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DISCRETE INTERPOLATION NORMS WITH APPLICATIONS*

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Abstract. We describe norm representations for interpolation spaces generated by finite-dimensional subspaces of Hilbert spaces. These norms are products of integer and noninteger powers of the Grammian matrices associated with the generating pair of spaces for the interpolation space. We include a brief description of some of the algorithms which allow the efficient computation of matrix powers. We consider in some detail the case of fractional Sobolev spaces both for positive and negative indices together with applications arising in preconditioning techniques. Numerical experiments are included.

Key words. interpolation spaces, Hilbert spaces, finite element method, domain decomposition

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1. Introduction.

Interpolation spaces arise naturally in the formulation of many modeling applications ranging from domain decomposition methods [22], [8], [11], [6], [45], [53] and multilevel methods [9], [14] to image processing [41], [42], [33], [52], [25], [24], advection-diffusion problems [47, 48], and elasticity [30]. It is therefore desirable to characterize the corresponding finite-dimensional spaces with the aim of enabling new numerical approaches and algorithms. In particular, we are interested in deriving norm representations corresponding to interpolation spaces generated by finite-dimensional subspaces of a given pair of Hilbert spaces. As a major application we derive discrete representations of norms corresponding to conforming finite element discretizations of fractional Sobolev spaces. We show that they involve fractional powers of products of certain Grammian matrices associated with the bases of the finite element spaces employed. We note that alternative representations of interpolation norms for Sobolev spaces have been considered in [8] in the context of domain decomposition, while [9] gives a multilevel representation of fractional Sobolev norms. For the case where wavelet spaces are of interest, some recent results can be found in [14], [13], where matrix representations in wavelet bases are given for Sobolev spaces of noninteger orders.

One apparent limitation associated with discrete representations of interpolation norms is that for large-scale computations they are seemingly expensive to compute. We show that this need not be so in the case of finite element norms for which inexpensive factorizations can be devised using standard approximation procedures such as projection onto Krylov subspaces.

The paper is organized as follows. In section 2, we introduce the concept of interpolation between abstract Hilbert spaces as described in [38]. In section 3, we also consider the corresponding finite-dimensional subspaces and derive expressions for the associated norm representations. In section 4, we derive the norms resulting from projection onto finite element spaces of fractional Sobolev spaces. Section 5 contains

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a brief review of existing algorithms for the computation of matrix noninteger powers which arise in the definition of discrete representations of interpolation norms; we also include in this section the details of a Lanczos procedure employed for the computation of interpolation norms. Section 6 includes applications arising in preconditioning of domain decomposition methods and methods for the biharmonic equation. The paper concludes with some numerical experiments.

In the following we will use the following notation: let A and B be positive definite matrices of order n; then $A \sim B$ iff there exist $c_1, c_2 \in \mathbb{R}_+$ such that for all $x \in \mathbb{R}^n \backslash \{\mathbf{0}\}$, $c_1 \leq x^T Ax/x^T Bx \leq c_2$ with c_1, c_2 independent of n. Furthermore, given a Hilbert space X and two norms $\|\cdot\|_1$ and $\|\cdot\|_2$ defined on it, we have that $\|u\|_1 \sim \|u\|_2$ iff there exist $c_1, c_2 \in \mathbb{R}_+$ such that for all $u \in X$, $c_1\|u\|_1 \leq \|u\|_2 \leq c_2\|u\|_1$ with c_1, c_2 independent of X. The constants are specified, where necessary.

2. Interpolation spaces.

We review here the presentation from [38, Chapter 1]; we also recall results from [1].

Let X, Y denote two separable Hilbert spaces and let $(\cdot,\cdot)_X, (\cdot,\cdot)_Y$ denote the corresponding inner products and $\|\cdot\|_X, \|\cdot\|_Y$ the respective norms.

DEFINITION 2.1. *We say X, Y form a compatible pair denoted by (X, Y) if*

(i) *X is a dense subset of Y;*

(ii) *the injection $i : X \to Y$ is continuous; i.e., there exists $c > 0$ such that*

$$\|v\|_Y = \|iv\|_Y \leq c\|v\|_X.$$

Let $w \in Y$. By the Riesz representation theorem [55, page 90], w defines a bounded linear functional $f_w := (\cdot, w)_Y$ on Y. This functional is bounded also on X since

$$f_w(u) = (u, w)_Y \leq \|u\|_Y\|w\|_Y \leq c\|w\|_Y\|u\|_X.$$

Hence, by the Riesz representation theorem, there exists $v = v_w \in X$ such that for all $u \in X$ there holds

$$(u, v)_X = f_w(u) = (u, w)_Y\,.$$

Let $\mathcal{J} : X \to Y$ denote the linear map $v_w \mapsto w$. Then for all $u, v \in X$

$$(u, v)_X = (u, \mathcal{J}v)_Y\,. \tag{2.1}$$

The operator $\mathcal{J}$ can be shown to be positive and self-adjoint with respect to $(\cdot,\cdot)_Y$. Using the spectral decomposition of $\mathcal{J}$ we define the operator $\mathcal{E} = \mathcal{J}^{1/2} : X \to Y$, which in turn is positive self-adjoint. Moreover (see [38, Chapter 1, section 2.2]), the space X can be seen to be the domain $D(\mathcal{E})$ of $\mathcal{E}$ and the norm of X is equivalent to the graph norm $\|\cdot\|_{\mathcal{E}}$:

$$\|u\|_X \sim \|u\|_{\mathcal{E}} := \left(\|u\|_Y^2 + \|\mathcal{E}u\|_Y^2\right)^{1/2}.$$

Similarly, the spectral decomposition of $\mathcal{E}$ can be used to define any real power of $\mathcal{E}$. Let $\theta \in [0, 1]$ and let $\|\cdot\|_\theta$ denote the scale of graph norms

$$\|u\|_\theta := \left(\|u\|_Y^2 + \|\mathcal{E}^{1-\theta}u\|_Y^2\right)^{1/2}. \tag{2.2}$$

One can then show that the domain of $\mathcal{E}^{1-\theta}$ endowed with the inner product

$$(u, v)_\theta = (u, v)_Y + \left(u, \mathcal{E}^{1-\theta}v\right)_Y$$

is a Hilbert space [38]. This is an *interpolation space of index θ for the pair* (X, Y) and is denoted by $[X, Y]_\theta$:

$$[X, Y]_\theta := D(\mathcal{E}^{1-\theta}), \qquad 0 \le \theta \le 1.$$

Note that $[X, Y]_0 = X$ and $[X, Y]_1 = Y$. Moreover, if $0 < \theta_1 < \theta_2 < 1$, then

$$X \subset [X, Y]_{\theta_1} \subset [X, Y]_{\theta_2} \subset Y \tag{2.3}$$

with dense inclusions. Let $\mathcal{L}(A; B)$ denote the space of continuous linear operators from A into B. The following classic interpolation theorem can be found in [38, Theorem 5.1].

THEOREM 2.2. *Let (X, Y), $(\mathcal{X}, \mathcal{Y})$ be two sets of compatible pairs of Hilbert spaces. Let $\pi \in \mathcal{L}(X; \mathcal{X}) \cap \mathcal{L}(Y; \mathcal{Y})$. Then for all $\theta \in (0, 1)$, $\pi \in \mathcal{L}([X, Y]_\theta; [\mathcal{X}, \mathcal{Y}]_\theta)$.*

Remark 2.1. An alternative definition of interpolation spaces is based on the K-method [1, Chapter 7] (see also [38, Chapter 15]), which employs the equivalent norm

$$|||u|||_\theta := \left(\|u\|_Y^2 + c\|\mathcal{E}^{1-\theta} u\|_Y^2\right)^{1/2},$$

where

$$c = \int_0^\infty \frac{s^{1-2\theta}}{1+s^2} \mathrm{d}s = \frac{\pi}{2} \frac{1}{\sin \pi\theta}.$$

For this choice of norm one can show that if

$$\|\pi u\|_{\mathcal{X}} \le M_0 \|u\|_X \quad \forall u \in X \quad \text{and} \quad \|\pi u\|_{\mathcal{Y}} \le M_1 \|u\|_Y \quad \forall u \in Y$$

with constants M_0, M_1 independent of $\mathcal{X}, \mathcal{Y}$, then

$$|||\pi u|||_{[\mathcal{X},\mathcal{Y}]_\theta} \le M_0^{1-\theta} M_1^\theta |||u|||_{[X,Y]_\theta}.$$

Since $|||\cdot|||_\theta, \|\cdot\|_\theta$ are equivalent, we deduce that a similar bound holds with respect to the norm $\|\cdot\|_\theta$ defined in (2.2):

$$\|\pi u\|_{[\mathcal{X},\mathcal{Y}]_\theta} \le C M_0^{1-\theta} M_1^\theta \|u\|_{[X,Y]_\theta} \tag{2.4}$$

with constants C, M_0, M_1 independent of $\mathcal{X}, \mathcal{Y}$.

Under certain assumptions, the graph norm on the interpolation space corresponding to a compatible pair $(\mathcal{X}, \mathcal{Y})$ of subspaces of X, Y is equivalent to the graph norm on the interpolation space generated by the pair (X, Y).

LEMMA 2.3. *Let $(\mathcal{X}, \mathcal{Y}), (X, Y)$ be compatible pairs and let $\mathcal{X}, \mathcal{Y}$ denote subspaces of X, Y, respectively, which are equipped with the subspace topology. Assume there exists an operator $I \in \mathcal{L}(X; \mathcal{X}) \cap \mathcal{L}(Y; \mathcal{Y})$ such that $Iu = u$ for all $u \in \mathcal{Y}$ and*

$$\|Iu\|_{\mathcal{X}} \le M_0 \|u\|_X \quad (\forall u \in X), \qquad \|Iu\|_{\mathcal{Y}} \le M_1 \|u\|_Y \quad (\forall u \in Y) \tag{2.5}$$

with constants M_0, M_1 independent of $\mathcal{X}, \mathcal{Y}$. Then for all $u \in [\mathcal{X}, \mathcal{Y}]_\theta$

$$\|u\|_{[X,Y]_\theta} \sim \|u\|_{[\mathcal{X},\mathcal{Y}]_\theta}$$

with constants of equivalence independent of $\mathcal{X}, \mathcal{Y}$.

Proof. Let $i \in \mathcal{L}(\mathcal{X}; X) \cap \mathcal{L}(\mathcal{Y}; Y)$ denote the continuous injection operator between the indicated spaces. By Theorem 2.2, $i \in \mathcal{L}([\mathcal{X}, \mathcal{Y}]_\theta; [X, Y]_\theta)$. By (2.4) (see Remark 2.1), there exists a constant C_1 independent of $\mathcal{X}, \mathcal{Y}$ such that for all $u \in [\mathcal{X}, \mathcal{Y}]_\theta$

$$\|u\|_{[X,Y]_\theta} = \|iu\|_{[X,Y]_\theta} \leq C_1 \|u\|_{[\mathcal{X},\mathcal{Y}]_\theta}. \tag{2.6}$$

By Theorem 2.2, $I \in \mathcal{L}([X, Y]_\theta; [\mathcal{X}, \mathcal{Y}]_\theta)$, and from (2.4) there exists a constant C_2 independent of $\mathcal{X}, \mathcal{Y}$ such that for all $u \in [\mathcal{X}, \mathcal{Y}]_\theta$

$$\|u\|_{[\mathcal{X},\mathcal{Y}]_\theta} = \|Iu\|_{[\mathcal{X},\mathcal{Y}]_\theta} \leq C_2 \|u\|_{[X,Y]_\theta}, \tag{2.7}$$

and the result of the lemma follows. ☐

Remark 2.2. The lemma holds also when the spaces $\mathcal{X}, \mathcal{Y}$ are equipped with norms equivalent to the norms induced by X, Y, with constants of equivalence independent of $\mathcal{X}, \mathcal{Y}$. This is particularly relevant for the case when $\mathcal{X}, \mathcal{Y}$ are finite-dimensional subspaces equipped with discrete norms which do not have a continuous representation.

