell(x) = \frac{\tilde{\gamma}_\ell(x)}{\bar{\gamma}(x)}, \quad \ell = 1, \dots, m, \quad \text{with } \bar{\gamma}(x) := \sum_{i=1}^m \tilde{\gamma}_i(x).$$

Then

$$\bar{\gamma}(x) \geq \psi(\alpha^2) > 0, \quad x \in \mathcal{M},$$

each function g_ℓ is supported in the ball of radius ρ_ℓ/h_ℓ centered at the origin, and for y in this ball,

$$g_\ell(y) = \frac{\Psi(h_\ell y / \rho_\ell)}{\bar{\gamma}(\varphi_\ell^{-1}(y_\ell + h_\ell y))}.$$

Here

$$\begin{aligned} \bar{\gamma}(\varphi_\ell^{-1}(y_\ell + h_\ell y)) &= \sum_{i \in I_\ell(y)} \Psi\left(\frac{(\varphi_i \circ \varphi_\ell^{-1})(y_\ell + h_\ell y) - y_i}{\rho_i}\right), \\ I_\ell(y) &:= \{i : \varphi_\ell^{-1}(y_\ell + h_\ell y) \in U_i\} \subset \{i : U_i \cap U_\ell \neq \emptyset\}. \end{aligned}$$

Then by the Leibniz and the chain rules it is easy to see that $\eta_r(\mathcal{A})$ can be bounded above in terms of (the upper bounds for)

$$\chi_{\mathcal{A}}, \quad \mu_{\mathcal{A}}, \quad q_{\mathcal{A}} \quad \text{and} \quad 1/\psi(\alpha^2),$$

as well as the constant

$$\max_{i,j=1,\dots,\hat{n}} \max_{|\alpha|\leq r} \|\partial^\alpha(\hat{\varphi}_i \circ \hat{\varphi}_j^{-1})\|_{L^\infty(\hat{\varphi}_j(\hat{U}_j))}$$

that depends only on the atlas $\hat{\mathcal{A}}$ that defines (8). Note that more general domains e.g. unions of ellipsoids may be used instead of balls as supports of the partition of unity functions γ_ℓ if we want to estimate the smallest possible constant $\eta_r(\mathcal{A})$ for a given choice of U_ℓ and $X_\ell = X \cap U_\ell$ and given r . The size of $\eta_r(\mathcal{A})$ for $r = s + \kappa$ influences the constants in the error bounds below.

We stress that in contrast to the partition of unity methods [5, 35, 40], Γ is not used in the computation of the discrete solution $\hat{u} \approx u|_X$, and we only need to choose a partitions of unity in order to prove the error bounds.

Theorem 1 *Let L be an elliptic differential operator of order 2κ with smooth coefficients and trivial null space, and let K be a reproducing kernel for a Sobolev space $H^s(\mathcal{M})$ with an integer s satisfying $s > 2\kappa + d/2$, such that L is positive and self-adjoint with respect to the inner product defined by K . Assume that a set of nodes X and an atlas $\mathcal{A} = \{(U_\ell, \varphi_\ell)\}_{\ell=1}^m$ satisfy (A1)–(A3). For any $f \in H^{s-\kappa}(\mathcal{M})$, let $u \in H^{s+\kappa}(\mathcal{M})$ be the solution of $Lu = f$, and let \hat{u} be the discrete approximate solution determined by (26). Then there exists a function $\tilde{u} \in H^{s+2\kappa}(\mathcal{M})$ such that $\tilde{u}|_X = \hat{u}$ and for all $0 \leq r < s - \kappa$,*

$$\|u - \tilde{u}\|_{H^{2\kappa+r}(\mathcal{M})} \leq C_1 h_{\mathcal{A}}^{s-2\kappa-d-r} \|u\|_{H^s(\mathcal{M})} + C_2 h_{\mathcal{A}}^{s-\kappa-d/2-r} \|u\|_{H^{s+\kappa}(\mathcal{M})}, \tag{53}$$

where $C_1, C_2 < \infty$ are independent of f, u and $h_{\mathcal{A}}$. If $\mu_{\mathcal{A}} \leq \mu, \lambda_{s+\kappa}(\mathcal{A}, X) \leq \lambda, \chi_{\mathcal{A}} \leq \chi, \nu_{X,\mathcal{A}} \leq \nu, q_{X,\mathcal{A}} \leq q, \eta_{s+\kappa}(\mathcal{A}) \leq \eta, P_{\mathcal{A}} \leq P, M_{\mathcal{A}} \leq M, \tau_{\mathcal{A}} \geq \tau, c_{\mathcal{A}} \geq c$, for some positive real $\mu, \lambda, \chi, \nu, q, \eta, P, M, \tau, c$, then (53) holds with C_1, C_2 depending only on $\mu, \lambda, \chi, \nu, q, \eta, P, M, \tau, c$, in addition to $\mathcal{M}, L, K, \hat{\mathcal{A}}$ and $\hat{\Gamma}$. Moreover,

$$\|u|_X - \hat{u}\|_\infty \leq \|u - \tilde{u}\|_{C(\mathcal{M})} \leq C_1 h_{\mathcal{A}}^{s-2\kappa-d-r_0} \|u\|_{H^s(\mathcal{M})} + C_2 h_{\mathcal{A}}^{s-\kappa-d/2-r_0} \|u\|_{H^{s+\kappa}(\mathcal{M})}, \tag{54}$$

where $r_0 = \max\{0, \lfloor \frac{d}{2} \rfloor - 2\kappa + 1\}$, with the same properties of C_1, C_2 .

Proof Recall that we assume that $\mu_{\mathcal{A}} \leq \mu, \lambda_{s+\kappa}(\mathcal{A}, X) \leq \lambda, c_{\mathcal{A}} \geq c, \chi_{\mathcal{A}} \leq \chi, \nu_{X,\mathcal{A}} \leq \nu, q_{X,\mathcal{A}} \leq q, \eta_{s+\kappa}(\mathcal{A}) \leq \eta$. Then also $\lambda_r(\mathcal{A}, X) \leq \lambda$ for all $r \leq s + \kappa$, in particular for $r = s$ and $r = s - \kappa$. The constants denoted by C, C_1, C_2, \dots in the proof will be independent of $f, u, h_{\mathcal{A}}$ and the Lipschitz cover parameters $P_{\mathcal{A}}, M_{\mathcal{A}}, \tau_{\mathcal{A}}$. They in general depend on \mathcal{M}, L, K , the atlas $\hat{\mathcal{A}}$ and the partition of unity $\hat{\Gamma}$ that we use to fix the Sobolev norms, as well as on $\mu, \lambda, \chi, \nu, q, \eta, c$. The constants in (53) and (54) will also depend on P, M, τ via the final application of Lemma 10 to (71). We assume without loss of generality that $h_{\mathcal{A}} \leq 1$.

Since $s > 2\kappa + d/2$, we obtain by (44) and (A1)–(A3),

$$\|W_\ell u|_{X_\ell} - Lu|_{X_\ell}\|_\infty \leq C \mathcal{E}_s(U_\ell^\varphi) h_{\mathcal{A}}^{s-2\kappa-d/2} \|u \circ \varphi_\ell^{-1}\|_{H^s(U_\ell^\varphi)}, \quad \ell = 1, \dots, m. \tag{55}$$

Since, in view of (26) and (28),

$$\|WM\hat{u} - Mf|_X\|_2^2 \leq \|WMu|_X - Mf|_X\|_2^2 = \sum_{\ell=1}^m \|W_\ell u|_{X_\ell} - Lu|_{X_\ell}\|_2^2,$$

we obtain by (55) and Lemma 7,

$$\varepsilon_1 := \|WM\hat{u} - Mf|_X\|_2 \leq C\mathcal{E}_s(\mathcal{A})h_{\mathcal{A}}^{s-2\kappa-d/2}\|u\|_{H^s(\mathcal{M})}. \tag{56}$$

We will construct a function $\tilde{u} \in H^{s+\kappa}(\mathcal{M})$ such that $\tilde{u}|_X = \hat{u}$, and estimate its distance to u in Sobolev spaces of lower order as in (53). We define local interpolants \tilde{u}_ℓ on the sets X_ℓ and then combine them together with the help of a partition of unity.

