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Matrix square-root preconditioners for the Steklov-Poincaré operator

Mario Arioli and Daniel Loghin

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Matrix square-root preconditioners for the Steklov-Poincaré operator

M. Arioli[1] and D. Loghin[2]

ABSTRACT
A key computational ingredient in domain decomposition methods for scalar elliptic problems is the preconditioning of a discrete Steklov-Poincaré operator defined on the union of the boundaries of each subdomain. This operator is norm-equivalent to a discrete fractional Sobolev norm-matrix of index 1/2. This norm-matrix is related to the matrix square-root of a certain generalised Laplacian operator defined on the subdomain boundaries. In this work we introduce a Krylov subspace approach to approximate the action of the inverse of such a norm-matrix in a sparse fashion. The resulting algorithm is shown to be optimal for preconditioning domain decomposition methods for elliptic problems. Numerical experiments demonstrate that it is also quasi-scalable.

Keywords: Generalized Laplace operators, Fractional Sobolev spaces, Krylov methods, Generalised Lanczos method, Domain decomposition, Matrix square root.

AMS(MOS) subject classifications: 35J15, 35J50, 47G30, 65F10, 65F15, 65F30, 65N30.

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[1] m.arioli@rl.ac.uk, Rutherford Appleton Laboratory.
[2] d.loghin@bham.ac.ukm.arioli@rl.ac.uk, School of Mathematics
University of Birmingham, UK.
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Computational Science and Engineering Department
Atlas Centre
Rutherford Appleton Laboratory
Oxon OX11 0QX

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1 Introduction

The usefulness of any domain decomposition method (DD) rests on the ability to solve a problem involving a pseudo-differential operator: the Steklov-Poincaré operator. Since under discretisation this gives rise to a system with a dense matrix, for large problems this needs to be solved approximately via a procedure which computes the action of the inverse of the discrete operator on a given vector. To this aim, a great number of iterative approaches have been suggested in the literature; classical algorithms include Dirichlet-Neumann, Neumann-Neumann, FETI methods, Schwarz methods, together with two-level and overlapping variants. For descriptions and analyses see Toselli and Widlund, 2005, Quarteroni and Valli, 1999.

An alternative that has not been considered to date and which can be shown to be competitive is based on a well-known property of the discrete Steklov-Poincaré operator: it is norm-equivalent to a Sobolev norm-matrix of index 1/2 (Quarteroni and Valli 1999), the discrete representation of which can be written in terms of the square-root of a discrete Laplacian defined on the union of the boundaries of each subdomain (Peisker 1988). This discrete norm has a non-sparse representation; however, since only the action of its inverse on a vector is required, we can achieve this using a standard approach based on a Krylov subspace approximation. The resulting algorithm is a generalised Lanczos procedure and the ensuing preconditioning procedure is independent of the size of the problem.

The paper is organised as follows. In Section 2 we introduce notation and background results. In Section 3 we present our theoretical results. We conclude with numerical experiments in Section 4.

2 Background results

To illustrate ideas and introduce notation in a simplified manner we consider a standard test problem for a two-domain DD method.

2.1 A model problem

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

$$\left\{ \begin{aligned} -\Delta u &= f && \text{in } \Omega, \\ u &= 0 && \text{on } \partial\Omega. \end{aligned} \right. \tag{1}$$

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

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

with the 'interface conditions'

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

Let now $\lambda_1, \lambda_2 \in H_{00}^{1/2}(\Gamma)$ 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

$$\left\{ \begin{aligned} -\Delta \psi_i &= 0 && \text{in } \Omega_i, \\ \psi_i &= \lambda_i && \text{on } \Gamma, \\ \psi_i &= 0 && \text{on } \partial\Omega_i \setminus \Gamma. \end{aligned} \right.$$

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

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

Note that we also defined a bilinear form $s(\cdot,\cdot) : H_{00}^{1/2}(\Gamma) \times H_{00}^{1/2}(\Gamma) \to 0$ 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 $\lambda \in H_{00}^{1/2}(\Gamma)$,

$$c_1\|\lambda\|^2_{H^{1/2}(\Gamma)} \leq s(\lambda, \lambda) \leq c_2\|\lambda\|^2_{H^{1/2}(\Gamma)}. \tag{3}$$