We turn now to the case where the spaces generating the scale of interpolation spaces are finite-dimensional. In particular, we are interested in the discrete representations of norms associated with these spaces.

3. Finite-dimensional interpolation spaces. Let $V_h \subset X$ denote a subset of X with $\dim V_h = n$. Let $X_h = (V_h, \|\cdot\|_X)$, $Y_h = (V_h, \|\cdot\|_Y)$ be finite-dimensional subspaces of X, Y, respectively, with the indicated induced norm topologies. It follows that (X_h, Y_h) is a compatible pair of Hilbert spaces. We proceed analogously to the previous section and define $\mathcal{J}_h$ via

$$(u_h, v_h)_X = (u_h, \mathcal{J}_h v_h)_Y\,, \qquad u_h, v_h \in X_h. \tag{3.1}$$

One can show that $\mathcal{J}_h$ is positive self-adjoint in the inner product $(\cdot,\cdot)_Y$, and therefore we can define $\mathcal{E}_h = \mathcal{J}_h^{1/2}$. We define the finite-dimensional interpolation spaces

$$[X_h, Y_h]_\theta := D(\mathcal{E}_h^{1-\theta}) = (V_h, \|\cdot\|_{\theta,h}),$$

where

$$\|u_h\|_{\theta,h} := \left(\|u_h\|_Y^2 + \|\mathcal{E}_h^{1-\theta} u_h\|_Y^2\right)^{1/2}. \tag{3.2}$$

For this choice of spaces, the result of Lemma 2.3 holds with constants independent of n, provided there exists an operator $I_h \in \mathcal{L}(X; X_h) \cap \mathcal{L}(Y; Y_h)$ such that $I_h u_h = u_h$ for all $u_h \in V_h$ and I_h is bounded as in (2.7) with constants independent of n.

3.1. Matrix representations. We are interested in deriving the matrix representations of $\mathcal{J}_h, \mathcal{E}_h$ as well as those corresponding to the scale of norms (3.2). In particular, we wish to derive matrices $H_\theta \in \mathbb{R}^{n\times n}$ with $\theta \in (0, 1)$, which induce norms equivalent to $\|\cdot\|_{\theta,h}$ with constants of equivalence independent of n. We first introduce some definitions and notation.

Let $H \in \mathbb{R}^{n\times n}$ be a symmetric and positive definite matrix. Then H induces a vector norm $\|\cdot\|_H$ on $\mathbb{R}^n$:

$$\|\mathbf{v}\|_H := \left(\mathbf{v}^T H \mathbf{v}\right)^{1/2}.$$

Given two symmetric and positive definite matrices $H_1 \in \mathbb{R}^{n\times n}$, $H_2 \in \mathbb{R}^{m\times m}$ we define the following matrix norm for matrices $M \in \mathbb{R}^{m\times n}$ (see [35, page 311]):

$$\|M\|_{H_1,H_2} = \max_{\mathbf{v}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{\|M\mathbf{v}\|_{H_2}}{\|\mathbf{v}\|_{H_1}}. \tag{3.3}$$

Finally, we define the H-condition number of a matrix M to be the quantity

$$\kappa_H(M) = \|M\|_{H,H^{-1}}\|M^{-1}\|_{H^{-1},H}.$$

Let $\{\phi_i\}_{1\le i\le n}$ denote a basis of X_h, Y_h and let H_X, H_Y denote the Grammian (or Riesz) matrices corresponding to the inner products $(\cdot,\cdot)_X$, $(\cdot,\cdot)_Y$, respectively:

$$(H_X)_{ij} = (\phi_i,\phi_j)_X\,, \quad (H_Y)_{ij} = (\phi_i,\phi_j)_Y\,, \qquad 1 \le i,j \le n,$$

so that

$$\|u_h\|_X = \|\mathbf{u}\|_{H_X}, \quad \|u_h\|_Y = \|\mathbf{u}\|_{H_Y},$$

where $\mathbf{u}$ denotes the vector of coefficients of u_h expanded in the basis $\{\phi_i\}$. We first note that the discrete Riesz representation (3.1) becomes

$$\mathbf{u}^T H_X \mathbf{v} = \mathbf{u}^T H_Y J \mathbf{v}$$

so that $J = H_Y^{-1} H_X$ is a product of two symmetric and positive definite matrices. The matrix J is self-adjoint and positive definite in the discrete H_Y-inner product, as

$$(\mathbf{u}, J\mathbf{v})_{H_Y} = \mathbf{u}^T H_Y (H_Y^{-1} H_X)\mathbf{v} = \mathbf{v}^T H_X \mathbf{u} = \mathbf{v}^T H_Y (H_Y^{-1} H_X)\mathbf{u} = (\mathbf{v}, J\mathbf{u})_{H_Y}$$

and

$$(\mathbf{u}, J\mathbf{u})_{H_Y} = \mathbf{u}^T H_X \mathbf{u} > 0 \quad \forall \mathbf{u} \ne \mathbf{0}.$$

One can also write explicitly the eigenvalue decomposition of J: since H_X, H_Y are symmetric and positive definite, there exists a matrix Q such that [35, Corollary 7.6.2]

$$H_X = Q^T D Q, \quad H_Y = Q^T Q,$$

where D is a diagonal matrix with positive entries, so that

$$J = H_Y^{-1} H_X = Q^{-1} D Q.$$

Note that the diagonal entries of D are also the eigenvalues of the generalized eigenvalue problem involving the pencil $[H_X, H_Y]$:

$$H_X V = H_Y V D \qquad (V = Q^{-1}). \tag{3.4}$$

It is evident that the matrix representation of $\mathcal{E}_h$ in the basis $\{\phi_i\}$ is the matrix

$$E = Q^{-1} D^{1/2} Q;$$

furthermore, the matrix representation of $\mathcal{E}_h^{1-\theta}$ is similarly

$$E^{1-\theta} = Q^{-1} D^{(1-\theta)/2} Q.$$

We now turn to the matrix representation of the norm $\|\cdot\|_{\theta,h}$ which we denote by $H_{\theta,h}$. Definition (3.2) yields

$$\|\mathbf{u}\|^2_{H_{\theta,h}} = \|\mathbf{u}\|^2_{H_Y} + \|E^{1-\theta}\mathbf{u}\|^2_{H_Y}$$

so that

$$\begin{aligned} H_{\theta,h} &= H_Y + (E^{1-\theta})^T H_Y E^{1-\theta} = H_Y + Q^T D^{1-\theta} Q \\ &= H_Y + H_Y J^{1-\theta} = Q^T(I + D^{1-\theta})Q. \end{aligned} \tag{3.5}$$

The above representation can be shown to be equivalent to a reduced form, as the following result shows.

LEMMA 3.1. *Let*

$$H_\theta = H_Y J^{1-\theta} = Q^T D^{1-\theta} Q. \tag{3.6}$$

Then

$$H_\theta \sim H_{\theta,h}$$

with constants of equivalence independent of n.

Proof. By definition, the norm of X_h is equivalent to the discrete graph norm (3.2) with $\theta = 0$:

$$Q^T D Q = H_X \sim H_{0,h} = H_Y + H_Y J = Q^T(I + D)Q.$$

Hence, there exist two positive real constants α_1, α_2 independent of n such that

$$\alpha_1 D_{ii} \le (1 + D_{ii}) \le \alpha_2 D_{ii}, \qquad 1 \le i \le n.$$

It follows that, setting $\tilde{\alpha}_1 = 1, \tilde{\alpha}_2 = \max\{\alpha_2, 2\}$, there holds

$$\tilde{\alpha}_1 D_{ii}^{1-\theta} \le (1 + D_{ii}^{1-\theta}) \le \tilde{\alpha}_2 D_{ii}^{1-\theta}, \qquad 1 \le i \le n,$$

and the result follows. ∎

Remark 3.1. If the matrices H_X, H_Y are simultaneously diagonalizable, one can derive a simpler expression for $H_{\theta,h}, H_\theta$. Assuming there exists an invertible matrix Z such that

$$Z^{-1} H_X Z = D_X, \quad Z^{-1} H_Y Z = D_Y,$$

we find

$$J = H_Y^{-1} H_X = Z D_Y^{-1} D_X Z^{-1}, \quad J^{1-\theta} = H_Y^{\theta-1} H_X^{1-\theta}$$

and thus

$$H_{\theta,h} = H_Y + H_Y J^{1-\theta} = H_Y + H_Y H_Y^{\theta-1} H_X^{1-\theta} = H_Y + H_Y^\theta H_X^{1-\theta}$$

and

$$H_\theta = H_Y^\theta H_X^{1-\theta} = H_Y^{\theta/2} H_X^{1-\theta} H_Y^{\theta/2}.$$

The following is a corollary of Lemma 2.3.

PROPOSITION 3.2. *Let the assumptions of Lemma* 2.3 *hold with* $(\mathcal{X}, \mathcal{Y})$ *replaced by* (X_h, Y_h) *defined above. Let* $H_{\theta,h}, H_\theta \in \mathbb{R}^{n\times n}$ *be defined as in* (3.5), (3.6)*, respectively. Then there exist constants* c, C *independent of* n *such that*

$$\begin{aligned} c\|u_h\|_{[X,Y]_\theta} \leq \ \|\mathbf{u}\|_{H_{\theta,h}} &\leq C\|u_h\|_{[X,Y]_\theta}, \\ c\|u_h\|_{[X,Y]_\theta} \leq \ \|\mathbf{u}\|_{H_\theta} \ &\leq C\|u_h\|_{[X,Y]_\theta} \end{aligned}$$

for all $u_h \in [X_h, Y_h]_\theta$ *and with* $\theta \in (0,1)$.

The above result provides two matrix representations of a norm equivalent to the norm of the interpolation space $[X,Y]_\theta$ when restricted to a finite-dimensional subspace. We will see that in the case of finite element discretizations of elliptic PDEs, the requirements of Proposition 3.2 hold for standard choices of spaces, norms, and discretizations.

Finally, we end with the following result concerning the conditioning of H_θ.