For each $\ell = 1, \dots, m$, let

$$\tilde{u}_\ell(x) = \sum_{j \in J_\ell} c_j K(x, x_j),$$

where the coefficients c_j are uniquely determined by the interpolation conditions

$$\tilde{u}_\ell|_{X_\ell} = \hat{u}|_{J_\ell}. \tag{57}$$

By (24), $L\tilde{u}_\ell|_{X_\ell} = W_\ell\tilde{u}_\ell|_{X_\ell}$. Hence

$$L\tilde{u}_\ell|_{X_\ell} = W_\ell\hat{u}|_{J_\ell}. \tag{58}$$

Moreover, by Lemma 6, $\tilde{u}_\ell \in H^{s+2\kappa}(\mathcal{M})$. By (2) and Lemmas 3 and 5,

$$\|\tilde{u}_\ell\|_{H^{s+\kappa}(\mathcal{M})} \leq C\|L\tilde{u}_\ell\|_{K_L}. \tag{59}$$

It follows from (58) and (28) that

$$\sum_{\ell=1}^m \|L\tilde{u}_\ell|_{X_\ell} - Lu|_{X_\ell}\|_2^2 = \sum_{\ell=1}^m \|W_\ell\hat{u}|_{J_\ell} - Lu|_{X_\ell}\|_2^2 = \|WM\hat{u} - Mf|_X\|_2^2 = \varepsilon_1^2. \tag{60}$$

Our next goal is to estimate the K_L -norm of $L\tilde{u}_\ell$. Note that due to (15), $\|L\tilde{u}_\ell\|_{K_L} = \|L\tilde{u}_\ell\|_{K_{L,U_\ell}}$ since $X_\ell \subset U_\ell$. Let

$$u_\ell \in \text{span}\{K(\cdot, x_j) : j \in J_\ell\}$$

be the kernel sum determined by the interpolation conditions

$$Lu_\ell|_{X_\ell} = Lu|_{X_\ell}.$$

Then Lu_ℓ is the K_L -kernel interpolant of $f = Lu$. By Lemma 5, K_L is a reproducing kernel for $H^{s-\kappa}(\mathcal{M})$, and by Lemma 9 and (A2), $H_{K_L}(U_\ell) = H^{s-\kappa}(U_\ell^\varphi)$. Hence, by (15) and the minimum norm property (14), since $X_\ell \subset U_\ell$,

$$\|Lu_\ell\|_{K_L} = \|Lu_\ell\|_{K_L, U_\ell} \leq \|f\|_{K_L, U_\ell},$$

and by Lemma 9,

$$\|f\|_{K_L, U_\ell} \leq C\mathcal{E}_{s-\kappa}(U_\ell^\varphi)\|f \circ \varphi_\ell^{-1}\|_{H^{s-\kappa}(U_\ell^\varphi)}.$$

It follows by Lemma 7 that

$$\sum_{\ell=1}^m \|Lu_\ell\|_{K_L}^2 \leq C\mathcal{E}_{s-\kappa}^2(\mathcal{A})\|f\|_{H^{s-\kappa}(\mathcal{M})}^2. \tag{61}$$

Consider the functions $v_\ell = L\tilde{u}_\ell - Lu_\ell$, $\ell = 1, \dots, m$, that satisfy

$$\sum_{\ell=1}^m \|v_\ell|_{X_\ell}\|_2^2 \leq \varepsilon_1^2,$$

thanks to (60). Let

$$\psi_\ell = \sum_{j \in J_\ell} v_\ell(x_j) \Psi_{j, \delta_\ell}^\ell, \quad \Psi_{j, \delta}^\ell(x) := \begin{cases} \Psi\left(\frac{\varphi_\ell(x) - \varphi_\ell(x_j)}{\delta}\right), & x \in U_\ell, \\ 0, & x \in \mathcal{M} \setminus U_\ell, \end{cases}$$

where $\Psi(y) = \psi(\|y\|_2^2)$ is a radially symmetric bump function in $C^\infty(\mathbb{R}^d)$ supported on the unit ball, as in Example 1, and δ_ℓ is defined in (48). Then the supports of the functions $\Psi_{j, \delta_\ell}^\ell$, $j \in J_\ell$, are pairwise disjoint and hence

$$\psi_\ell|_{X_\ell} = v_\ell|_{X_\ell}$$

and

$$\|\psi_\ell \circ \varphi_\ell^{-1}\|_{H^r(U_\ell^\varphi)} = \delta_\ell^{-r+d/2} \|\Psi|_{H^r(\mathbb{R}^d)}\| v_\ell|_{X_\ell}\|_2, \quad r \in \mathbb{Z}_+.$$

Since $\delta_\ell^{-1} < 2v^{1/d}qh_{\mathcal{A}}^{-1}$ and $\delta_\ell < h_{\mathcal{A}} \leq 1$, we obtain

$$\begin{aligned} \sum_{\ell=1}^m \|\psi_\ell \circ \varphi_\ell^{-1}\|_{H^{s-\kappa}(U_\ell^\varphi)}^2 &\leq \sum_{r=0}^{s-\kappa} \|\Psi\|_{H^r(\mathbb{R}^d)}^2 \sum_{\ell=1}^m \delta_\ell^{-2r+d} \|v_\ell|_{X_\ell}\|_2^2 \\ &\leq C\varepsilon_1^2 \|\Psi\|_{H^{s-\kappa}(\mathbb{R}^d)}^2 h_{\mathcal{A}}^{-2(s-\kappa)+d}. \end{aligned}$$

By (15), the minimum norm property (14) of v_ℓ as the K_L -kernel interpolant of $\psi_\ell \in H_{K_L}(U_\ell)$, and by Lemma 9,

$$\|v_\ell\|_{K_L} = \|v_\ell\|_{K_L, U_\ell} \leq \|\psi_\ell\|_{K_L, U_\ell} \leq C\mathcal{E}_{s-\kappa}(U_\ell^\varphi)\|\psi_\ell \circ \varphi_\ell^{-1}\|_{H^{s-\kappa}(U_\ell^\varphi)},$$

and it follows from the above that

$$\sum_{\ell=1}^m \|v_\ell\|_{K_L}^2 \leq C\mathcal{E}_{s-\kappa}^2(\mathcal{A})\varepsilon_1^2 h_{\mathcal{A}}^{-2(s-\kappa)+d}.$$

Combining this with (61), we obtain for $L\tilde{u}_\ell = Lu_\ell + v_\ell$,

$$\left(\sum_{\ell=1}^m \|L\tilde{u}_\ell\|_{K_L}^2\right)^{1/2} \leq \mathcal{E}_{s-\kappa}(\mathcal{A})(C_1\|f\|_{H^{s-\kappa}(\mathcal{M})} + C_2\varepsilon_1 h_{\mathcal{A}}^{-s+\kappa+d/2}). \tag{62}$$

We set

$$\tilde{u} := \sum_{\ell=1}^m \gamma_\ell \tilde{u}_\ell,$$

where $\{\gamma_\ell\}_{\ell=1}^m$ is the smooth partition of unity (50) subordinate to \mathcal{A} . Note that $\tilde{u} \in H^{s+2\kappa}(\mathcal{M})$, which follows from the same property of \tilde{u}_ℓ . It follows from (57) and (50) that

$$\tilde{u}|_X = \hat{u}. \tag{63}$$

We now use (62) and the properties of the partition of unity in order to obtain an estimate for $\|L\tilde{u}\|_{H^{s-\kappa}(\mathcal{M})}$. By Lemma 7,

$$\|L\tilde{u}\|_{H^{s-\kappa}(\mathcal{M})}^2 \leq C \sum_{\ell=1}^m \|L\tilde{u} \circ \varphi_\ell^{-1}\|_{H^{s-\kappa}(U_\ell^\varphi)}^2.$$

For each $\ell = 1, \dots, m$,

$$\|L\tilde{u} \circ \varphi_\ell^{-1}\|_{H^{s-\kappa}(U_\ell^\varphi)} \leq \|L\tilde{u}_\ell \circ \varphi_\ell^{-1}\|_{H^{s-\kappa}(U_\ell^\varphi)} + \|L(\tilde{u} - \tilde{u}_\ell) \circ \varphi_\ell^{-1}\|_{H^{s-\kappa}(U_\ell^\varphi)}.$$

By Lemma 9 and (15),

$$\|L\tilde{u}_\ell \circ \varphi_\ell^{-1}\|_{H^{s-\kappa}(U_\ell^\varphi)} \leq C\|L\tilde{u}_\ell\|_{K_L},$$

and we will be able to estimate the terms of this type by applying (62). It follows from (17) and the Leibniz rule that

$$\|L(\tilde{u} - \tilde{u}_\ell) \circ \varphi_\ell^{-1}\|_{H^{s-\kappa}(U_\ell^\varphi)} \leq C\|(\tilde{u} - \tilde{u}_\ell) \circ \varphi_\ell^{-1}\|_{H^{s+\kappa}(U_\ell^\varphi)}.$$

