SParse Approximate Inverse (SPAI) based transmission conditions for optimized algebraic Schwarz methods

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1 Introduction

There have been various studies on algebraic domain decomposition methods, see e.g. [1], [2], [6], [7], [8] and references therein. Algebraic Optimized Schwarz Methods (AOSMs) were introduced in [4] to solve block banded linear systems arising from the discretization of PDEs on irregular domains. AOSMs mimic Optimized Schwarz Methods (OSMs) [5] algebraically by optimizing transmission blocks between subdomains. We propose here a new approach for obtaining transmission blocks using SParse Approximate Inverse (SPAI) techniques [9]. SPAI permits the approximation of the required parts of an inverse needed in the optimal transmission blocks, without knowing the entire inverse that would be infeasible in practice, and is naturally parallel, like the domain decomposition iteration itself. Using SPAI with different numbers of diagonals in a predefined sparsity pattern gives rise to approximations in the transmission blocks which can be interpreted as differential transmission operators at the continuous level of various degrees, and this can be used to compute a theoretical convergence factor of the resulting AOSM. We can therefore compare the performance of the SPAI AOSM also theoretically, and show that a direct SPAI application without taking into account the entire non-linear structure of the convergence estimate of AOSM leads to suboptimal performance. We thus propose also a modified SPAI-like technique that minimizes the entire convergence estimate and restores the expected performance.

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2 Algebraic Optimized Schwarz Methods

We are interested in solving linear systems of the form

$$Au = f,$$

where the $n \times n$ matrix A arises from a finite element or finite difference discretization of a partial differential equation, and has a block banded structure of the form

$$A = \begin{bmatrix} A_{11} & A_{12} & & \\ A_{21} & A_{22} & A_{23} & \\ & A_{32} & A_{33} & A_{34} \\ & & A_{43} & A_{44} \end{bmatrix}, \tag{1}$$

where A_{ij} are blocks of size $n_i \times n_j$, $i, j = 1, \ldots, 4$, and $n = \sum_i n_i$. We suppose that $n_1 \gg n_2$ and $n_4 \gg n_3$, representing two large subdomains; for generalizations to more subdomains, see [4, Section 6]. We consider Algebraic Optimized Schwarz methods of additive and multiplicative type, whose iteration operators are based on the following modifications inspired by OSM,

$$T_{ORAS} = I - \sum_{i=1}^{2} \tilde{R}_i^T \tilde{A}_i^{-1} R_i A, \text{ and } T_{ORMS} = \prod_{i=2}^{1} (I - \tilde{R}_i^T \tilde{A}_i^{-1} R_i A), \tag{2}$$

where

$$\tilde{A}_1 = \begin{bmatrix} A_{11} & A_{12} & \\ A_{21} & A_{22} & A_{23} \\ & A_{32} & S_1 \end{bmatrix}, \qquad \tilde{A}_2 = \begin{bmatrix} S_2 & A_{23} & \\ A_{32} & A_{33} & A_{34} \\ & A_{43} & A_{44} \end{bmatrix}, \tag{3}$$

with $S_1 = A_{33} + D_1$ and $S_2 = A_{22} + D_2$. Here D_1 and D_2 are transmission matrices to be chosen for fast convergence. The asymptotic convergence factor of AOSM depends on the product of the following two norms (see [4, Theorem 3.2]),

$$\| (I + D_1 B_{33})^{-1} [D_1 B_{12} - A_{34} B_{13}] \|, \ \| (I + D_2 B_{11})^{-1} [D_2 B_{32} - A_{21} B_{31}] \|, \tag{4}$$

where the B matrices involve certain columns of inverses of submatrices of A, namely

$$\begin{bmatrix} B_{31} \\ B_{32} \\ B_{33} \end{bmatrix} := \begin{bmatrix} A_{11} & A_{12} & \\ A_{21} & A_{22} & A_{23} \\ & A_{32} & A_{33} \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 0 \\ I \end{bmatrix}, \quad \begin{bmatrix} B_{11} \\ B_{12} \\ B_{13} \end{bmatrix} := \begin{bmatrix} A_{22} & A_{23} & \\ A_{32} & A_{33} & A_{34} \\ & A_{43} & A_{44} \end{bmatrix}^{-1} \begin{bmatrix} I \\ 0 \\ 0 \end{bmatrix}. \tag{5}$$