LEMMA 3.3. *Let* $\kappa := \kappa_{H_Y}(H_X)$ *denote the* H_Y*-condition number of* H_X*. Then*

$$\kappa_{H_Y}(H_\theta) = \kappa^{1-\theta}.$$

Proof. Using the decompositions $H_X = Q^T D Q, H_Y = Q^T Q$, we find

$$\begin{aligned} \|H_X\|_{H_Y, H_Y^{-1}} &= \max_{\mathbf{v}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{\mathbf{v}^T H_X \mathbf{v}}{\mathbf{v} H_Y \mathbf{v}} = \max_i D_{ii}, \\ \|H_X^{-1}\|_{H_Y^{-1}, H_Y} &= \max_{\mathbf{v}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{\mathbf{v}^T H_0^{-1} \mathbf{v}}{\mathbf{v} H_1^{-1} \mathbf{v}} = \left(\min_i D_{ii}\right)^{-1}, \end{aligned}$$

so that

$$\kappa_{H_Y}(H_X) = \kappa_2(D).$$

Similarly we find

$$\begin{aligned} \|H_\theta\|_{H_Y, H_Y^{-1}} &= \max_{\mathbf{v}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{\mathbf{v}^T H_\theta \mathbf{v}}{\mathbf{v} H_Y \mathbf{v}} = \max_i D_{ii}^{1-\theta}, \\ \|H_\theta^{-1}\|_{H_Y^{-1}, H_Y} &= \max_{\mathbf{v}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{\mathbf{v}^T H_0^{-1} \mathbf{v}}{\mathbf{v} H_1^{-1} \mathbf{v}} = \left(\min_i D_{ii}^{1-\theta}\right)^{-1}, \end{aligned}$$

so that

$$\kappa_{H_Y}(H_\theta) = \left(\kappa_2(D)\right)^{1-\theta},$$

which is the stated result. ∎

3.2. Dual spaces. The dense inclusion (2.3) leads to the following inclusion corresponding to the respective dual spaces:

$$Y' \subset [X,Y]'_\theta \subset X'. \tag{3.7}$$

Moreover, the following duality result can be found in [38, Theorem 6.2]:

$$[X,Y]'_\theta = [Y', X']_{\theta'}, \quad \theta' = 1-\theta. \tag{3.8}$$

Before we consider the matrix representation of norms on finite-dimensional subspaces of $[X,Y]'_\theta$ we introduce notation and some standard concepts regarding finite-dimensional dual spaces. Let V be a finite-dimensional linear space and let $\mathcal{H} =$

$(V, (\cdot,\cdot)_{\mathcal{H}})$ be a Hilbert space spanned by $\{\phi_i\}_{1\le i\le n}$, with dual $\mathcal{H}' = (V, (\cdot,\cdot)_{\mathcal{H}'})$ spanned by the basis $\{\phi'_i\}_{1\le i\le n}$ dual to $\{\phi_i\}$, i.e.,

$$\langle \phi'_i, \phi_j\rangle_{\mathcal{H}',\mathcal{H}} := \phi'_i(\phi_j) = \delta_{ij}.$$

Let $u \in \mathcal{H}, v' \in \mathcal{H}'$ have coefficients $(\mathbf{u})_i, (\mathbf{v}')_i$ with respect to the natural and dual bases of $\mathcal{H}, \mathcal{H}'$, respectively. Then

$$\langle v', u\rangle_{\mathcal{H}',\mathcal{H}} = v'(u) = (\mathbf{v}')^T\mathbf{u}.$$

By the Riesz representation theorem, given $v' \in \mathcal{H}'$, there is an element $v \in \mathcal{H}$ such that $v'(u) = (v,u)_{\mathcal{H}}$ for all $u \in \mathcal{H}$ with $\|v'\|_{\mathcal{H}'} = \|v\|_{\mathcal{H}}$. Let H, H' denote the Grammians

$$H_{ij} = (\phi_i, \phi_j)_{\mathcal{H}}, \quad H'_{ij} = \left(\phi'_i, \phi'_j\right)_{\mathcal{H}'}.$$

Then

$$\|\mathbf{v}\|_H = \|v\|_{\mathcal{H}} = \|v'\|_{\mathcal{H}'} = \sup_{w\in\mathcal{H}\setminus\{0\}} \frac{v'(w)}{\|w\|_{\mathcal{H}}} = \max_{\mathbf{w}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{(\mathbf{v}')^T\mathbf{w}}{\|\mathbf{w}\|_H} = \|\mathbf{v}'\|_{H^{-1}} = \|\mathbf{v}'\|_{H'}.$$

Hence, the matrix representation in the dual basis $\{\phi'_i\}$ of the norm $\|\cdot\|_{\mathcal{H}'}$ is $H' = H^{-1}$, with the representer v of v' having coefficients in the natural basis given by $\mathbf{v} = H^{-1}\mathbf{v}'$.

Let $X'_h = (V_h, \|\cdot\|_{X'}), Y'_h = (V_h, \|\cdot\|_{Y'})$ be finite-dimensional subspaces of X', Y', respectively, with the indicated induced norm topologies. As before, we define positive self-adjoint operators $\mathcal{J}'_h, \mathcal{E}'_h : Y'_h \to X'_h$:

$$(u'_h, v'_h)_{Y'} = (u'_h, \mathcal{J}'_h v'_h)_{X'}, \qquad u'_h, v'_h \in Y'_h, \tag{3.9}$$

where $\mathcal{J}'_h$ is positive self-adjoint and $\mathcal{E}'_h = (\mathcal{J}'_h)^{1/2}$. We define the discrete interpolation spaces

$$[Y'_h, X'_h]_\theta := D((\mathcal{E}'_h)^{\theta'}) = (V_h, \|\cdot\|_{\theta',h}),$$

where $\|\cdot\|_{\theta',h}$ is the scale of graph norms

$$\|u_h\|_{\theta',h} := \left(\|u_h\|^2_{X'} + \|\left(\mathcal{E}'_h\right)^{1-\theta'} u_h\|^2_{X'}\right)^{1/2}. \tag{3.10}$$

As before, the norm $\|\cdot\|_{\theta',h}$, with matrix representation $H'_{\theta',h}$, can be shown equivalent to a reduced norm with matrix representation $H'_{\theta'}$ which in turn can be seen to be simply the inverse of H_θ:

$$H'_{\theta',h} = H'_X + H'_X(J')^{1-\theta'} \sim H'_{\theta'} := H'_X(J')^{1-\theta'},$$

where

$$H'_{\theta'} = H_X^{-1}(H_X H_Y^{-1})^\theta = Q^{-1}D^{\theta-1}Q^{-T} = J^{\theta-1}H_Y^{-1} = H_\theta^{-1}. \tag{3.11}$$

Hence, H_θ^{-1} can be taken to be the matrix representation of a norm on $[X_h, Y_h]'_\theta$.

Remark 3.2. This choice corresponds to the definition of the matrix representation of a dual norm on a finite-dimensional space spanned by a dual basis as given in [35, page 275]:

$$\|\mathbf{z}\|^D := \max_{\mathbf{v}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{\mathbf{v}^T\mathbf{z}}{\|\mathbf{v}\|_H} = \|\mathbf{z}\|_{H^{-1}}.$$

Note, however, that $H'_{\theta',h}$ and $H^{-1}_{\theta,h}$ can be shown only to be spectrally equivalent.

4. Fractional Sobolev spaces. In this section we consider the case where X, Y are Sobolev spaces. In particular, we are interested in deriving the matrix representations of fractional Sobolev norms with a view to designing optimal iterative solution methods for finite element discretizations of PDEs. We start by reviewing some standard definitions and results.

Let Ω denote an open bounded subset of $\mathbb{R}^n$ with smooth boundary Γ and let $\boldsymbol{\alpha}$ denote a multi-index of order m, where m is a positive integer. Let

$$H^m(\Omega) = \left\{u : D^{\boldsymbol{\alpha}} u \in L^2(\Omega), \quad |\boldsymbol{\alpha}| \le m\right\}$$

denote the usual Sobolev space of order m, with the convention that $H^0(\Omega) = L^2(\Omega)$. Sobolev spaces of real index $0 \le s \le m$ are defined as interpolation spaces of index $\theta = 1 - s/m$ for the pair $[H^m(\Omega), H^0(\Omega)]$:

$$H^s(\Omega) := [H^m(\Omega), H^0(\Omega)]_\theta. \tag{4.1}$$

One can use this definition to characterize interpolation spaces for pairs of Sobolev spaces of real index:

$$[H^{s_1}(\Omega), H^{s_2}(\Omega)]_\theta = H^{(1-\theta)s_1+\theta s_2}(\Omega).$$

Now let $C_0^\infty(\Omega)$ denote the space of infinitely differentiable functions with compact support in Ω and let $H_0^s(\Omega)$ denote the completion of $C_0^\infty(\Omega)$ in $H^s(\Omega)$, where $s > 0$. Then

$$\begin{cases} H_0^s(\Omega) = H^s(\Omega), & s \le 1/2, \\ H_0^s(\Omega) \subset H^s(\Omega), & s > 1/2. \end{cases}$$

In fact, given $0 \le s_2 < s_1$, one has the following characterizations based on interpolation:

$$\begin{cases} [H_0^{s_1}(\Omega), H_0^{s_2}(\Omega)]_\theta = H_0^{(1-\theta)s_1+\theta s_2}(\Omega) & \text{if } (1-\theta)s_1 + \theta s_2 \ne k + 1/2, \\ [H_0^{s_1}(\Omega), H_0^{s_2}(\Omega)]_\theta \subset H_0^{(1-\theta)s_1+\theta s_2}(\Omega) & \text{if } (1-\theta)s_1 + \theta s_2 = k + 1/2, \end{cases} \tag{4.2}$$

with $k \in \mathbb{N}$. In particular, the choice $s_1 = k+1, s_2 = k$ yields

$$[H_0^{k+1}(\Omega), H_0^k(\Omega)]_\theta = H_0^{k+1-\theta}(\Omega) \quad \text{if } \theta \ne 1/2, \tag{4.3}$$

while for $\theta = 1/2$ we define

$$H_{00}^{k+1/2}(\Omega) := \left[H_0^{k+1}(\Omega), H_0^k(\Omega)\right]_{1/2} \subset H_0^{k+1/2}(\Omega). \tag{4.4}$$

Finally, we define for $s > 0$

$$H^{-s}(\Omega) = (H_0^s(\Omega))'.$$

Now let $0 \le s_1 < s_2$. Then, for $(1-\theta)s_1 + \theta s_2 \ne k + 1/2 \quad (k \in \mathbb{N})$

$$[H^{-s_1}(\Omega), H^{-s_2}(\Omega)]_\theta = H^{-(1-\theta)s_1-\theta s_2}(\Omega),$$

while if $(1-\theta)s_1 + \theta s_2 = k + 1/2 \quad (k \in \mathbb{N})$,

$$[H^{-s_1}(\Omega), H^{-s_2}(\Omega)]_\theta = \left(H_{00}^{k+1/2}(\Omega)\right)'.$$

4.1. Special domains. The open Ω can be replaced by a regular manifold, and the Sobolev spaces are built using a variational formulation based on the Laplace–Beltrami operator. The resulting Hilbert spaces can be used to build by the same techniques presented in section 2 the corresponding fractional Sobolev spaces (see [38, page 42]).

Another choice for Ω is to be a metric graph (in the literature these are also named quantum graphs). This choice will be used in section 7.1 (see Remark 7.1). A metric graph is a graph $G = (\mathbb{V}, \mathbb{E})$ made of vertices $v \in \mathbb{V}$ and edges $e \in \mathbb{E}$ each with associated length $\ell(e)$. For the sake of simplicity, we assume that $\ell(e) < \infty$ for all $e \in \mathbb{E}$ and that the number of vertices and edges is finite.