By the definition of \tilde{u} ,

$$\tilde{u} - \tilde{u}_\ell = \sum_{p \in I_\ell \setminus \{\ell\}} \gamma_p (\tilde{u}_p - \tilde{u}_\ell) \text{ in } U_\ell, \quad I_\ell = \{i : U_i \cap U_\ell \neq \emptyset\}.$$

Applying the Leibniz rule again, we obtain for $|\alpha| \leq s + \kappa$,

$$\partial^\alpha \left((\tilde{u} - \tilde{u}_\ell) \circ \varphi_\ell^{-1} \right) = \sum_{p \in I_\ell \setminus \{\ell\}} \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} \partial^{\alpha-\beta} (\gamma_p \circ \varphi_\ell^{-1}) \partial^\beta \left((\tilde{u}_p - \tilde{u}_\ell) \circ \varphi_\ell^{-1} \right) \text{ in } U_\ell^\varphi$$

By (51),

$$\|\partial^{\alpha-\beta} (\gamma_p \circ \varphi_\ell^{-1})\|_{L^\infty(U_\ell^\varphi)} = h_\ell^{|\beta-\alpha|} \|\partial^{\alpha-\beta} g_\ell\|_{L^\infty(\mathbb{R}^d)} \leq h_\ell^{|\beta-\alpha|} \eta_{s+\kappa}(\mathcal{A}) \leq \eta h_\ell^{|\beta-\alpha|}.$$

Hence

$$\|\partial^\alpha \left((\tilde{u} - \tilde{u}_\ell) \circ \varphi_\ell^{-1} \right)\|_{L^2(U_\ell^\varphi)} \leq C \sum_{p \in I_\ell \setminus \{\ell\}} \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} h_\ell^{|\beta-\alpha|} \|\partial^\beta \left((\tilde{u}_p - \tilde{u}_\ell) \circ \varphi_\ell^{-1} \right)\|_{L^2(U_\ell^\varphi)}.$$

Let $p \in I_\ell \setminus \{\ell\}$. By (57),

$$\tilde{u}_p|_{X_p \cap X_\ell} = \hat{u}|_{J_p \cap J_\ell} = \tilde{u}_\ell|_{X_p \cap X_\ell}.$$

Hence, it follows from (35) and (A3) that for $|\beta| < s + \kappa$,

$$\|\partial^\beta \left((\tilde{u}_p - \tilde{u}_\ell) \circ \varphi_\ell^{-1} \right)\|_{L^2(U_\ell^\varphi)} \leq C h_\ell^{s+\kappa-|\beta|} |(\tilde{u}_p - \tilde{u}_\ell) \circ \varphi_\ell^{-1}|_{H^{s+\kappa}(U_\ell^\varphi)}. \tag{64}$$

By Lemma 7,

$$|(\tilde{u}_p - \tilde{u}_\ell) \circ \varphi_\ell^{-1}|_{H^{s+\kappa}(U_\ell^\varphi)} \leq C \|\tilde{u}_p - \tilde{u}_\ell\|_{H^{s+\kappa}(\mathcal{M})}.$$

By (59),

$$\|\tilde{u}_p - \tilde{u}_\ell\|_{H^{s+\kappa}(\mathcal{M})} \leq C (\|L\tilde{u}_p\|_{K_L} + \|L\tilde{u}_\ell\|_{K_L}).$$

By combining these estimates, since $h_{\mathcal{A}} \leq 1$ and hence $h_\ell^{s+\kappa-|\alpha|} \leq 1$, we obtain

$$\|(\tilde{u} - \tilde{u}_\ell) \circ \varphi_\ell^{-1}\|_{H^{s+\kappa}(U_\ell^\varphi)} \leq C \sum_{p \in I_\ell} \|L\tilde{u}_p\|_{K_L}. \tag{65}$$

This implies

$$\sum_{\ell=1}^m \|L(\tilde{u} - \tilde{u}_\ell) \circ \varphi_\ell^{-1}\|_{H^{s-\kappa}(U_\ell^\varphi)}^2 \leq C \sum_{\ell=1}^m \|L\tilde{u}_\ell\|_{K_L}^2.$$

Summarizing the estimates, we get

$$\|L\tilde{u}\|_{H^{s-\kappa}(\mathcal{M})} \leq C \left(\sum_{\ell=1}^m \|L\tilde{u}_\ell\|_{K_L}^2 \right)^{1/2}$$

and hence by (62),

$$\|L\tilde{u}\|_{H^{s-\kappa}(\mathcal{M})} \leq C_1 \|f\|_{H^{s-\kappa}(\mathcal{M})} + C_2 \varepsilon_1 h_{\mathcal{A}}^{-s+\kappa+d/2}. \tag{66}$$

Finally, we will estimate Sobolev norms of $Lu - L\tilde{u}$ by applying Lemma 11 locally, which in turn will give us estimates for $u - \tilde{u}$ thanks to (2). Since $X = \cup_{\ell=1}^m X_\ell$, it follows from (60) that

$$\|L\tilde{u}|_X - Lu|_X\|_2 \leq \left(\sum_{\ell=1}^m \|L\tilde{u}|_{X_\ell} - Lu|_{X_\ell}\|_2^2 \right)^{1/2} \leq \varepsilon_1 + \varepsilon_2, \tag{67}$$

where

$$\varepsilon_2 := \left(\sum_{\ell=1}^m \|L\tilde{u}|_{X_\ell} - L\tilde{u}_\ell|_{X_\ell}\|_2^2 \right)^{1/2}.$$

By (58) and (63),

$$L\tilde{u}_\ell|_{X_\ell} = W_\ell \hat{u}|_{J_\ell} = W_\ell \tilde{u}|_{X_\ell}.$$

By construction, \tilde{u}_ℓ is the kernel interpolant to \tilde{u} on X_ℓ , compare (57) and (63). Hence by (42),

$$\|L\tilde{u}|_{X_\ell} - L\tilde{u}_\ell|_{X_\ell}\|_\infty = \|L\tilde{u}|_{X_\ell} - W_\ell \tilde{u}|_{X_\ell}\|_\infty \leq Ch_\ell^{s-\kappa-d/2} |(\tilde{u} - \tilde{u}_\ell) \circ \varphi_\ell^{-1}|_{H^{s+\kappa}(U_\ell^\varphi)}.$$

In view of (65),

$$\varepsilon_2^2 \leq \nu \sum_{\ell=1}^m \|L\tilde{u}|_{X_\ell} - L\tilde{u}_\ell|_{X_\ell}\|_\infty^2 \leq Ch_{\mathcal{A}}^{2s-2\kappa-d} \sum_{\ell=1}^m \|L\tilde{u}_\ell\|_{K_L}^2.$$

and by (62) we get

$$\varepsilon_2 \leq \mathcal{E}_{s-\kappa}(\mathcal{A}) (C_1 h_{\mathcal{A}}^{s-\kappa-d/2} \|Lu\|_{H^{s-\kappa}(\mathcal{M})} + C_2 \varepsilon_1). \tag{68}$$

Let $v = L\tilde{u} - Lu$. Then $v \in H^{s-\kappa}(\mathcal{M})$ and

$$\varepsilon_3 := \|v\|_{H^{s-\kappa}(\mathcal{M})} \leq \|L\tilde{u}\|_{H^{s-\kappa}(\mathcal{M})} + \|Lu\|_{H^{s-\kappa}(\mathcal{M})}.$$

Hence by (66),

$$\varepsilon_3 \leq \mathcal{E}_{s-\kappa}(\mathcal{A}) (C_1 \|Lu\|_{H^{s-\kappa}(\mathcal{M})} + C_2 \varepsilon_1 h_{\mathcal{A}}^{-s+\kappa+d/2}). \tag{69}$$

By Lemma 11, for any integer r with $0 \leq r < s - \kappa$, and each $\ell = 1, \dots, m$,

$$|v \circ \varphi_\ell^{-1}|_{H^r(U_\ell^\varphi)} \leq Ch_\ell^{-r} (h_\ell^{d/2} \|v\|_{X_\ell} + h_\ell^{s-\kappa} |v \circ \varphi_\ell^{-1}|_{H^{s-\kappa}(U_\ell^\varphi)}).$$