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

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

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

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

The resulting solution is

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

2.2 Algebraic formulation

Conforming finite element discretisations of model problem (1) give rise to a linear system involving a matrix which is structured in the following way

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

where $A_{II,i}, i = 1, 2$ are discrete 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

$$\text{(i) } A_{II,i}\mathbf{u}_i^{\{1\}} = \mathbf{f}_{I,i},$$

$$\text{(ii) } S\mathbf{u}_B = \mathbf{f}_B - A_{IB,1}^T\mathbf{u}_1^{\{1\}} - A_{IB,2}^T\mathbf{u}_2^{\{2\}},$$

$$\text{(iii) } A_{II,i}\mathbf{u}_i^{\{2\}} = -A_{IB,1}^T\mathbf{u}_B - A_{IB,2}^T\mathbf{u}_B,$$

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 discretisations of the three continuous problems listed above (see Quarteroni and Valli, 1999 for full details). In particular, the Schur complement S is the finite element discretisation of the variational definition (2) of the Steklov-Poincaré operator $\mathcal{S}$. Since $s(\cdot,\cdot)$ is $H^{1/2}_{00}(\Gamma)$-elliptic, we deduce that for any piecewise polynomial function λ_h defined on Γ there holds

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

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

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

One expects that a discrete representation of the norm $\|\cdot\|_{H^{1/2}(\Gamma)}$, say a symmetric and positive-definite matrix H, would provide a useful spectral equivalence between S and H. This is indeed the case as we show below.

3 $H^{1/2}$-preconditioners

3.1 Discrete fractional Sobolev norms

Let X, Y be two Hilbert spaces with norms $\|\cdot\|_X, \|\cdot\|_Y$ and with $X \subset Y$ and X dense in Y. Let $X_h \subset Y_h$ denote finite-dimensional subspaces of X, Y, respectively, which for given bases have discrete norms L, M, i.e., given $u_h \in X_h$, we have

$$\|u_h\|^2_X = \|\mathbf{u}\|^2_L = \mathbf{u}^T L \mathbf{u}, \quad \|u_h\|^2_Y = \|\mathbf{u}\|^2_M = \mathbf{u}^T M \mathbf{u}.$$

Let $[X, Y]_\theta$ denote the interpolation space with norm $\|\cdot\|_\theta$ and such that $[X, Y]_0 = X,\ [X, Y]_1 = Y$. We are clearly interested in the choice of spaces $X = H^1_0(\Gamma)$ and $Y = L^2(\Gamma)$ and the case $\theta = 1/2$ which yields $[X, Y]_{1/2} \equiv H^{1/2}_{00}(\Gamma)$. Before we introduce a discrete norm for $H^{1/2}_{00}(\Gamma)$ we remark that, since M, L are symmetric and positive definite matrices, there exists a matrix Q such that (Horn and Johnson 1985)

$$M = Q^T Q, \quad L = Q^T D_L Q,$$

where D_L is a diagonal matrix with positive diagonal entries. Since, $M^{-1}L = Q^{-1}D_L Q$, we define $(M^{-1}L)^{1/2} = Q^{-1}D_L^{1/2}Q$, so that

$$M(M^{-1}L)^{1/2} = Q^T D_L^{1/2} Q$$

is a symmetric and positive definite matrix. The following Lemma can be found in (Arioli and Loghin 2008) (see also (Burstedde 2007) for an alternative derivation).

Lemma 3.1. *Let $\Gamma \subset \mathbb{R}^d$ be an open set and let $Y = L^2(\Gamma), X = H^1_0(\Gamma)$, with $\|u\|_X = \|\nabla u\|_Y$. Let L, M be discrete norm-matrices corresponding to some conforming finite element basis for $X_h \subset X$ and $Y_h \subset Y$. Let $\lambda_h \in X_h$ have vector of coefficients $\boldsymbol{\lambda}$ with respect to the finite element basis and let*

$$H_{1/2} = M + M(M^{-1}L)^{1/2}.$$

Then $H_{1/2}$ is a symmetric positive definite matrix and there exist constants k_1, k_2 such that

$$k_1\|\lambda_h\|_{1/2} \leq \|\boldsymbol{\lambda}\|_{H_{1/2}} \leq k_2\|\lambda_h\|_{1/2}.$$

Hence, since $[X,Y]_{1/2} \equiv H_{00}^{1/2}(\Gamma)$, we can use the $H_{00}^{1/2}(\Gamma)$-ellipticity of the bilinear form $s(\cdot,\cdot)$ to derive the following equivalence.