The degree of a vertex is the number of incident edges on it, and the boundary of G consists of the vertices of degree one. Moreover, an edge can be identified with a finite segment of the real line such that we can introduce a coordinate $x(e)$ and a preferred direction of the edge. This defines a natural topology on the graph and makes it a one-dimensional simplicial complex. As a consequence we can define a function $f(x)$ on G at all points of the graph and not only at its vertices. Moreover, we can define the Lebesgue measure on G which allows the introduction of some standard Sobolev function spaces on the graph.

DEFINITION 4.1. *The space $L^2(G)$ consists of all measurable and square integrable functions on each edge e and such that*

$$||f||^2_{L^2(G)} = \sum_{e\in\mathbb{E}} ||f||^2_{L^2(e)} < \infty.$$

DEFINITION 4.2. *The Sobolev space $H^1(G)$ consists of all continuous functions on G that belong to $H^1(e)$ for each edge e and such that*

$$\sum_{e\in\mathbb{E}} ||f||^2_{H^1(e)} < \infty.$$

We can also define the space $H^1_0(G)$ adding the condition that the functions $f(x) \in H^1(G)$ take zero values at the boundary vertices.

A friendly but accurate introduction and survey on quantum graphs is given by Kuchment [37]. In [37] is also observed that there is no natural definition of Sobolev spaces $H^k(G)$ of order k higher than 1, due to the lack of natural conditions at the vertices. For the Laplace operators and the case $k = 2$ it is possible to introduce Neumann–Kirchoff conditions at the internal vertices that allow a consistent definition of the eigenvalue problem (see [29]).

However, taking into account the two previous definitions and the Hilbert structure of $L^2(G)$ and $H^1(G)$ we can still introduce the corresponding fractional Sobolev spaces by the interpolation method.

4.2. Discrete fractional Sobolev norms. The results from the previous section can be used to derive discrete Sobolev norms for some standard pairs. We consider below some examples which arise naturally in the formulation of elliptic PDEs. In particular, Sobolev spaces of index "integer+1/2" will be the focus of our discussion since they arise naturally as ranges of boundary operators.

We start, however, with the general case and derive the matrix representation of a norm defined on a finite-dimensional subspace of the interpolation space (see (4.3))

$$H_0^{k+1-\theta}(\Omega) = [H_0^{k+1}(\Omega), H_0^k(\Omega)]_\theta, \quad \theta \neq 1/2.$$

Let $X = H_0^{k+1}(\Omega), Y = H_0^k(\Omega)$ and let $V_h = \text{span}\{\phi\}_{1\leq i\leq n}$ be a subset of X. Let $X_h = (V_h, (\cdot,\cdot)_X), Y_h = (V_h, (\cdot,\cdot)_Y)$ be two finite-dimensional subspaces of X, Y with the induced topology. Let $L_k \in \mathbb{R}^{n\times n}$ denote the Grammian matrices corresponding to the $H^k(\Omega)$-inner product:

$$(L_k)_{ij} = (\phi_i, \phi_j)_{H^k(\Omega)}.$$

Using the results of section 2, we find $J = L_k^{-1}L_{k+1}$ and a matrix representation for a norm on the interpolation space $[X_h, Y_h]_\theta$ is given by

$$H_{k+1-\theta} := L_k J^{1-\theta} = L_k(L_k^{-1}L_{k+1})^{1-\theta}.$$

Similarly, a matrix representation for a norm on a finite-dimensional subspace of

$$H_{00}^{k+1/2}(\Omega) := [H_0^{k+1}(\Omega), H_0^k(\Omega)]_{1/2}$$

is given by setting $\theta = 1/2$ in the expression for $H_{k+1-\theta}$ above:

$$H_{k+1/2} := L_k J^{1/2} = L_k(L_k^{-1}L_{k+1})^{1/2},$$

which simplifies in the case when the matrices L_k are simultaneously diagonalizable to the expression derived in [14] for the case of wavelet bases

$$H_{k+1/2} = L_k^{1/4}L_{k+1}^{1/2}L_k^{1/4}.$$

Note the abuse of notation: the matrix H_θ in the previous section and the matrices $H_{k+\theta}$ defined above have different definitions. Note also that different choices of L_k lead to different discrete norms, though they are all equivalent with constants of equivalence independent of n. We illustrate the above derivation with examples corresponding to $k = 0$ and $k = 1$.

Example 4.1. *Let $X = H_0^1(\Omega), Y = L^2(\Omega)$. We wish to derive the matrix representation of a norm defined on a discrete subspace of the interpolation space*

$$H_{00}^{1/2}(\Omega) = [H_0^1(\Omega), L^2(\Omega)]_{1/2}.$$

Using the notation introduced above we let $L_1, L_0 \in \mathbb{R}^{n\times n}$ denote the Grammian matrices of the basis functions $\{\phi_i\}$ in the following inner products:

$$(L_1)_{ij} = (\nabla\phi_i, \nabla\phi_j)_{L^2(\Omega)}, \qquad (L_0)_{ij} = (\phi_i, \phi_j)_{L^2(\Omega)}.$$

The matrix L_0 is a discrete identity, while the matrix L_1 is a discrete Dirichlet Laplacian. Therefore, $J = L_0^{-1}L_1$ and a norm for the interpolation space $[X_h, Y_h]_\theta$ is induced by the matrix

$$H_\theta = L_0 J^{1-\theta} = L_0(L_0^{-1}L_1)^{1-\theta}.$$

If L_0, L_1 are simultaneously diagonalizable (as is the case for a uniform subdivision of Ω), the expression for H_θ becomes

$$H_\theta = L_0^\theta L_1^{1-\theta} = L_0^{\theta/2}L_1^{1-\theta}L_0^{\theta/2}.$$

In particular, if $\theta = 1/2$, we find

$$H_{1/2} = L_0^{1/4}L_1^{1/2}L_0^{1/4}.$$

EXAMPLE 4.2. *Let $X = H_0^2(\Omega), Y = H_0^1(\Omega)$. We wish to derive a matrix representation for a norm defined on a finite-dimensional subspace of $H_{00}^{3/2}(\Omega)$. We consider two characterizations for this space (cf.* (4.2)*):*

$$H_{00}^{3/2}(\Omega) = [H_0^2(\Omega), H_0^1(\Omega)]_{1/2} = [H_0^2(\Omega), L^2(\Omega)]_{1/4}.$$

We similarly define the following Grammian matrices:

$$(L_2)_{ij} = (\Delta\phi_i, \Delta\phi_j)_{L^2(\Omega)}, \qquad (L_1)_{ij} = (\nabla\phi_i, \nabla\phi_j)_{L^2(\Omega)}, \qquad (L_0)_{ij} = (\phi_i, \phi_j)_{L^2(\Omega)}.$$

The matrix L_0 is a discrete identity and the matrix L_1 is a discrete Dirichlet Laplacian, while the matrix L_2 is the discretization of a biharmonic operator with homogeneous boundary conditions. A discrete norm is therefore induced by either of the following matrices:

$$H_{3/2} = L_1(L_1^{-1}L_2)^{1/2} \quad \text{or} \quad H_{3/2} = L_0(L_0^{-1}L_2)^{3/4},$$

which, in the case of simultaneous diagonalization, simplifies to

$$H_{3/2} = L_1^{1/4}L_2^{1/2}L_1^{1/4} \quad \text{or} \quad H_{3/2} = L_0^{1/8}L_2^{3/4}L_0^{1/8}.$$

Remark 4.1. In both examples above, the choice of norms for the spaces $H_0^k(\Omega)$ is not unique. One could choose to define L_1 in terms of the (equivalent) full norm of $H_0^1(\Omega)$:

$$(L_1)_{ij} = (\phi_i, \phi_j)_{L^2(\Omega)} + (\nabla\phi_i, \nabla\phi_j)_{L^2(\Omega)}.$$

The same can be said about L_2. The resulting discrete norms will therefore be different from, but equivalent to, the norms derived above.

Remark 4.2. The spectral condition number of the matrices L_k (and therefore $\kappa_{L_0}(L_k)$) is known to be of the order n^{2k} for certain finite-dimensional spaces, such as those arising from quasi-uniform finite element or finite difference discretizations (see Proposition 6.2). One can then use Lemma 3.3 to establish the conditioning of the above matrix representations:

$$\kappa_2(H_{1/2}) \sim \kappa_{L_0}(L_1) = (n^2)^{(1-1/2)} = n,$$
$$\kappa_2(H_{3/2}) \sim \kappa_{L_0}(L_2) = (n^4)^{(1-1/4)} = n^3.$$

We consider now the case of fractional Sobolev spaces of negative index and the corresponding discrete norms. Consider the dual of the interpolation space

$$\left(H_0^{k+1-\theta}(\Omega)\right)' = [H^{-k}(\Omega), H^{-(k+1)}(\Omega)]_{1-\theta} = \left([H_0^{k+1}(\Omega), H_0^k(\Omega)]_\theta\right)' =: H^{-k+\theta-1}(\Omega).$$

Let X_h, Y_h be defined as above. Let $\{\phi_i'\}_{1\le i\le n}$ be a basis of V_h dual to $\{\phi_i\}$ with respect to the duality pairing $\langle\cdot,\cdot\rangle_{Y_h'\times Y_h}$. We are interested in deriving a matrix representation for a norm on $[X_h, Y_h]_\theta' = [Y_h', X_h']_{\theta'}$. We define a reduced matrix representation of the norm on this space in the usual way using the fact that the matrix representations of norms on $H^{-k}(\Omega) = (H_0^k(\Omega))'$ are $L_{-k} := L_k^{-1}$:

$$H'_{-k-\theta'} := L_{-(k+1)}(L_{-(k+1)}^{-1}L_{-k})^{1-\theta'}.$$

Then it is easy to see that

$$H'_{-k-\theta'} = H'_{-k+\theta-1} = H^{-1}_{k+1-\theta},$$

which corresponds to derivation (3.11).

The matrix $H'_{-k+\theta-1}$ is the representation *with respect to the dual basis* for a norm on a finite-dimensional subspace of $H^{-k+\theta-1}(\Omega)$. We wish to derive a representation also with respect to the (natural) basis $\{\phi_i\}_{1\leq i\leq n}$. Let $v' \in Y'_h$ have representer $v \in Y_h$. The corresponding coefficients $\mathbf{v}', \mathbf{v}$ will satisfy $\mathbf{v}' = L_k\mathbf{v}$ (see section 3.2). Hence

$$\|\mathbf{v}'\|_{H'_{-k-\theta'}} = \|L_k\mathbf{v}\|_{H'_{-k-\theta'}} = \|\mathbf{v}\|_{L_k H'_{-k-\theta'} L_k}$$

so that the matrix representation for a norm on $[X_h, Y_h]'_\theta$ with respect to the basis $\{\phi_i\}_{1\leq i\leq n}$ is

$$H_{-k-\theta'} := L_k H'_{-k-\theta'} L_k = L_k H^{-1}_{k+1-\theta} L_k = L_k(L_k^{-1}L_{k+1})^{\theta-1}.$$

In particular, in the case $\theta = 1/2$ we find a matrix representation for a norm defined on a finite-dimensional subspace of $(H^{1/2}_{00}(\Omega))'$:

$$H_{-k-1/2} = L_k(L_k^{-1}L_{k+1})^{-1/2}.$$

EXAMPLE 4.3. *Let $X = H^1_0(\Omega), Y = L^2(\Omega)$ and let X_h, Y_h be defined as above. Then a discrete norm on $[X_h, Y_h]'_{1/2} \subset (H^{1/2}_{00}(\Omega))'$ is given by*

$$H_{-1/2} = L_0(L_0^{-1}L_1)^{-1/2}, \tag{4.5}$$

which in the case of simultaneous diagonalization of L_0, L_1 can be written as

$$H_{-1/2} = L_0^{3/4}L_1^{-1/2}L_0^{3/4}.$$

We end with a remark concerning finite element subspaces of Sobolev spaces, which is the choice we employ when we consider the numerical examples of section 6.