Hence by Lemma 7,

$$\begin{aligned} \|v\|_{H^r(\mathcal{M})}^2 &\leq C \sum_{\ell=1}^m \|v \circ \varphi_\ell^{-1}\|_{H^r(U_\ell^\varphi)}^2 \\ &\leq C \left(\sum_{\ell=1}^m h_\ell^{d-2r} \|v\|_{X_\ell}^2 + h_{\mathcal{A}}^{2(s-\kappa-r)} \sum_{\ell=1}^m |v \circ \varphi_\ell^{-1}|_{H^{s-\kappa}(U_\ell^\varphi)}^2 \right) \\ &\leq C_1 h_{\mathcal{A}}^{d-2r} \|v\|_X^2 + C_2 h_{\mathcal{A}}^{2(s-\kappa-r)} \|v\|_{H^{s-\kappa}(\mathcal{M})}^2. \end{aligned}$$

By (67) and definitions of v and ε_3 , we get

$$\|Lu - L\tilde{u}\|_{H^r(\mathcal{M})} \leq C_1 h_{\mathcal{A}}^{d/2-r} (\varepsilon_1 + \varepsilon_2) + C_2 h_{\mathcal{A}}^{s-\kappa-r} \varepsilon_3.$$

It follows in view of (2) that for any $0 \leq r < s - \kappa$,

$$\|u - \tilde{u}\|_{H^{r+2\kappa}(\mathcal{M})} \leq C_1 h_{\mathcal{A}}^{d/2-r} (\varepsilon_1 + \varepsilon_2) + C_2 h_{\mathcal{A}}^{s-\kappa-r} \varepsilon_3. \tag{70}$$

By (56), (68) and (69),

$$\begin{aligned} \varepsilon_1 + \varepsilon_2 &\leq C_1 \mathcal{E}_s(\mathcal{A}) h_{\mathcal{A}}^{s-2\kappa-d/2} \|u\|_{H^s(\mathcal{M})} + C_2 \mathcal{E}_{s-\kappa}(\mathcal{A}) h_{\mathcal{A}}^{s-\kappa-d/2} \|Lu\|_{H^{s-\kappa}(\mathcal{M})}, \\ \varepsilon_3 &\leq \mathcal{E}_{s-\kappa}(\mathcal{A}) (C_1 \|Lu\|_{H^{s-\kappa}(\mathcal{M})} + C_2 \mathcal{E}_s(\mathcal{A}) h_{\mathcal{A}}^{-\kappa} \|u\|_{H^s(\mathcal{M})}). \end{aligned}$$

Hence by (70),

$$\|u - \tilde{u}\|_{H^{r+2\kappa}(\mathcal{M})} \leq \mathcal{E}_{s-\kappa}(\mathcal{A}) (C_1 \mathcal{E}_s(\mathcal{A}) h_{\mathcal{A}}^{s-2\kappa-r} \|u\|_{H^s(\mathcal{M})} + C_2 h_{\mathcal{A}}^{s-\kappa-r} \|Lu\|_{H^{s-\kappa}(\mathcal{M})}).$$

By using (2) again, we arrive at

$$\|u - \tilde{u}\|_{H^{r+2\kappa}(\mathcal{M})} \leq \mathcal{E}_{s-\kappa}(\mathcal{A}) (C_1 \mathcal{E}_s(\mathcal{A}) h_{\mathcal{A}}^{s-2\kappa-r} \|u\|_{H^s(\mathcal{M})} + C_2 h_{\mathcal{A}}^{s-\kappa-r} \|u\|_{H^{s+\kappa}(\mathcal{M})}), \tag{71}$$

which implies (53) in view of Lemma 10.

To show (54) we use (63) and Sobolev embedding of $H^{2\kappa+r}(\mathcal{M})$ into $C(\mathcal{M})$ as soon as $2\kappa + r > d/2$. It is easy to see that r_0 in (54) is the smallest nonnegative integer r satisfying this inequality. \square

Note that convergence in the norm of $H^{2\kappa+r}(\mathcal{M})$ as $h_{\mathcal{A}} \rightarrow 0$ follows from (53) only when $0 \leq r < s - 2\kappa - d$, thus under the assumption

$$s > 2\kappa + d,$$

which is stricter than (46), and the discrete convergence follows from (54) under the assumption that

$$s > \max\{2\kappa, \frac{d}{2} + 1\} + d.$$

In particular, in the discrete case in order for the power of $h_{\mathcal{A}}$ to be positive, we need

$$s > 2\kappa + d + r_0 = \max\{2\kappa + d, d + \lfloor \frac{d}{2} \rfloor + 1\},$$

which is equivalent to $s > \max\{2\kappa, \frac{d}{2} + 1\} + d$ since s is integer.

For example, for $\kappa = 1$ and $d \leq 3$ we obtain the Sobolev norm convergence with the order

$$\|u - \tilde{u}\|_{H^{2+r}(\mathcal{M})} = \mathcal{O}(h_{\mathcal{A}}^{s-d-2-r}) \quad \text{if } s \geq d + 3, \quad 0 \leq r \leq s - d - 3, \quad (72)$$

and the discrete norm convergence

$$\|u|_X - \hat{u}\|_{\infty} = \mathcal{O}(h_{\mathcal{A}}^{s-d-2}) \quad \text{if } s \geq d + 3. \quad (73)$$

Remark 2 The function \tilde{u} of the proof of Theorem 1 may be used for the approximate evaluation of the solution and derived quantities such as gradient at any points in \mathcal{M} , which however requires construction of a suitable partition of unity Γ . Instead, for the same purpose we may employ the local interpolation functions \tilde{u}_{ℓ} determined by (57). Indeed, since \tilde{u}_{ℓ} is a kernel interpolant to \tilde{u} on X_{ℓ} , the sampling inequality (36) applied to $v = (\tilde{u} - \tilde{u}_{\ell}) \circ \varphi_{\ell}^{-1}$ on $\Omega = U_{\ell}^{\varphi}$ with $r = s$ leads to the estimate

$$|\tilde{u}(x) - \tilde{u}_{\ell}(x)| \leq Ch_{\mathcal{A}}^{s-d/2} \|\tilde{u}\|_{H^s(\mathcal{M})}, \quad x \in U_{\ell},$$

where the factor C is independent of u and $h_{\mathcal{A}}$, compare the proof of (43) in the above. By (66) and (56) we have

$$\|\tilde{u}\|_{H^s(\mathcal{M})} \leq Ch_{\mathcal{A}}^{-\kappa} \|u\|_{H^s(\mathcal{M})}.$$

By taking into account (54), we arrive at the bound

$$|u(x) - \tilde{u}_{\ell}(x)| \leq C_1 h_{\mathcal{A}}^{s-2\kappa-d-r_0} \|u\|_{H^s(\mathcal{M})} + C_2 h_{\mathcal{A}}^{s-\kappa-d/2-r_0} \|u\|_{H^{s+\kappa}(\mathcal{M})}, \quad x \in U_{\ell}, \quad (74)$$

which shows that \tilde{u}_{ℓ} may be used as approximation of u on U_{ℓ} as soon as $s > \max\{2\kappa, \frac{d}{2} + 1\} + d$.

Remark 3 Condition (A3) prohibits small non-empty intersections $X_p \cap X_{\ell}$ because the images of any such set under φ_p and φ_{ℓ} are required to be $(s + \kappa)$ -determining sets. In fact, we only need that sufficiently many intersections have this property. More precisely, we may replace (A3) by the following assumption:

(A3') Given $\sigma \in \mathbb{N}$, $\chi < \infty$, $R < \infty$ and $\lambda < \infty$, assume that for each pair ℓ, p with $U_{\ell} \cap U_p \neq \emptyset$, there is a set $U_{\ell,p} \subset \mathcal{M}$ and a chain $U_{p_0}, U_{p_1}, \dots, U_{p_S}$, with $p_0 = \ell, p_S = p$ and $S \leq \sigma$, such that

- $\bigcup_{i=0}^S U_{p_i} \subset U_{\ell,p} \subset \hat{U}_k^c$ for some $1 \leq k \leq \hat{n}$,
- $\chi(\hat{\varphi}_k(U_{\ell,p})) \leq \chi$,
- $\text{diam}(\hat{\varphi}_k(U_{\ell,p})) \leq R \max \{ \text{diam}(U_\ell^\varphi), \text{diam}(U_p^\varphi) \}$,
- $\lambda_{s+\kappa}(\hat{\varphi}_k(U_{\ell,p}), \hat{\varphi}_k(X_{p_i} \cap X_{p_{i-1}})) \leq \lambda, i = 1, \dots, S,$ and
- in the case $\ell = p$ we choose $S = 1, U_{\ell,p} = U_\ell$ and k such that $\varphi_\ell = \hat{\varphi}_k|_{U_\ell}$.