Theorem 3.1. *Let $s(\cdot,\cdot)$ be defined by* (2) *and let* (3) *and the hypotheses of Lemma 3.1 hold. Let*

$$H = H_{1/2} = M + M(M^{-1}L)^{1/2}.$$

Then

$$\frac{1}{k_2 c_1}\|\boldsymbol{\lambda}\|_H^2 \leq \boldsymbol{\lambda}^T S \boldsymbol{\lambda} \leq c_2 k_1 \|\boldsymbol{\lambda}\|_H^2.$$

The above result indicates that H and S are spectrally-equivalent. In other words, the eigenvalues of $H^{-1}S$ are bounded independently of the size of the problem and therefore H is an optimal preconditioner for S. While this result may have been known previously for special cases ((Dryja 1982) and (Dryja and Widlund 1988)), the actual implementation of this preconditioner was never attempted due to its computational cost: the matrix H is a full matrix, as is each of the three matrices in the second term in its definition. One way of circumventing this issue is to use a Krylov subspace approximation for the matrix square-root.

3.2 Krylov subspace approximation

The preconditioning procedure requires at each iteration the action of the inverse of H on a given vector. First note that H and $M(M^{-1}L)^{1/2}$ are spectrally equivalent. Hence we can focus on the following reduced version of the preconditioner $H := M(M^{-1}L)^{1/2}$ with the main task of approximating the following product

$$\mathbf{z} = H^{-1}\mathbf{b}.$$

Consider now the following generalised Lanczos factorisation

$$LV = MVT, \quad V^T M V = I$$

where V is an M orthonormal matrix with $\mathbf{v}_1 = M^{-1}\mathbf{b}/\|\mathbf{b}\|_{M^{-1}}$ as its first column and T is a symmetric positive definite tridiagonal matrix. A simple calculation shows that

$$H^{-1} = VT^{-1/2}V^T$$

so that

$$\mathbf{z} = H^{-1}\mathbf{b} = VT^{-1/2}V^T\mathbf{b} = VT^{-1/2}\mathbf{e}_1\|\mathbf{b}\|_{M^{-1}}.$$

In practice, this computation is expensive; an approximation is provided by computing a generalised Lanczos procedure for a small number of steps k. The resulting approximation is

$$\mathbf{z} = H^{-1}\mathbf{v} \approx V_k T_k^{-1/2}\mathbf{e}_1\|\mathbf{b}\|_{M^{-1}}.$$

Complexity The approach indicated above has sub-linear complexity. Indeed, if n denotes the size of the Schur complement matrix, the Lanczos factorisation itself requires $O(n^{(d-1)/d})$ operations, while the actual computation requires $O(k^3)$ operations for computing $\tilde{\mathbf{z}} = T_k^{-1/2}\mathbf{e}_1$ and $O(n^{(d-1)/d})$ again for the matrix-vector product $V_k\tilde{\mathbf{z}}$.

Remark 1. *The approach described above requires knowledge of a suitable k so that the preconditioning step is not affected by a poor approximation of the product $H^{-1}\mathbf{b}$. In practice, the values of k for which we get a useful approximation are low and easy to prescribe. Another issue to highlight is the fact that the generalised Lanczos factorisation will need to be computed with each application of the preconditioner as the choice of* $\mathbf{b}$ *will be different. This should not pose a problem given the sub-linear complexity of our procedure.*

4 Numerical experiments

We present in this section results obtained using the reduced discrete $H^{1/2}$-norm preconditioner introduced in the previous section using the generalised Lanczos procedure described above. The test problems are the model problem (1) as well as the following convection-diffusion problem

$$\begin{cases} -\nu\Delta u + \vec{b}\cdot\nabla u &= f \qquad \text{in } \Omega, \\ \qquad\qquad u &= 0 \qquad \text{on } \partial\Omega. \end{cases} \tag{4}$$

In both cases the domain Ω was the unit square which was subdivided into 4,16,64 equal subdomains. The mesh size was subdivided in each case a couple of times in order to validate indirectly the theoretical result of Theorem 3.1. The matrices L, M were assembled on the one-dimensional set of boundaries for each subdomain; in this sense, L and M can be seen as quasi-global operators.