Remark 4.3. Let the basis functions $\{\phi_i\}_{1\leq i\leq n}$ for X_h be continuous piecewise polynomials defined on a given subdivision of a polyhedral domain Ω into regular simplices of maximum diameter h. In this case, it is known (see [10]) that the piecewise polynomial interpolant I_h satisfies

$$\|v - I_h v\|_{H^m(\Omega)} \leq C\|v\|_{H^m(\Omega)}$$

so that

$$\|I_h v\|_{H^m(\Omega)} \leq (1 + C)\|v\|_{H^m(\Omega)}$$

for some constant C independent of h. Thus, $I_h \in \mathcal{L}(X, X_h) \cap \mathcal{L}(Y, Y_h)$ and also I_h satisfies the inequalities (2.5). Hence, Lemma 2.3 applies for general conforming finite element discretizations under standard regularity conditions on Ω and its corresponding subdivision into simplices. In particular, the fractional Sobolev scale of norms $\|\cdot\|_{k+1-\theta}$ is equivalent on $[X_h, Y_h]_\theta$ to the discrete norms induced by the family of matrices $H_{k+1-\theta}$ introduced above for $\theta \in (0, 1)$.

5. Evaluation of $\boldsymbol{H_\theta}$. In order to construct and apply in a practical application any of the discrete norms derived in the previous discussion we are required to evaluate (noninteger) powers of a matrix. This task may be achieved in different ways for different applications. In general, if the dimension of the problem is low, one can employ a direct method based on a generalized eigenvalue decomposition. This approach has complexity of order $O(n^3)$. Another direct approach is available in the case when the matrices involved have a Toeplitz structure; in this case the evaluation can be achieved via an FFT (see [44]) and the complexity is $O(n \log n)$. In both cases the storage requirements are of order $O(n^2)$. For larger problems, iterative techniques may represent a cheaper alternative. An example in case is Newton's method [34], which has attractive convergence properties under a suitable implementation. However, the complexity of the method is that of a direct method, even if the original matrix is sparse. One expects that for sparse matrices one can devise efficient techniques for evaluating H_θ or its action applied to a given vector. This is indeed the case. In [32] the authors propose a method based on representing a function of a matrix as an integral which they go on to evaluate using efficient quadrature rules. The method can be adapted to provide a sparse algorithm for the evaluation of H_θ. Another approach is to construct approximations of Krylov type which are known to take advantage of the sparsity of the matrices involved. Several authors have considered this approach for general matrix functions [20], [15], [21], [19], [46], [2], [26], and some convergence analysis is available for certain algorithms proposed for the computation of the matrix square root function [20]. We illustrate below the Krylov subspace approximation for the case $\theta = 1/2$.

5.1. A generalized Lanczos algorithm. Given a pair of symmetric and positive definite matrices (M, A), the generalized Lanczos algorithm constructs a set of M-orthogonal vectors $\mathbf{v}_i$ such that

$$AV_k = MV_kT_k + \beta_{k+1}M\mathbf{v}_{k+1}\mathbf{e}_k^T, \quad V_k^TMV_k = I_k,$$

where the columns $\mathbf{v}_i$ of $V_k = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k]$ are known as the Lanczos vectors and $I_k \in \mathbb{R}^{k\times k}$ is the identity matrix with kth column denoted by $\mathbf{e}_k$, while the matrix $T_k \in \mathbb{R}^{k\times k}$ is a symmetric and tridiagonal matrix [43]. The standard algorithm corresponds to the case $M = I$. Note that T_k can be seen as a projection of A onto the space spanned by the M-orthogonal columns of V_k:

$$V_k^TAV_k = T_k, \quad V_k^TMV_k = I_k. \tag{5.1}$$

In exact arithmetic, when $k = n$, the algorithm can be seen as providing simultaneous factorizations of the matrix pair (M, A) as

$$A = V_n^{-T}T_nV_n^{-1}, \quad M = V_n^{-T}V_n^{-1}.$$

We recall the algorithm below [43].

The explicit form of T_k is given below:

$$T_k = \mathrm{tridiag}[\boldsymbol{\beta}, \boldsymbol{\alpha}, \boldsymbol{\beta}] = \begin{pmatrix} \alpha_1 & \beta_2 & & 0 \\ \beta_2 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \beta_k \\ 0 & & \beta_k & \alpha_k \end{pmatrix}.$$

ALGORITHM 1. Generalized Lanczos Algorithm

Input: $A, M \in \mathbb{R}^{n\times n}(\text{spd}), \mathbf{v} \in \mathbb{R}^n$
Output: $V_k \in \mathbb{R}^{n\times k}, T_k \in \mathbb{R}^{k\times k}$

```
Set β_1 = 0, v_0 = 0, v_1 = v/‖v‖_M
for i = 1 : k
   w_i = M^{-1} A v_i − β_i v_{i−1}
   α_i = (w_i, v_i)_M
   w_i = w_i − α_i v_i
   β_{i+1} = ‖w_i‖_M
   if β_{i+1} = 0 stop
   v_{i+1} = w_i/β_{i+1}
end
T_k = tridiag[β, α, β]
```

Consider now the generalized Lanczos factorization for the matrix pair (H_Y, H_X):

$$H_X V = H_Y V T, \qquad V^T H_Y V = I, \tag{5.2}$$

where we used the notation $V = V_n, T = T_n$. We can immediately derive the following result.

LEMMA 5.1. *Let* (5.2) *hold and let* $H_{\theta,h} = H_Y + H_Y J^{1-\theta}$ *and* $H_\theta = H_Y J^{1-\theta}$ *with* $J = H_Y^{-1} H_X$. *Then*

$$H_\theta = \left(V T^{\theta-1} V^T\right)^{-1} = H_Y V T^{1-\theta} V^T H_Y \tag{5.3}$$

and

$$H_{\theta,h} = \left(V(I + T^{1-\theta})^{-1} V^T\right)^{-1} = H_Y V (I + T^{1-\theta}) V^T H_Y. \tag{5.4}$$

5.2. Sparse evaluation of $H_\theta \mathbf{z}$. The complexity of the full ($k = n$) generalized Lanczos algorithm is in general $O(n^3)$. However, in many applications of interest we do not need to compute H_θ but simply apply it (or its inverse) to a given vector $\mathbf{z} \in \mathbb{R}^n$. In such cases, a truncated version of the algorithm is used in practice with only k Lanczos vectors being constructed. As we are interested in approximations of $H_\theta \mathbf{z}$ we note first that if we start the Lanczos process with $\mathbf{v} = \mathbf{z}$, then

$$V_k^T H_Y \mathbf{z} = \mathbf{e}_1 \|\mathbf{z}\|_{H_Y},$$

where $\mathbf{e}_1 \in \mathbb{R}^k$ is the first column of the identity I_k. This leads us to consider the following approximations of the matrix-vector products:

$$H_\theta \mathbf{z} \approx H_Y V_k T_k^{1-\theta} \mathbf{e}_1 \|\mathbf{z}\|_{H_Y}$$

and

$$H_{\theta,h} \mathbf{z} \approx H_Y V_k (I_k + T_k^{1-\theta}) \mathbf{e}_1 \|\mathbf{z}\|_{H_Y}.$$

Similarly, if we wish to apply the inverse of H_θ to a given vector $\mathbf{z}$, we first note that if we start the iteration with $\mathbf{v} = H_Y^{-1}\mathbf{z}$, then

$$V_k^T \mathbf{z} = V_k^T H_Y (H_Y)^{-1} \mathbf{z} = \mathbf{e}_1 \|H_Y^{-1}\mathbf{z}\|_{H_Y} = \mathbf{e}_1 \|\mathbf{z}\|_{H_Y^{-1}}.$$

This leads us to consider the following approximations (cf. Lemma 5.1):

$$H_\theta^{-1}\mathbf{z} \approx V_k T_k^{\theta-1} V_k^T \mathbf{z} = V_k T_k^{\theta-1} \mathbf{e}_1 \|\mathbf{z}\|_{H_Y^{-1}}$$

and

$$H_{\theta,h}^{-1}\mathbf{z} \approx V_k \left(I_k + T_k^{1-\theta}\right)^{-1} V_k^T \mathbf{z} = V_k \left(I_k + T_k^{1-\theta}\right)^{-1} \mathbf{e}_1 \|\mathbf{z}\|_{H_Y^{-1}}.$$

The complexity of the above operations depends on the complexity corresponding to the application of the inverse of H_Y. If this operation can be achieved in $O(n)$ operations, then the overall complexity of computing $H_\theta \mathbf{z}, H_\theta^{-1}\mathbf{z}$ is of order $O(kn)$ for $k \ll n$, with storage requirements of the same order.

6. Applications.

6.1. Preconditioners for the Steklov–Poincaré operator. Domain decomposition (DD) methods require the solution of a problem which involves a pseudo-differential operator defined on a Sobolev space of functions with domain the set of boundaries defined by the decomposition of the domain. This operator is generally known as the Steklov–Poincaré operator or the Dirichlet–Neumann map, though this definition was introduced for DD methods applied to second-order problems involving the Laplacian operator. A great number of iterative approaches have been proposed in the literature over the last two decades; classical algorithms include Dirichlet–Neumann, Neumann–Neumann, FETI methods, and Schwarz methods together with two-level and overlapping variants. Complete descriptions and analyses can be found in a range of references; see, for example, [53] and [45]. While most methods approximate implicitly the Steklov–Poincaré operator, there are also some approaches which target it directly: Dryja considered the square root of the Laplacian operator in [22], [23] (also analyzed in [16]), while Bramble, Pasciak, and Schatz [8] considered another local representation of discrete fractional Sobolev norms for preconditioning this interface operator (see also the multilevel representation of fractional Sobolev norms in [9]). Finally, [54] considered the restriction to the interface of the fundamental solution defined on an imbedding domain, while Chan and Mathew [17] proposed an algebraic construction through a so-called probing technique. We present below an alternative using discrete interpolation norms, which in some sense is related to the square root Laplacian of Dryja but which is cast in a different context, is more general, and affords a general analysis.