The last condition ensures that (A2) follows from (A3'), with $\chi_{\mathcal{A}} \leq \chi$, and that $\lambda_{s+\kappa}(U_\ell^\varphi, X_\ell^\varphi) \leq \lambda$. If we assume (A3') instead of (A2) and (A3), then Theorem 1 still holds, with C_1 and C_2 depending in addition on σ and R . Indeed, we apply (A3) in the proof twice, namely to show (55) and (64). While (55) uses the case $\ell = p$, where there is no difference between (A3') and (A3), in order to replace (64) we write

$$\tilde{u}_p - \tilde{u}_\ell = \sum_{i=1}^S \tilde{u}_{p_i} - \tilde{u}_{p_{i-1}},$$

and deduce

$$\begin{aligned} \|\partial^\beta((\tilde{u}_p - \tilde{u}_\ell) \circ \varphi_\ell^{-1})\|_{L^2(U_\ell^\varphi)} &\leq C \|\partial^\beta((\tilde{u}_p - \tilde{u}_\ell) \circ \hat{\varphi}_k^{-1})\|_{L^2(\hat{\varphi}_k(U_{\ell,p}))} \\ &\leq C \sum_{i=1}^S \|\partial^\beta((\tilde{u}_{p_i} - \tilde{u}_{p_{i-1}}) \circ \hat{\varphi}_k^{-1})\|_{L^2(\hat{\varphi}_k(U_{\ell,p}))}. \end{aligned}$$

In view of (57),

$$\tilde{u}_{p_i}|_{X_{p_i} \cap X_{p_{i-1}}} = \hat{u}|_{J_{p_i} \cap J_{p_{i-1}}} = \tilde{u}_{p_{i-1}}|_{X_{p_i} \cap X_{p_{i-1}}}, \quad i = 1, \dots, S,$$

and hence by (35) and (A3') we have for $|\beta| < s + \kappa$ and all $i = 1, \dots, S$,

$$\|\partial^\beta((\tilde{u}_{p_i} - \tilde{u}_{p_{i-1}}) \circ \hat{\varphi}_k^{-1})\|_{L^2(\hat{\varphi}_k(U_{\ell,p}))} \leq C h_{\ell,p}^{s+\kappa-|\beta|} |(\tilde{u}_{p_i} - \tilde{u}_{p_{i-1}}) \circ \hat{\varphi}_k^{-1}|_{H^{s+\kappa}(\hat{\varphi}_k(U_{\ell,p}))},$$

where $h_{\ell,p} := \text{diam}(\hat{\varphi}_k(U_{\ell,p}))$, which may serve as a replacement for (64) in the arguments leading to (65) since $h_{\ell,p} \leq R h_{\mathcal{A}}$ by (A3'), and as in the proof of Lemma 7 it can be shown that

$$|(\tilde{u}_{p_i} - \tilde{u}_{p_{i-1}}) \circ \hat{\varphi}_k^{-1}|_{H^{s+\kappa}(\hat{\varphi}_k(U_{\ell,p}))} \leq C \|\tilde{u}_{p_i} - \tilde{u}_{p_{i-1}}\|_{H^{s+\kappa}(\mathcal{A})}, \quad i = 1, \dots, S.$$

Remark 4 Theorem 1 remains valid if we define $\hat{u} \in \mathbb{R}^n$ by minimizing a p -norm (29) instead of least squares as in (26). Indeed, the proof goes through with obvious changes. In particular, to show (56) with

$$\varepsilon_1 := \|WM\hat{u} - Mf|_X\|_p \leq \|WMu|_X - Mf|_X\|_p = \left\| \left\{ \|W_\ell u|_{X_\ell} - Lu|_{X_\ell}\|_p \right\}_{\ell=1}^m \right\|_p$$

we need a p -norm version of Lemma 7, which holds with $\sqrt{\mu_{\mathcal{A}}}$ replaced by $\mu_{\mathcal{A}}^{1/p}$.

6 Numerical examples

The goal of this section is numerical verification of the convergence orders suggested by the error bounds of Theorem 1, in particular by the discrete maximum norm bound of (73).

We consider the d -dimensional sphere $\mathcal{M} = \mathbb{S}^d$ embedded into \mathbb{R}^{d+1} ,

$$\mathbb{S}^d = \{x \in \mathbb{R}^{d+1} : \|x\|_2 = 1\},$$

and solve the equation

$$Lu := -\Delta_{\mathcal{M}}u + u = f \quad \text{in } \mathcal{M}, \tag{75}$$

w.r.t. $u : \mathbb{S}^d \rightarrow \mathbb{R}$, where $\Delta_{\mathcal{M}}$ is the spherical Laplace-Beltrami operator, and $f : \mathbb{S}^d \rightarrow \mathbb{R}$ is given by

$$f(x) = (4d + 5 - s^2(x)) \sin s(x) + d s(x) \cos s(x), \quad x \in \mathbb{S}^d,$$

where $s(x) := 2 \sum_{i=1}^{d+1} x_i$. The exact solution of (75) is

$$u(x) = \sin s(x) = \sin \left(2 \sum_{i=1}^{d+1} x_i \right), \quad x \in \mathbb{S}^d.$$

The operator L in (75) is the special case of (22) with $\alpha = \kappa = 1$. As discussed in Section 2.3, it satisfies all assumptions required for the least squares method of Section 3 and for the error bounds of Theorem 1, as soon as K is a zonal reproducing kernel for the Sobolev space $H^s(\mathcal{M})$ for sufficiently large s .

We use the (scaled) Matérn kernels

$$K(x, y) = M_{s,d}^\varepsilon(x, y) = M_{s,d}(\varepsilon x, \varepsilon y), \quad x, y \in \mathbb{S}^d,$$

where $M_{s,d}$ is given in (16). As noticed in Section 2.2, $M_{s,d}^\varepsilon$ restricted to \mathcal{M} is a reproducing kernel for $H^s(\mathcal{M})$ whenever $s > d/2$. We discussed in Section 2.3 that these kernels are zonal and satisfy the hypotheses of Lemma 5 with respect to the operator L . Since the order of L is two, the method of Section 3 is well defined as soon as $s > d/2 + 1$. The assumption (46) used in the error bounds is satisfied whenever s is an integer greater than $d/2 + 2$, in particular $s \geq 3$ for $d = 1$, $s \geq 4$ for $d = 2$ or 3.

In order to compute the differentiation matrices (24) we need evaluations of the kernel $K_L(x, y) = L_1 K(x, y)$ for arbitrary $x, y \in \mathbb{S}^d$. For this, we use the following general formula for the application of the Laplace-Beltrami operator $\Delta_{\mathcal{M}}$ to the first argument of any zonal kernel K in the f -form $K(x, y) = f(t)$, where $t = \|x - y\|_2^2/2 = 1 - x^T y$, $x, y \in \mathbb{S}^d$,

$$K_{\Delta_{\mathcal{M}}}(x, y) = t(2 - t)f''(t) + d(1 - t)f'(t). \tag{76}$$

The formula can be easily shown by using [15, Lemma 1.4.2]. For more information on the f -form, see [57] and [19].

For $d \in \{2, 3\}$ we generate rather regular sets of nodes on the unit sphere \mathbb{S}^d by first producing a quasi-random set with uniform probability distribution on \mathbb{S}^d , and then applying a thinning algorithm to increase the minimum separation of the nodes. More precisely, for a given $\delta > 0$, we first generate N_0 points in \mathbb{R}^{d+1} with normally distributed components, where N_0 is obtained by rounding $\text{vol}_d(\mathbb{S}^d)/\delta^d$ to the nearest integer. We then project these points to the sphere \mathbb{S}^d , and run on them MATLAB's command `unique_tol` with absolute tolerance 2δ , to produce the final set X whose cardinality will be denoted by N . For each $d \in \{2, 3\}$ we create five sets of this type obtained with $\delta = 4^{-i/d}\delta_0$, $i = 0, 1, \dots, 4$, where we choose $\delta_0 = 0.1$ in 2D and $\delta_0 = 0.15$ in 3D. The cardinalities N of the resulting sets X can be found in Table 2 below. An example of a node set X obtained this way for the sphere \mathbb{S}^2 is shown in Fig. 1.