Given the generally non-symmetric nature of the system matrix the solver chosen was flexible GMRES with relative tolerance 10^{-6} and with global preconditioner of the form

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

with $A_I I = \nu L_{II} + N_{II}$ 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. We remark here that this choice of preconditioner is known to be useful provided we have a good approximation to the Schur complement. Thus, if H is replaced by S convergence is achieved in 2 iterations (Murphy, Golub and Wathen 2000). Our choice of preconditioner will never achieve this, since H does not approximate S itself but is an equivalent operator. However, we will see that the resulting performance remains attractive.

4.1 The model problem

In this case we preconditioned the Poisson problem with the exact preconditioner $H = M + M(M^{-1}L)^{1/2}$ and also using the generalised Lanczos procedure described in Section 3 with a fixed value of k. The number of iterations is displayed in Table 1. 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. The Krylov approximation also appears to be robust with respect to the choice of

domains=	4	16	64	4	16	64
level=1	9	10	13	9	10	13
2	10	11	14	10	11	14
3	10	11	14	11	12	15

Table 1: *GMRES iterations for model problem* (1) *for* $k = n$ *and* $k = 50$.

k. Indeed, the convergence features are maintained for a fixed choice of k which is small relative to the size of the problem.

4.2 Convection-diffusion problem

We solved test problem (4) for the choice of ‘rotating wind’

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

domains=	4	16	64	4	16	64	4	16	64
level=1	10	12	16	12	18	27	25	42	68
2	10	13	16	13	18	27	25	43	68
3	11	13	17	13	18	26	25	43	67

Table 2: *GMRES iterations for model problem* (4) *for* $\nu = 1, 0.1, 0.01$ *and* $k = 50$.

We chose to approximate only the action of H^{-1} for the same fixed value of $k = 50$. The range of diffusion coefficients was $\nu = 1, 0.1, 0.01$. 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 subdomain 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.

5 Summary

We presented a new preconditioner for the discrete Steklov-Poincaré operator arising in domain decomposition methods. Our preconditioner is a discrete fractional Sobolev norm of index 1/2 which was shown to be optimal both theoretically and numerically. For moderately nonsymmetric elliptic problems, the preconditioner is also quasi-scalable. Experiments were included for the two-dimensional case, though the analysis is general and three-dimensional experiments are expected to exhibit the same performance.

References

Arioli, M. and Loghin, D. (2008), Discrete fractional Sobolev norms with applications, Technical report, STFC-RAL. In preparation.

Burstedde, C. (2007), 'On the numerical evaluation of fractional Sobolev norms', *Comm. Pure and Appl. Math* **6**(3), 587–605.

Dryja, M. (1982), 'A capacitance matrix method for Dirichlet problem on polygon region', *Numer. Math.* **39**, 51–64.

Dryja, M. and Widlund, O. (1988), Some domain decomposition algorithms for elliptic problems, *in* 'Proceedings of the Conference on Iterative Methods for Large Linear Systems, Austin, Texas'.

Horn, R. A. and Johnson, C. R. (1985), *Matrix Analysis*, Cambridge University Press.

Murphy, M. F., Golub, G. H. and Wathen, A. J. (2000), 'A note on preconditioning for indefinite linear systems', *SIAM J. Sci. Comp.* **21**, 1969–1972.

Peisker, P. (1988), 'On the numerical solution of the first biharmonic equation', *Mathematical Modelling and Numerical Analysis* **22**(4), 655–676.

Quarteroni, A. and Valli, A. (1999), *Domain Decomposition Methods for Partial Differential Equations*, Numerical Mathematics and Scientific Computation, Oxford University Press.

Toselli, A. and Widlund, O. (2005), *Domain Decomposition Methods – Algorithms and Theory*, Springer.