6.1.1. A model problem. Let Ω be an open subset of $\mathbb{R}^d$ with boundary $\partial\Omega$ and consider the model problem

$$\left\{\begin{array}{rll} -\Delta u & = f & \text{in } \Omega, \\ u & = 0 & \text{on } \partial\Omega. \end{array}\right. \tag{6.1}$$

Given a partition of Ω into two subdomains $\Omega \equiv \Omega_1 \cup \Omega_2$ with common boundary Γ this problem can be equivalently written as

$$\left\{\begin{array}{rll} -\Delta u_1 & = f & \text{in } \Omega_1, \\ u_1 & = 0 & \text{on } \partial\Omega_1 \setminus \Gamma, \end{array}\right. \qquad \left\{\begin{array}{rll} -\Delta u_2 & = f & \text{in } \Omega_2, \\ u_2 & = 0 & \text{on } \partial\Omega_2 \setminus \Gamma, \end{array}\right.$$

with the "interface conditions"

$$\left\{\begin{array}{rcl} u_1 & = & u_2, \\ \frac{\partial u_1}{\partial n_1} & = & -\frac{\partial u_2}{\partial n_2} \end{array}\right. \quad \text{on } \Gamma.$$

Now let $\lambda_1, \lambda_2 \in H_{00}^{1/2}(\Gamma)$ and, correspondingly, let ψ_1, ψ_2 denote the harmonic extensions of λ_1, λ_2, respectively, into Ω_1, Ω_2; i.e., for $i = 1, 2$, ψ_i satisfy

$$\begin{cases} -\Delta\psi_i &= 0 \qquad \text{in } \Omega_i, \\ \quad \psi_i &= \lambda_i \qquad \text{on } \Gamma, \\ \quad \psi_i &= 0 \qquad \text{on } \partial\Omega_i \setminus \Gamma. \end{cases}$$

Let $H_{00}^{1/2}(\Gamma) = [H_0^1(\Gamma), L_2(\Gamma)]_{1/2}$. We define the Steklov–Poincaré operator $\mathcal{S}$: $H_{00}^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ via

$$(\mathcal{S}\lambda_1, \lambda_2)_{H^{1/2}(\Gamma)} = (\nabla\psi_1, \nabla\psi_2)_{L^2(\Omega)} =: s(\lambda_1, \lambda_2). \tag{6.2}$$

Note that we also defined a bilinear form $s(\cdot, \cdot) : H_{00}^{1/2}(\Gamma) \times H_{00}^{1/2}(\Gamma) \to \mathbb{R}$ which can be seen to be symmetric and positive definite. One can show further that this bilinear form is also $H_{00}^{1/2}(\Gamma)$-elliptic; i.e., there exist constants c_1, c_2 such that for all $\lambda \in H_{00}^{1/2}(\Gamma)$

$$c_1\|\lambda\|^2_{H^{1/2}(\Gamma)} \leq s(\lambda, \lambda) \leq c_2\|\lambda\|^2_{H^{1/2}(\Gamma)}. \tag{6.3}$$

With this definition of $\mathcal{S}$ our model problem can be recast as a sequence of three decoupled problems involving Poisson problems on each subdomain together with a problem set on the interface Γ:

$$\text{(i)} \quad \begin{cases} -\Delta u_i^{\{1\}} &= f \quad \text{in } \Omega_i, \\ \quad u_i^{\{1\}} &= 0 \quad \text{on } \partial\Omega_i, \end{cases}$$

$$\text{(ii)} \quad \left\{ \ \mathcal{S}\lambda = -\frac{\partial u_1^{\{1\}}}{\partial n_1} - \frac{\partial u_2^{\{1\}}}{\partial n_2} \quad \text{on } \Gamma, \right.$$

$$\text{(iii)} \quad \begin{cases} -\Delta u_i^{\{2\}} &= 0 \quad \text{in } \Omega_i, \\ \quad u_i^{\{2\}} &= \lambda \quad \text{on } \partial\Omega_i. \end{cases}$$

The resulting solution is

$$u|_{\Omega_i} = u_i^{\{1\}} + u_i^{\{2\}}.$$

6.1.2. Discrete formulation. Let $P_r(U)$ denote the space of polynomials in two variables of degree r defined on a set $U \subset \mathbb{R}^2$. Let

$$V^h = V^{h,r} := \left\{ w \in C^0(\Omega) : w|_T \in P_k \ \ \forall T \in \mathcal{T}_h \right\} \subset H^1(\Omega) \tag{6.4}$$

be a finite-dimensional space of piecewise polynomial functions defined on some subdivision $\mathcal{T}_h$ of Ω into simplices T of maximum diameter h. Further, let $V_I^h, V_B^h \subset V^h$ satisfy $V_I^h \oplus V_B^H \equiv V^h$, where $V_I^h = \left\{ w \in V^h : w|_{\partial\Omega} = 0 \right\}$. Let $X_h \subset H_0^1(\Gamma)$ denote the space spanned by the restriction of the basis functions of V_I^h to the internal boundary Γ. The discrete variational formulation of model problem (6.1) reads as follows:

$$\begin{cases} \text{Find } u_h \in V_I^h \text{ such that } \forall v_h \in V_I^h \\ \qquad\qquad a(u_h, v_h) = f(v_h), \end{cases}$$

where

$$a(v,w) = (\nabla v, \nabla w)\,, \quad f(v) = (f, v)\,.$$

This formulation give rise to a linear system with the following structure:

$$\begin{pmatrix} A_{II,1} & 0 & A_{IB,1} \\ 0 & A_{II,2} & A_{IB,2} \\ A_{IB,1}^T & A_{IB,2}^T & A_{BB,1} + A_{BB,2} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{I,1} \\ \mathbf{u}_{I,2} \\ \mathbf{u}_B \end{pmatrix} = \begin{pmatrix} \mathbf{f}_{I,1} \\ \mathbf{f}_{I,2} \\ \mathbf{f}_B \end{pmatrix},$$

where $A_{II,i}, i = 1, 2$, are discrete Dirichlet Laplacians corresponding to the interior nodes of the computational domain Ω_i and $A_{BB,i}, i = 1, 2$, are the corresponding interior boundary contributions from each domain. The above system can be "decoupled" into three problems:

$$\begin{array}{ll} \text{(i)} & A_{II,i}\mathbf{u}_i^{\{1\}} = \mathbf{f}_{I,i}, \\ \text{(ii)} & S\mathbf{u}_B = \mathbf{f}_B - A_{IB,1}^T \mathbf{u}_1^{\{1\}} - A_{IB,2}^T \mathbf{u}_2^{\{2\}}, \\ \text{(iii)} & A_{II,i}\mathbf{u}_i^{\{2\}} = -A_{IB,1}^T \mathbf{u}_B - A_{IB,2}^T \mathbf{u}_B, \end{array}$$

where S is the Schur complement corresponding to the boundary nodes

$$S = S_1 + S_2, \quad S_i = A_{BB,i} - A_{IB,i}^T A_{II,i}^{-1} A_{IB,i}.$$

The resulting solution is $(\mathbf{u}_{I,1},\ \mathbf{u}_{I,2},\ \mathbf{u}_B)$, where

$$\mathbf{u}_{I,i} = \mathbf{u}_i^{\{1\}} + \mathbf{u}_i^{\{2\}}.$$

It is evident that these algebraic problems are finite element discretizations of the three continuous problems listed above (see [45] for full details). In particular, the Schur complement S is the finite element discretization of the variational definition (6.2) of the Steklov–Poincaré operator $\mathcal{S}$. Since $s(\cdot,\cdot)$ is $H_{00}^{1/2}(\Gamma)$-elliptic, we deduce that for any $\lambda_h \in X_h$ there holds

$$c_1 \|\lambda_h\|_{H^{1/2}(\Gamma)}^2 \le s(\lambda_h, \lambda_h) \le c_2 \|\lambda_h\|_{H^{1/2}(\Gamma)}^2. \tag{6.5}$$

Note that if we denote by $\boldsymbol{\lambda}$ the vector of coefficients of λ_h expanded in a finite element basis, then

$$s(\lambda_h, \lambda_h) = \boldsymbol{\lambda}^T S \boldsymbol{\lambda}.$$

6.1.3. $H_{00}^{1/2}$-preconditioners. For large problems, constructing and applying the inverse of the Schur complement S in step (ii) above is computationally prohibitive. Instead, the problem can be solved using a preconditioned iterative technique. For symmetric and positive definite problems it is known that optimal acceleration of an iterative method is achieved when a spectrally equivalent preconditioner P_S is employed. We show below that the matrix representation of an $H_{00}^{1/2}(\Gamma)$-norm has this property and can therefore be employed as a preconditioner for DD methods of scalar elliptic problems.

The inequalities (6.5) describe essentially the spectral equivalence between the discrete operator induced by the bilinear form $s(\cdot,\cdot)$ acting on a finite-dimensional subspace of $H_{00}^{1/2}(\Gamma) \times H_{00}^{1/2}(\Gamma)$ and a discrete representation of the $H_{00}^{1/2}$-norm. We make this statement precise below.

PROPOSITION 6.1. *Let* $X_h = \operatorname{span}\{\phi_i, 1 \le i \le m\}$ *be defined as above and let* $(L_k)_{ij} = (\phi_i, \phi_j)_{H_0^k(\Gamma)}$ *for* $k = 0, 1$. *Let*

$$H_{1/2} := L_0(L_0^{-1}L_1)^{1/2}.$$

Then for all $\boldsymbol{\lambda} \in \mathbb{R}^m \setminus \{\mathbf{0}\}$

$$\kappa_1 \le \frac{\boldsymbol{\lambda}^T S \boldsymbol{\lambda}}{\boldsymbol{\lambda}^T H_{1/2} \boldsymbol{\lambda}} \le \kappa_2$$

with κ_1, κ_2 *independent of* h.

Proof. Since Lemma 2.3 holds (see Remark 4.3) there exist constants η_1, η_2 such that for all $\lambda_h \in X_h$

$$\eta_1 \|\lambda_h\|_{1/2} \le \|\lambda_h\|_{\theta,h} \le \eta_2 \|\lambda_h\|_{1/2}.$$

The norm $\|\cdot\|_{\theta,h}$ has matrix representation $H_{1/2,h}$ which, by (3.6), is spectrally equivalent to $H_{1/2}$. Hence, there exist constants $\tilde{\eta}_1, \tilde{\eta}_2$ such that

$$\tilde{\eta}_1 \|\lambda_h\|_{1/2} \le \|\boldsymbol{\lambda}\|_{H_{1/2}} \le \tilde{\eta}_2 \|\lambda_h\|_{1/2}.$$

Using the $H_{00}^{1/2}$-ellipticity (6.5) of $s(\cdot,\cdot)$ we get

$$\frac{c_1}{\tilde{\eta}_2^2} \|\boldsymbol{\lambda}\|_{H_{1/2}}^2 \le \boldsymbol{\lambda}^T S \boldsymbol{\lambda} \le \frac{c_2}{\tilde{\eta}_1^2} \|\boldsymbol{\lambda}\|_{H_{1/2}}^2,$$

which is the required result. ∎

Remark 6.1. The matrix $H_{1/2}$ is the reduced version of the matrix representation for the norm $\|\cdot\|_{1/2,h}$. It is evident that the above result holds with $H_{1/2}$ replaced with $L_0 + L_0(L_0^{-1}L_1)^{1/2}$.

The above result indicates that S and $H_{1/2}$ exhibit the same spectral properties. In particular, the following result holds (cf. Remark 4.2).