We run our method using the kernels $M_{s,d}^\varepsilon$, $s = 3, \dots, 7$, with the shape parameter ε reported in Table 1. We choose the set X_ℓ of (47) for each $\ell = 1, \dots, N$ by collecting $n_\ell = 2 \dim \Pi_{s-1}^d$ nearest neighbors of the node x_ℓ in X with respect to the Euclidian distance in \mathbb{R}^{d+1} . The numbers n_ℓ are also included in Table 1. In all cases these numbers were big enough in our experiments so that the approximation order would not increase if n_ℓ were increased, even though Conditions (A3) or (A3') are not guaranteed with this choice of X_ℓ .

Recall that the error bound (73) is given in terms of the maximum diameter $h_{\mathcal{A}}$ of the sets U_ℓ^φ that depend on the choice of the atlas \mathcal{A} . However, we do not generate either the sets U_ℓ , the atlas \mathcal{A} , or the partition of unity Γ as they are not needed for

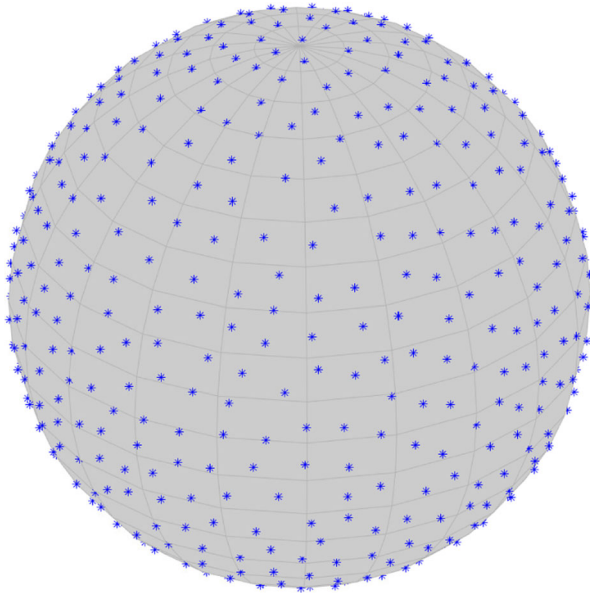


Fig. 1 Example of a node set X in \mathbb{S}^2 : 604 nodes obtained with $\delta = 0.05$

Table 1 The number of nearest neighbors n_ℓ used to generate the sets X_ℓ and the shape parameter ε of the kernel $M_{s,d}^\varepsilon$, chosen individually for each $s = 3, \dots, 7$ in both 2D and 3D

s	\mathbb{S}^2		\mathbb{S}^3	
	n_ℓ	ε	n_ℓ	ε
3	6	2^{-6}	8	2^{-9}
4	12	0.5	20	2^{-4}
5	20	2	40	0.25
6	30	3	70	1

the computation of the discrete approximate solution \hat{u} . Therefore we replace $h_{\mathcal{A}}$ by the easily computable quantity

$$h_{\mathcal{X}} := \max_{1 \leq \ell \leq N} \tilde{h}_\ell,$$

where \tilde{h}_ℓ denotes the Euclidean diameter of $X_\ell \subset \mathbb{R}^{d+1}$. By choosing the primary atlas $\hat{\mathcal{A}}$ for example as a number of half-spheres projected to appropriate tangent hyperplanes to \mathbb{S}^d in \mathbb{R}^{d+1} , we may achieve that the quantities $h_{\mathcal{A}}$ and $h_{\mathcal{X}}$ are equivalent in order when one of them goes to zero, for any admissible atlas \mathcal{A} . The numbers $h_{\mathcal{X}}$ depending on d, N and s are reported in Table 2. We have also estimated the quasi-uniformity of \mathcal{X} and X by computing

$$q_{\mathcal{X}} := \max_{1 \leq i, j \leq N} \frac{\tilde{h}_i}{\tilde{h}_j}, \quad q_{X, \mathcal{A}} := \max_{1 \leq \ell \leq N} \frac{h_{\mathcal{X}}}{2n_\ell^{1/d} \delta_\ell}$$

as replacement for $q_{\mathcal{A}}$ and $q_{X, \mathcal{A}}$. In all experiments both quantities were below 2.1.

Table 2 $h_{\mathcal{X}}$: maximum diameter of subsets X_ℓ for (a) \mathbb{S}^2 and (b) \mathbb{S}^3 , depending on N and s

N	s			
	3	4	5	6
(a) \mathbb{S}^2				
152	0.82	1.19	1.40	1.62
604	0.45	0.61	0.78	0.90
2,414	0.22	0.31	0.39	0.48
9,560	0.12	0.16	0.21	0.25
38,358	0.06	0.08	0.10	0.13
(b) \mathbb{S}^3				
257	1.06	1.41	1.68	1.90
1,014	0.73	0.93	1.16	1.35
4,048	0.45	0.60	0.74	0.88
16,276	0.29	0.39	0.49	0.57
65,164	0.19	0.25	0.31	0.36

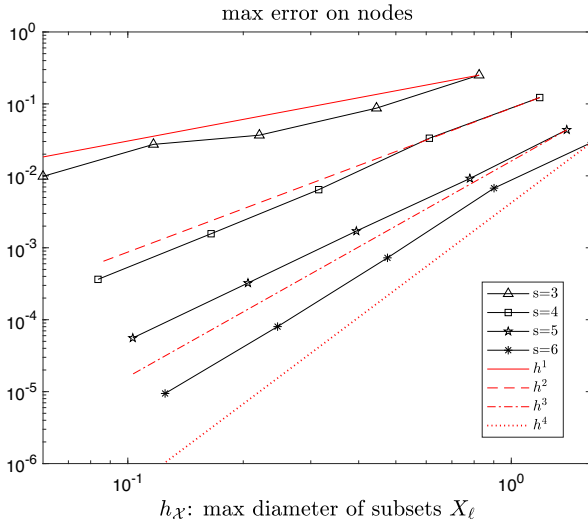


Fig. 2 Maximum error $\|u|_X - \hat{u}\|_\infty$ in 2D as function of h_X . For comparison we also include straight lines with slopes corresponding to convergence orders between h_X and h_X^4

We plot the error $\|u|_X - \hat{u}\|_\infty$ against h_X in Fig. 2 for S^2 and in Fig. 3 for S^3 . The plots indicate convergence orders between h_X^{s-3} and h_X^{s-2} for both $d = 2, 3$, which is higher than the theoretical estimate (73) that justifies h_X^{s-4} in 2D and h_X^{s-5} in 3D. Numerical convergence is observed for $s \geq 3$ in 2D and $s \geq 4$ in 3D.

Note that the values for ε in Table 1 are chosen as small as possible such that the results are not yet affected by the rounding errors. In most cases we choose ε as an

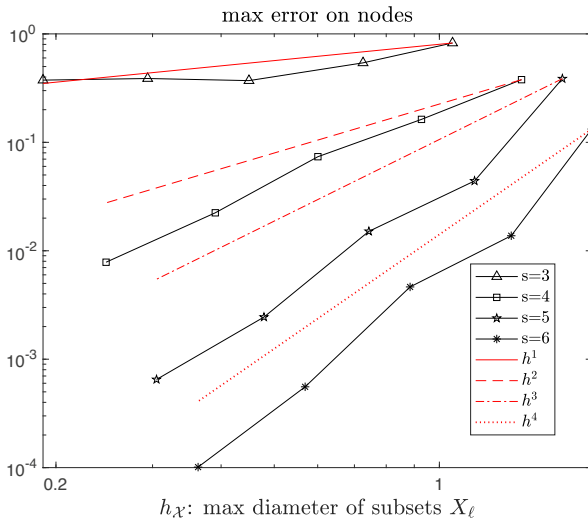


Fig. 3 Maximum error $\|u|_X - \hat{u}\|_\infty$ in 3D as function of h_X

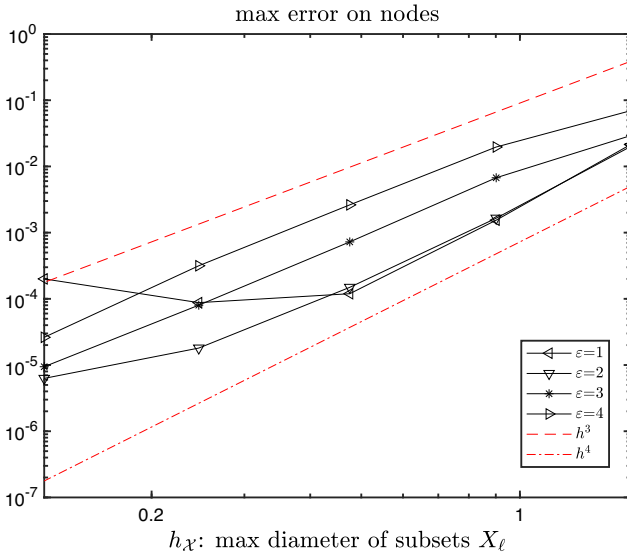


Fig. 4 Maximum error $\|u|_X - \hat{u}\|_\infty$ in 2D for $s = 6$ and several choices of ϵ

integer power of two, $\epsilon = 2^j$ for some $j \in \mathbb{Z}$. However, in the case $s = 6$ in 2D we make an exception and take $\epsilon = 3$ because $\epsilon = 2$ gives errors severely affected by rounding for the largest set X produced with $\delta = 1/16$, whereas $\epsilon = 4$ leads to solutions whose errors are too high, see Fig. 4. This figure illustrates that the errors tend to be smaller for smaller $\epsilon > 0$, without changing the approximation order. However, when we decrease ϵ , we get to the point that the kernel matrices $M_{s,d}^\epsilon|_{X_\ell}$ become too ill-conditioned, affecting the computation of W_ℓ in (24), which leads to a high error of the solution on denser sets X , as we see for $\epsilon \in \{1, 2\}$ in the figure.

7 Conclusion

In this paper we introduced a discrete least squares version of the meshless finite difference method for elliptic differential equations on closed manifolds, based on invertible local differentiation matrices for overlapping subsets of nodes. We obtained error bounds for this method by a new technique, and tested its convergence properties numerically. The sparse overdetermined linear system this method relies on has full rank without any additional assumptions like sufficient density of nodes. In particular, it is not related to a discretization of any variational or continuous least squares formulation of the differential equation. Since no exact or approximate integration is involved, the scheme does not require any partition of the manifold or its ambient space and is purely meshless.

Numerical examples suggest better convergence orders of the method than predicted by the error bounds, which indicates that theoretical results may be improved by refining the techniques introduced in the proof of Theorem 1. In particular, we expect

that the factor $h^{-d/2}$ in the estimate of Lemma 10 may be removed, which would allow to somewhat improve the bounds (53) and (54), but will not be sufficient for explaining numerical results. The assumption that the nodes are quasi-uniform in the sense that $q_{X,\mathcal{A}}$ is uniformly bounded does not seem natural, but is essential for the proof.

New ideas are needed in order to extend the method with guaranteed full rank of the system matrix to boundary value problems, conditionally positive definite kernels, or to the case when the elliptic operator L is not necessarily self-adjoint with respect to the inner product of $H^s(\mathcal{M})$ generated by the kernel K . In particular, conditionally positive definite kernels may help to improve the conditioning of the least squares problem (28), as they are known to do in the RBF-FD method on domains in \mathbb{R}^d [6], and remove the need for tuning the shape parameter ε we observed in Section 6.

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Declarations

Conflict of interest The author has no competing interests to declare that are relevant to the content of this article.

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References

1. Adams, R., Fournier, J.: Sobolev Spaces, 2nd edn. Academic Press, Amsterdam (2003)
2. Agranovich, M.S.: Elliptic operators on closed manifolds. In: Egorov, Y.V., Shubin, M.A. (eds.) Partial Differential Equations VI: Elliptic and Parabolic Operators, pp. 1–130. Heidelberg, Springer, Berlin Heidelberg, Berlin (1994)
3. Agranovich, M.S.: Sobolev spaces, their generalizations and elliptic problems in smooth and Lipschitz domains. Springer, (2015)
4. Aronszajn, N.: Theory of reproducing kernels. Transactions of the American Mathematical Society **68**(3), 337–404 (1950)
5. Babuška, I., Melenk, J.M.: The partition of unity method. International journal for numerical methods in engineering **40**(4), 727–758 (1997)
6. Bayona V., Flyer, N., Fornberg, B., Barnett, G.A.: On the role of polynomials in RBF-FD approximations: II. Numerical solution of elliptic PDEs. Journal of Computational Physics, **332**, 257 – 273 (2017)
7. Belytschko, T., Krongauz, Y., Organ, D., Fleming, M., Krysl, P.: Meshless methods: an overview and recent developments. Computer Methods in Applied Mechanics and Engineering, special issue **139**, 3–47 (1996)
8. Björck, Å.: Numerical methods for least squares problems. SIAM, (1996)
9. Brenner, S., Scott, R.: The mathematical theory of finite element methods, 3rd Edition. Springer Science & Business Media, (2008)
10. Buhmann, M.D.: Radial Basis Functions. Cambridge University Press, New York, NY, USA (2003)

11. Burenkov, V.: Sobolev Spaces on Domains. Teubner-Texte zur Mathematik. Teubner B.G, GmbH (1998)
12. Chen, M., Ling, L.: Extrinsic meshless collocation methods for PDEs on manifolds. *SIAM Journal on Numerical Analysis* **58**(2), 988–1007 (2020)
13. Cheney, E.: Introduction to Approximation Theory, ser. AMS Chelsea Publishing Series, AMS Chelsea Pub (1982)
14. Cheung, K.C., Ling, L.: A kernel-based embedding method and convergence analysis for surfaces PDEs. *SIAM Journal on Scientific Computing* **40**(1), A266–A287 (2018)
15. Dai, F., Xu, Y.: Approximation theory and harmonic analysis on spheres and balls. Springer, (2013)
16. Davies, M.: Linear approximation using the criterion of least total deviations. *Journal of the Royal Statistical Society: Series B (Methodological)* **29**(1), 101–109 (1967)
17. Davydov, O.: Error bound for radial basis interpolation in terms of a growth function. In: Cohen, A., Merrien, J.L., Schumaker, L.L. (eds.) *Curve and Surface Fitting: Avignon 2006*, pp. 121–130. Nashboro Press, Brentwood (2007)
18. Davydov, O.: Selection of sparse sets of influence for meshless finite difference methods, [arXiv:1908.01567v1](https://arxiv.org/abs/1908.01567v1), (2019)
19. Davydov, O.: mFDlab: A laboratory for meshless finite difference (mFD) methods, <https://bitbucket.org/meshlessFD/mfdlab>, (2020)
20. Davydov, O.: Approximation with conditionally positive definite kernels on deficient sets. In: Gregory, M.N., Fasshauer, E., Schumaker, L.L. (eds.) *Approximation Theory XVI: Nashville 2019*, pp. 27–38. Springer, Berlin Heidelberg (2021)
21. Davydov, O., Oanh, D.T.: Adaptive meshless centres and RBF stencils for Poisson equation. *J. Comput. Phys.* **230**, 287–304 (2011)
22. Davydov, O., Oanh, D.T., Tuong, N.M.: Octant-based stencil selection for meshless finite difference methods in 3D. *Vietnam Journal of Mathematics* **48**, 93–106 (2020)
23. Davydov, O., Oanh D.T., Tuong, N.M.: Improved stencil selection for meshless finite difference methods in 3D. *Journal of Computational and Applied Mathematics*, **115031**, (2023)
24. Davydov, O., Safarpoor, M.: A meshless finite difference method for elliptic interface problems based on pivoted QR decomposition. *Applied Numerical Mathematics* **161**, 489–509 (2021)
25. Davydov, O., Schaback, R.: Error bounds for kernel-based numerical differentiation. *Numerische Mathematik* **132**(2), 243–269 (2016)
26. Davydov, O., Schaback, R.: Minimal numerical differentiation formulas. *Numerische Mathematik* **140**(3), 555–592 (2018)
27. Davydov, O., Schaback, R.: Optimal stencils in Sobolev spaces. *IMA Journal of Numerical Analysis* **39**(1), 398–422 (2019)
28. Demkowicz, L., Karafiat, A., Liszka, T.: On some convergence results for FDM with irregular mesh. *Computer Methods in Applied Mechanics and Engineering* **42**(3), 343–355 (1984)
29. Fasshauer, G.: *Meshfree Approximation Methods with MATLAB*. World Scientific Publishing Co., Inc, River Edge, NJ, USA (2007)
30. Fasshauer, G., McCourt, M.: *Kernel-based Approximation Methods using MATLAB*. World Scientific Publishing Co., Inc, River Edge, NJ, USA (2015)
31. Flyer, N., Lehto, E., Blaise, S., Wright, G.B., St-Cyr, A.: A guide to RBF-generated finite differences for nonlinear transport: Shallow water simulations on a sphere. *Journal of Computational Physics* **231**(11), 4078–4095 (2012)
32. Fornberg, B., Flyer, N.: *A Primer on Radial Basis Functions with Applications to the Geosciences*. Society for Industrial and Applied Mathematics, Philadelphia, PA, USA (2015)
33. Freeden, W., Gervens, T., Schreiner, M.: *Constructive approximation on the sphere with applications to geomathematics*. Oxford University Press, (1998)
34. Fuselier, E., Wright, G.B.: Scattered data interpolation on embedded submanifolds with restricted positive definite kernels: Sobolev error estimates. *SIAM Journal on Numerical Analysis* **50**(3), 1753–1776 (2012)
35. Griebel, M., Schweitzer, M.: A particle-partition of unity method-part II: Efficient cover construction and reliable integration. *SIAM Journal on Scientific Computing* **23**(5), 1655–1682 (2002)
36. Hangelbroek, T., Narcowich, F.J., Rieger, C., Ward, J.D.: Direct and inverse results on bounded domains for meshless methods via localized bases on manifolds. In: Dick, J., Kuo, F.Y., Woźniakowski, H. (eds.) *Contemporary Computational Mathematics - A Celebration of the 80th Birthday of Ian Sloan*, pp. 517–543. Springer International Publishing, Cham (2018)