PROPOSITION 6.2. *Let* $L_0, L_1 \in \mathbb{R}^m$ *be defined as in Proposition* 6.1. *Then*

$$\kappa_{L_0}(H_{1/2}) = O(h^{-1}) \quad \textit{and} \quad \kappa_{L_0}(S) = O(h^{-1}).$$

Proof. Since L_0 is a mass matrix and L_1 is a discrete Laplacian, by the Poincaré inequality there exists a constant γ_1 independent of h such that

$$\|\boldsymbol{\lambda}\|_{L_0} \le \gamma_1^{-1} \|\boldsymbol{\lambda}\|_{L_1}.$$

Furthermore, the following standard discrete inverse inequality is assumed to hold:

$$\|\boldsymbol{\lambda}\|_{L_1}^2 \le \gamma_2 h^{-2} \|\boldsymbol{\lambda}\|_{L_0}^2,$$

where γ_2 is also independent of h. Hence,

$$\gamma_1 \le \frac{\boldsymbol{\lambda}^T L_1 \boldsymbol{\lambda}}{\boldsymbol{\lambda}^T L_0 \boldsymbol{\lambda}} \le \gamma_2 h^{-2}$$

and therefore $\kappa_{L_0}(L_1) = O(h^{-2})$. Hence, by Lemma 3.3,

$$\kappa_{L_0}(H_{1/2}) = (\kappa_{L_0}(L_1))^{1/2} = O(h^{-1}).$$

The second statement follows from the spectral equivalence of $H_{1/2}$ and S derived in Proposition 6.1. ∎

Since $\|\cdot\|_{L_0}$ is equivalent to the Euclidean (l_2-) norm, we conclude that $\kappa_2(S) = O(h^{-1})$, which is the standard result on the condition number of the discrete Steklov–Poincaré operator [45]. This indicates that an iterative technique which ignores the Schur complement problem will be suboptimal. We verify in the numerical experiments section below that this is indeed the case and demonstrate that $H_{1/2}$ is a suitable preconditioner in this sense.

6.2. Boundary preconditioners for the biharmonic operator. Consider the biharmonic problem in a polygonal convex open domain $\Omega \subset \mathbb{R}^2$ with boundary $\Gamma = \cup_{i=1}^{K}\Gamma_i$:

$$\left\{\begin{aligned} \Delta^2 u &= f && \text{in } \Omega, \\ u = \partial u/\partial n &= 0 && \text{on } \Gamma. \end{aligned}\right. \tag{6.6}$$

A standard approach to solving (6.6) is to introduce another variable $v = -\Delta u$ and solve the resulting system:

$$\left\{\begin{aligned} -\Delta u &= f && \text{in } \Omega, \\ v + \Delta u &= 0 && \text{in } \Omega, \\ u = \partial u/\partial n &= 0 && \text{on } \Gamma. \end{aligned}\right. \tag{6.7}$$

There is a considerable literature on the topic of this model problem, both from the approximation point of view [39], [30], [5], [12], [18], [28] and also an algorithmic one [30], [44], [7], [50]. A notable approach is provided by Glowinski and Pironneau [30], who suggested for the first time preconditioning with a discrete $H^{-1/2}(\Gamma)$-norm. An analysis of their preconditioner was provided by Peisker [44] for the case of uniform discretizations. We briefly review this approach below.

6.2.1. The Pironneau–Glowinski method. The following reformulation of the biharmonic problem was introduced in [30]. Let $\lambda = v\,|_\Gamma$. The solution (u, v) of system (6.7) can be obtained by solving the following three problems:

$$\text{(i)} \quad \left\{\begin{aligned} -\Delta v_0 &= f && \text{in } \Omega, \\ v_0 &= 0 && \text{on } \Gamma, \end{aligned}\right. \qquad \left\{\begin{aligned} -\Delta u_0 &= v_0 && \text{in } \Omega, \\ u_0 &= 0 && \text{on } \Gamma, \end{aligned}\right. \tag{6.8}$$

$$\text{(ii)} \quad \mathcal{S}\lambda = \partial u_0/\partial \nu \quad \text{on } \Gamma, \tag{6.9}$$

$$\text{(iii)} \quad \left\{\begin{aligned} -\Delta v_1 &= 0 && \text{in } \Omega, \\ v_1 &= \lambda && \text{on } \Gamma, \end{aligned}\right. \qquad \left\{\begin{aligned} -\Delta u_1 &= v_1 && \text{in } \Omega, \\ u_1 &= 0 && \text{on } \Gamma, \end{aligned}\right. \tag{6.10}$$

the final solution being $(u, v) = (u_0 + u_1, v_0 + v_1)$. The aim of considering this formulation is to split the problem into smaller, easier to solve problems. While (i) and (iii) may indeed be classified as easy from a computational point of view, the crux of the problem becomes equation (ii). As in the case of DD methods, $\mathcal{S}$ is a boundary operator which is defined on $H^{-1/2}(\Gamma)$ and which induces a bilinear form $s(\cdot,\cdot) : H^{-1/2}(\Gamma) \times H^{-1/2}(\Gamma)$ via

$$(S\lambda_1, \lambda_2) = (\Delta\psi_1, \Delta\psi_2) := s(\lambda_1, \lambda_2).$$

The functions ψ_i are biharmonic extensions of $\lambda_i \in H^{-1/2}(\Gamma)$ into Ω; i.e., they are solutions of the biharmonic problems

$$\left\{\begin{aligned} \Delta^2 \psi_i &= 0 && \text{in } \Omega, \\ \psi_i &= 0 && \text{on } \Gamma, \\ -\partial\psi_i/\partial n &= \lambda_i && \text{on } \Gamma. \end{aligned}\right. \tag{6.11}$$

It is shown in [30] that the bilinear form $s(\cdot,\cdot)$ is symmetric, positive definite, and $H^{-1/2}(\Gamma)$-elliptic; i.e., there exist constants c_1, c_2 such that for all $\lambda \in H^{-1/2}(\Gamma)$

$$c_1\|\lambda\|^2_{H^{-1/2}(\Gamma)} \leq s(\lambda,\lambda) \leq c_2\|\lambda\|^2_{H^{-1/2}(\Gamma)}. \tag{6.12}$$

6.2.2. Discrete formulation. Consider now the following standard mixed finite element method for (6.7). Let V^h, V_I^h, V_B^h be defined as above (see (6.4)). The discrete weak formulation is then the following:

Find $(u_h, v_h) \in V_I^h \times V^h$ such that $\forall (w_h, z_h) \in V_I^h \times V^h$

$$\left\{ \begin{array}{rl} l(v_h, w_h) & = (f, w_h)\,, \\ l(u_h, z_h) - m(v_h, z_h) & = 0, \end{array} \right. \tag{6.13}$$

where

$$l(z,w) := (\nabla z, \nabla w)\,, \quad m(z,w) := (z,w)\,.$$

As described in [30], (6.13) is equivalent to the discrete versions of (6.8)–(6.10) given by the following three weak formulations:

(i) Find $(u_{0h}, v_{0h}) \in V_I^h \times V_I^h$ such that $\forall (w_h, z_h) \in V_I^h \times V_I^h$

$$\left\{ \begin{array}{rl} l(v_{0h}, w_h) & = (f, w_h)\,, \\ l(u_{0h}, z_h) - m(v_{0h}, z_h) & = 0. \end{array} \right. \tag{6.14}$$

(ii) Find $\lambda_h \in V_B^h$ such that $\forall \mu_h \in V_B^h$

$$\left\{ \; s(\lambda_h, \mu_h) \quad = -s(\lambda_{0h}, \mu_h). \right. \tag{6.15}$$

(iii) Find $(u_{1h}, v_{1h}) \in V_I^h \times V^h$, $v_{1h} - \lambda_h \in V_I^h$, such that $\forall (w_h, z_h) \in V_I^h \times V^h$

$$\left\{ \begin{array}{rl} l(v_{1h}, w_h) & = 0, \\ l(u_{1h}, z_h) - m(v_{1h}, z_h) & = 0. \end{array} \right. \tag{6.16}$$

Now let $\operatorname{span}\{\phi_i, 1 \leq i \leq n\} = V^h$ so that $w_h \in V^h, z_h \in V_I^h$ can be written

$$w_h = \sum_{i=1}^{n} \mathbf{w}_i \phi_i, \quad z_h = \sum_{i=1}^{n_I} \mathbf{z}_i \phi_i,$$

where $n = |V^h|, n_I = |V_I^h|$. Problem (6.13) is then equivalent to the following linear system of equations:

$$\begin{pmatrix} 0 & L_{II} & L_{IB} \\ L_{II} & -M_{II} & -M_{IB} \\ L_{IB}^T & -M_{IB}^T & -M_{BB} \end{pmatrix} \begin{pmatrix} \mathbf{u}_I \\ \mathbf{v}_I \\ \mathbf{v}_B \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ 0 \\ 0 \end{pmatrix}, \tag{6.17}$$

where

$$(L_{II})_{ij} = l(\phi_j, \phi_i), \quad (L_{IB})_{ik} = l(\phi_k, \phi_i)$$

and

$$(M_{II})_{ij} = m(\phi_j, \phi_i), \quad (M_{IB})_{ik} = m(\phi_k, \phi_i), \quad (M_{BB})_{kl} = m(\phi_l, \phi_k)$$

for $1 \le i, j \le m, 1 \le k, l \le n - n_I$. We also write (6.17) in the more compact form

$$\begin{pmatrix} L & Z \\ Z^T & -M_{BB} \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{v}_B \end{pmatrix} = \begin{pmatrix} \mathbf{g} \\ 0 \end{pmatrix}, \tag{6.18}$$

where

$$L = \begin{pmatrix} 0 & L_{II} \\ L_{II} & -M_{II} \end{pmatrix}, \quad Z = \begin{pmatrix} L_{IB} \\ -M_{IB} \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} \mathbf{u}_I \\ \mathbf{v}_I \end{pmatrix}.$$

It can be seen (see, for example, [4]) that the discrete problems (6.14)–(6.16) represent a boundary Schur complement approach to solving (6.17). As before, the task is therefore the efficient solution of problem (ii), in particular the derivation of optimal preconditioners for this step. The Schur complement associated with L in the matrix of (6.18) is

$$S = -M_{BB} - Z^T L^{-1} Z.$$

Let $X_h \subset H^1(\Gamma)$ denote the space spanned by the restriction of the basis functions of V_I^h to the boundary Γ. As in the case of DD methods, the Schur complement is the matrix representation of the bilinear form $s(\cdot,\cdot)$ with respect to the basis $\{\phi_i\}$. In particular, if $\lambda_h \in X_h$ has a vector of coefficients $\boldsymbol{\lambda}$, then

$$s(\lambda_h, \lambda_h) = \boldsymbol{\lambda}^T S \boldsymbol{\lambda}.$$

6.2.3. $\boldsymbol{H^{-1/2}(\Gamma)}$-preconditioners. A discrete $H^{-1/2}$-norm on X_h can be defined as a sum of norms corresponding to each *open* segment of the polygonal boundary Γ:

$$\|\lambda_h\|_{H^{-1/2}(\Gamma)} := \left(\sum_{i=1}^{K} \|\lambda_h\|^2_{H^{-1/2}(\Gamma_i)} \right)^{1/2}.$$

In particular, $H^{-1/2}(\Gamma_i)$ is understood here to be the dual of $H_{00}^{1/2}(\Gamma_i)$. For this space, a matrix representation for its norm was derived in section 4 (see (4.5)). However, Peisker [44] uses a different, algebraic, definition of the norms corresponding to each boundary segment, based on *linear and uniform* discretizations of Laplacian and mass matrices. This results in a matrix representation for the discrete norm $\|\cdot\|_{H^{-1/2}(\Gamma)}$ which is a direct sum of matrix representations of norms corresponding to the interior of each boundary segment. There are two drawbacks to this approach. First, the linear case ($r = 1$) does not yield stable mixed finite element discretizations of the biharmonic problem [49]. Second, the resulting preconditioner is not defined for nonuniform meshes. Following the presentation from section 4 we introduce the following representation of a discrete $H^{-1/2}(\Gamma)$-norm which is based on the above broken norm:

$$\|\lambda_h\|^2_{H^{-1/2}(\Gamma)} = \|\boldsymbol{\lambda}\|^2_{H_{\{-1/2\}}}$$

for $\lambda_h \in X_h$, where

$$H_{\{-1/2\}} = \bigoplus_{i=1}^{K} H^{\{i\}}_{-1/2}, \tag{6.19}$$

where

$$H^{\{i\}}_{-1/2} = L_{0,i}(L_{0,i}^{-1}L_{1,i})^{-1/2}$$

with $(L_{k,r})_{ij} = (\phi_i, \phi_j)_{H_0^k(\Gamma_r)}$, $k = 0, 1$, discrete operators defined on the interior of each boundary Γ_i. The following result can be proved immediately.

PROPOSITION 6.3. *Let $X_h = \operatorname{span}\{\phi_i, 1 \le i \le m\}$ be defined as above and let $H_{\{-1/2\}}$ be defined as in* (6.19). *Then for all $\boldsymbol{\lambda} \in \mathbb{R}^m \setminus \{\mathbf{0}\}$*

$$\kappa_1 \le \frac{\boldsymbol{\lambda}^T S \boldsymbol{\lambda}}{\boldsymbol{\lambda}^T H_{\{-1/2\}} \boldsymbol{\lambda}} \le \kappa_2$$

with constants κ_1, κ_2 independent of h.

Proof. The proof is similar to that of Proposition 6.1. ∎

7. Numerical experiments.

We present in this section numerical experiments corresponding to the two applications of the previous section. In both cases the solutions are obtained using preconditioned iterative methods with a combination of two- and one-dimensional preconditioners. The latter type are matrix representations of norms defined on finite-dimensional subspaces of fractional Sobolev spaces of index 1/2 which are constructed on the boundaries of the computational domain.

7.1. Domain decomposition for elliptic problems.

We solve the test problem (6.1) as well as the following convection-diffusion problem:

$$\begin{cases} -\nu\Delta u + \vec{b}\cdot\nabla u &= f \qquad \text{in } \Omega, \\ \qquad\qquad\quad u &= 0 \qquad \text{on } \partial\Omega. \end{cases} \tag{7.1}$$

We note here that Proposition 6.1 applies only in the symmetric case (6.1). However, one can derive suitable convergence results for the nonsymmetric case also which we did not include here. We refer the reader to [3] for further details. The domain is the unit square which was subdivided into equal squares. We used the finite element method to discretize the problems and constructed the corresponding representations of the norms required. The choice of finite-dimensional space was V^h defined in (6.4) with $r = 1$ and also $r = 2$. The choice $r = 2$ is relevant in the context of preconditioning discrete Laplacians (respectively, discrete convection-diffusion operators) arising from so-called P2-P1 discretizations of the Stokes [51], [31] (respectively, Oseen) problems [27], [36] which employ quadratic piecewise polynomial spaces for the approximation of the momentum equations.

Due to nonsymmetry, we choose to work with nonsymmetric iterative methods (flexible GMRES), coupled with nonsymmetric preconditioners of the form

$$P = \begin{pmatrix} A_{II} & A_{IB} \\ 0 & P_S \end{pmatrix}$$

with $A_{II} = \nu L_{II} + N_{II}$, where L_{II} is the direct sum of Laplacians assembled on each subdomain and N_{II} is the direct sum of the convection operator $\vec{b}\cdot\nabla$ assembled also on each subdomain. This choice of preconditioner is known to be useful, provided we have a good approximation P_S to the Schur complement. Thus, if P_S is replaced by S, convergence is achieved in two iterations [40]. Our choice of preconditioner will never achieve this, since the norms derived above do not approximate S itself but are equivalent operators. However, we will see that the resulting performance remains attractive.

The Schur complement preconditioner P_S is chosen to be each of $H_{1/2}$ and $H_{1/2,h}$, the discrete $H^{1/2}(\Gamma)$-norms defined in Proposition 6.1 and Remark 6.1, respectively. We also chose to work with a simplified version $\widehat{H}_{1/2}$ of $H_{1/2}$ obtained by replacing the mass matrix L_0 by a lumped version $\widehat{L}_0$:

$$\widehat{H}_{1/2} := \widehat{L}_0(\widehat{L}_0^{-1}L_1)^{1/2}.$$

The action of the inverses of $H_{1/2,h}, H_{1/2}, \widehat{H}_{1/2}$ was computed using the iterative method presented in section 5.2 which uses the Lanczos algorithm with $k = O(m^{1/2})$.

Remark 7.1. In the case where the domain is subdivided into several subdomains the boundary Γ will be the union of internal faces or boundaries (a so-called skeleton or wirebasket)

$$\Gamma = \bigcup_{i=1}^{K} \Gamma_i.$$

One can generalize the definition of a $H^{1/2}(\Gamma)$-norm to a broken $H^{1/2}(\Gamma)$-norm which results in a direct sum of symmetric and positive definite matrices as in (6.19) for the biharmonic problem. However, we choose to work with a related generalization which involves assembling the Grammians L_0, L_1 on the whole wirebasket Γ. In particular, L_1 will incorporate Dirichlet conditions corresponding to the set $\partial\Omega \cap \Gamma$ and will include additional contributions at each internal vertex. The resulting matrix is symmetric and positive definite and can be seen to be a discrete representation of a norm on $[X_h, Y_h]_{1/2} \subset H^{1/2}(\Gamma)$ with improved spectral properties [3].

7.1.1. The Poisson problem. The number of iterations is displayed in Table 7.1 for the cases $r = 1$, $r = 2$ (linear and quadratic finite elements), respectively. The size m of the skeleton is also displayed; it is obvious that a direct calculation of the matrix square root function is becoming prohibitive for an increasing number of domains and an increasing mesh size. As expected, the number of iterations is independent of the size of the problem. Moreover, the preconditioning procedure appears to be quasi-scalable with only a slight, possibly logarithmic dependence on the number of subdomains. A notable result is the performance of the preconditioner $\widehat{H}_{1/2}$ which is a simplified version of the other two which employs a lumped approximation of the mass matrix.

7.1.2. The convection-diffusion problem. We solved test problem (7.1) for the choice of "rotating wind"

$$\vec{b} = (2(2y-1)(1-(2x-1)^2), -2(2x-1)(1-(2y-1)^2)).$$

We chose to approximate only the action of $\widehat{H}_{1/2}^{-1}$ using the generalized Lanczos process with the same choice of k. The range of diffusion coefficients was $\nu = 1, 0.1, 0.01$. The results are displayed in Table 7.2. In all cases the number of iterations is independent of the size of the problem, though it grows with reducing ν. The dependence on the number of subdomains also grows with reducing ν. This reflects the inability of our symmetric preconditioner to remain equivalent in some sense to an increasingly more nonsymmetric Schur complement.

Table 7.1
FGMRES iterations for model problem (6.1) *for* $r = 1, 2$.

			$r=1$			$r=2$		
#dom	n	m	$H_{1/2,h}$	$H_{1/2}$	$\widehat{H}_{1/2}$	$H_{1/2,h}$	$H_{1/2}$	$\widehat{H}_{1/2}$
4	45,377	449	10	9	9	11	11	11
	180,865	897	10	10	10	11	11	11
	722,177	1793	11	11	11	11	11	11
16	45,953	1149	13	12	12	13	13	13
	183,041	2301	13	13	13	13	13	13
	730,625	4605	13	13	13	13	13	13
64	66,049	3549	16	14	14	16	15	15
	263,169	7133	16	15	15	16	15	15
	1,050,625	14,301	17	16	15	17	15	15

Table 7.2
FGMRES iterations for model problem (7.1) *for* $r = 1$, $r = 2$, $\nu = 1, 0.1, 0.01$, *and* $P_S = \widehat{H}_{1/2}$.

			$r=1$			$r=2$		
#dom	n	m	$\nu=1$	$\nu=0.1$	$\nu=0.01$	$\nu=1$	$\nu=0.1$	$\nu=0.01$
4	45,377	449	10	12	21	12	13	20
	180,865	897	11	11	20	12	13	19
	722,177	1793	11	11	19	12	12	18
16	45,953	1149	12	17	37	13	17	35
	183,041	2301	13	17	35	13	16	32
	730,625	4605	12	15	32	12	15	30
64	66,049	3549	16	22	55	17	21	51
	263,169	7133	17	22	52	16	20	46
	1,050,625	14,301	15	19	47	16	19	43

7.2. Biharmonic problem. We solved the biharmonic problem using the formulation (6.7), which was discretized using the weak formulation (6.13), where V^h is the finite element space defined in (6.4) with $r = 2$ (quadratic approximation). This is known to be a stable mixed finite element method for the biharmonic problem [49]. As the Glowinski–Pironneau method is a boundary Schur complement approach, we choose to work again with a block-triangular preconditioner of the form (cf. (6.18))

$$P = \begin{pmatrix} L & Z \\ & P_S \end{pmatrix},$$

where $P_S = H_{\{-1/2\}}$ was defined in (6.19). We ignore the symmetry of our problem and again use flexible GMRES, given the changing nature of our preconditioner due to the Lanczos approximation. As in the case of the previous example, we consider an approximation $\tilde{H}_{\{-1/2\}}$ resulting from replacing the mass matrix L_0 with a lumped version $\widehat{L}_0$. The results are displayed in Table 7.3. As expected, the number of iterations is independent of n; moreover, the preconditioner reduces greatly the iteration count compared to the case where no preconditioner is employed. We notice that in the unpreconditioned case the dependence on h is evident as predicted by [7], though mild ($O(h^{-1/2})$); we also notice that in this case there is a considerable additional computational effort, particularly compared to the minimal effort that the above preconditioners require. The same behavior can be noticed for stretched meshes. Table 7.4 displays the iteration count corresponding to a finite element discretization on an exponentially stretched mesh, with nodes clustered near the boundary and the mesh aspect ratio ranging from 1 to 20.

TABLE 7.3
FGMRES iterations for problem (6.6) *for a range of preconditioners* P_S*: Isotropic meshes.*

n	m	I	$H_{\{-1/2,h\}}$	$H_{\{-1/2\}}$	$\widehat{H}_{\{-1/2\}}$
84,610	640	26	10	12	12
337,154	1280	30	9	11	11
1,346,050	2560	36	9	11	11

TABLE 7.4
FGMRES iterations for problem (6.6) *for a range of preconditioners* P_S*: Stretched meshes.*

n	m	I	$H_{\{-1/2,h\}}$	$H_{\{-1/2\}}$	$\widehat{H}_{\{-1/2\}}$
31,250	496	37	8	9	9
128,018	1008	43	8	9	9
518,162	2032	52	7	8	8

8. Summary. We presented a derivation of norm representations of norms associated with interpolation spaces. In particular, we focused on projections onto conforming finite element spaces of fractional Sobolev norms. A notable result is that interpolation norms can be represented as products of generally real powers of Grammian matrices associated with the pair of spaces generating the scale of interpolation spaces. The issue of algorithmic complexity in the construction of discrete interpolation norms was also considered with the presentation of some sparse matrix algorithms for the approximation of real powers of matrices. Some applications arising from PDE modeling were considered to illustrate the usefulness of interpolation norms in large-scale computing.

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