37. Hangelbroek, T., Narcowich, F.J., Ward, J.D.: Kernel approximation on manifolds I: Bounding the Lebesgue constant. *SIAM Journal on Mathematical Analysis* **42**(4), 1732–1760 (2010)
38. Jetter, K., Stöckler, J., Ward, J.: Error estimates for scattered data interpolation on spheres. *Mathematics of Computation of the American Mathematical Society* **68**(226), 733–747 (1999)
39. Kansa, E.J.: Multiquadrics - a scattered data approximation scheme with applications to computational fluid-dynamics - II: Solutions to parabolic, hyperbolic and elliptic partial differential equations. *Comput. Math. Appl.* **19**, 147–161 (1990)
40. Larsson, E., Shcherbakov, V., Heryudono, A.: A least squares radial basis function partition of unity method for solving PDEs. *SIAM Journal on Scientific Computing* **39**(6), A2538–A2563 (2017)
41. Lee, J.: *Introduction to Smooth Manifolds*. Graduate Texts in Mathematics. Springer, New York (2013)
42. Levesley, J., Luo, Z.: Error estimates for Hermite interpolation on spheres. *Journal of mathematical analysis and applications* **281**(1), 46–61 (2003)
43. Levesley, J., Ragozin, D.L.: Radial basis interpolation on homogeneous manifolds: convergence rates. *Advances in Computational Mathematics* **27**(2), 237–246 (2007)
44. Maz'ya, V., Poborchii, S.: *Differentiable Functions on Bad Domains*. World Scientific, (1997)
45. Morton, T.M., Neamtu, M.: Error bounds for solving pseudodifferential equations on spheres by collocation with zonal kernels. *Journal of Approximation Theory* **114**(2), 242–268 (2002)
46. Narcowich, F.: Generalized Hermite interpolation and positive definite kernels on a Riemannian manifold. *Journal of Mathematical Analysis and Applications* **190**(1), 165–193 (1995)
47. Narcowich, F., Rowe, S., Ward, J.: A novel Galerkin method for solving PDEs on the sphere using highly localized kernel bases. *Mathematics of Computation* **86**(303), 197–231 (2017)
48. Narcowich, F.J., Ward, J.D., Wendland, H.: Sobolev bounds on functions with scattered zeros, with applications to radial basis function surface fitting. *Mathematics of Computation* **74**, 743–763 (2005)
49. Nguyen, V.P., Rabczuk, T., Bordas, S., Duflot, M.: Meshless methods: A review and computer implementation aspects. *Math. Comput. Simul.* **79**(3), 763–813 (2008)
50. Oanh, D.T., Davydov, O., Phu, H.X.: Adaptive RBF-FD method for elliptic problems with point singularities in 2D. *Applied Mathematics and Computation* **313**, 474–497 (2017)
51. Paulsen, V.I., Raghupathi, M.: *An Introduction to the Theory of Reproducing Kernel Hilbert Spaces*. Cambridge Studies in Advanced Mathematics. Cambridge University Press, (2016)
52. Petras, A., Ling, L., Ruuth, S.J.: An RBF-FD closest point method for solving PDEs on surfaces. *Journal of Computational Physics* **370**, 43–57 (2018)
53. Pham, T.D., Tran, T.: Strongly elliptic pseudodifferential equations on the sphere with radial basis functions. *Numerische Mathematik* **128**(3), 589–614 (2014)
54. Power, H., Barraco, V.: A comparison analysis between unsymmetric and symmetric radial basis function collocation methods for the numerical solution of partial differential equations. *Computers and Mathematics with Applications* **43**, 551–583 (2002)
55. Rieger, C., Schaback, R., Zwicknagl, B.: Sampling and stability. In: Dæhlen, M., Floater, M., Lyche, T., Merrien, J.L., Mørken, K., Schumaker, L.L. (eds.) *International Conference on Mathematical Methods for Curves and Surfaces*, pp. 347–369. Springer, Berlin Heidelberg (2008)
56. Schaback, R.: Unsymmetric meshless methods for operator equations. *Numerische Mathematik* **114**(4), 629–651 (2010)
57. Schaback, R.: MATLAB programming for kernel-based methods. Technical report, University of Göttingen, (2011). Available at <http://num.math.uni-goettingen.de/schaback/research/papers/MPfKBM.pdf>
58. Schaback, R.: All well-posed problems have uniformly stable and convergent discretizations. *Numerische Mathematik* **132**(3), 597–630 (2016)
59. Schaback, R.: Error analysis of nodal meshless methods. In: Griebel, M., Schweitzer, M.A. (eds.) *Mesh-free Methods for Partial Differential Equations VIII*, pages 117–143. Springer International Publishing, (2017)
60. Seibold, B.: Minimal positive stencils in meshfree finite difference methods for the Poisson equation. *Comput. Methods Appl. Mech. Eng.* **198**(3–4), 592–601 (2008)
61. Shankar, V.: The overlapped radial basis function-finite difference (RBF-FD) method: A generalization of RBF-FD. *Journal of Computational Physics* **342**, 211–228 (2017)
62. Shankar, V., Wright, G.B., Kirby, R.M., Fogelson, A.L.: A radial basis function (RBF)-Finite Difference (FD) method for diffusion and reaction-diffusion equations on surfaces. *Journal of Scientific Computing* **63**(3), 745–768 (2015)

63. Sokolov, A., Davydov, O., Kuzmin, D., Westermann, A., Turek, S.: A flux-corrected RBF-FD method for convection dominated problems in domains and on manifolds. *Journal of Numerical Mathematics*, published online 2019
64. Sokolov, A., Davydov, O., Turek, S.: Numerical study of the RBF-FD level set based method for partial differential equations on evolving-in-time surfaces. In: Griebel, M., Schweitzer, M.A. (eds.) *Meshfree Methods for Partial Differential Equations IX*, pp. 117–134. Springer, Berlin Heidelberg (2019)
65. Stein, E.M.: *Singular Integrals and Differentiability Properties of Functions*. Princeton University Press, (1970)
66. Suchde, P., Kuhnert, J.: A meshfree generalized finite difference method for surface PDEs. *Computers & Mathematics with Applications* **78**(8), 2789–2805 (2019)
67. Tominec, I., Larsson, E., Heryudono, A.: A least squares radial basis function finite difference method with improved stability properties. *SIAM Journal on Scientific Computing* **43**(2), A1441–A1471 (2021)
68. Weidmann, J.: *Linear Operators in Hilbert Spaces*. Springer-Verlag, New York (1980)
69. Wendland, H.: *Scattered Data Approximation*. Cambridge University Press, (2004)
70. Wendland, H., Rieger, C.: Approximate interpolation with applications to selecting smoothing parameters. *Numerische Mathematik* **101**(4), 729–748 (2005)

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