We can easily derive the optimal choice for the transmission matrices, see [4],

$$D_{1,\text{opt}} = -A_{34} A_{44}^{-1} A_{43} \qquad \text{and} \qquad D_{2,\text{opt}} = -A_{21} A_{11}^{-1} A_{12}, \tag{6}$$

which make (4) zero. The corresponding AOSM then converges in two iterations for ORAS, so one can not do better than this. Computing these optimal blocks $D_{1,\text{opt}}$ and $D_{2,\text{opt}}$ is however equivalent to computing the Schur complements

$$S_{1,\mathrm{opt}} = A_{33} - A_{34}A_{44}^{-1}A_{43} \quad \text{and} \quad S_{2,\mathrm{opt}} = A_{22} - A_{21}A_{11}^{-1}A_{12} \tag{7}$$

corresponding to the submatrices

$$\begin{bmatrix} A_{33} & A_{34} \\ A_{43} & A_{44} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \tag{8}$$

and is thus very expensive, due to the large inverses A_{44}^{-1} and A_{11}^{-1}. In the next section we propose sparse approximations of the optimal transmission blocks using predefined sparsity patterns.

3 Sparse approximations of optimal transmission blocks

The new idea to determine approximations $D_{1,\mathrm{app}}$ and $D_{2,\mathrm{app}}$ that make the norms in (4) small and are cheap to compute is to use a SParse Approximate Inverse (SPAI) technique to make the differences

$$||D_1 B_{12} - A_{34}B_{13}|| \quad \text{and} \quad ||D_2 B_{32} - A_{21}B_{31}|| \tag{9}$$

small by approximating the inverse blocks A_{11}^{-1} and A_{44}^{-1} in (6). Due to the sparsity of A_{34}, A_{43}, A_{21}, and A_{12}, we only need to approximate small subblocks of A_{11}^{-1} and A_{44}^{-1} only using.

To gain insight into the quality and performance of such SPAI approximations of $D_{1,\mathrm{opt}}$ and $D_{2,\mathrm{opt}}$, we consider the model problem $\Delta u = f$ in $\Omega = (0,1)^2$, discretized by a standard five point finite difference stencil, which leads to a system matrix of the form (1) with, e.g.,

$$A_{11} = \frac{1}{h^2}\begin{bmatrix} T & I & & \\ I & \ddots & \ddots & \\ & \ddots & \ddots & I \\ & & I & T \end{bmatrix}, \; A_{12} = \frac{1}{h^2}\begin{bmatrix} 0 & 0 & 0 \\ \vdots & & \vdots \\ 0 & 0 & 0 \\ I & 0 & 0 \end{bmatrix}, \; A_{21} = \frac{1}{h^2}\begin{bmatrix} 0 \dots 0 & I \\ 0 \dots 0 & 0 \\ 0 \dots 0 & 0 \end{bmatrix}, \tag{10}$$

where $T = \mathrm{spdiag}([1,-4,1])$. To approximate the block inverse A_{11}^{-1} in $D_{2,\mathrm{opt}} = -A_{21}A_{11}^{-1}A_{12}$ with matrices from (10) using SPAI naively, we would solve for a matrix M of the same large size as A_{11} with given sparsity pattern the minimization problem $||A_{11}M - I||_F \longrightarrow \min$, which requires solving a least squares problem for each column, and where one specifies a sparsity pattern for M. Because of the sparsity structure of A_{12} and A_{21} however in (10), we see that we need the SPAI approximation only of the last diagonal block (bottom right) of M, which we denote by M^{br}. Thus, it is not necessary to compute the entire SPAI approximation M, it is sufficient to just solve the least squares problems corresponding to the last few columns in M which contain M^{br}, and furthermore these least squares problems are also small due to the sparsity of A_{11}. Doing this for our model problem using a diagonal sparsity pattern for M leads to

$$D_{2,\mathrm{app}}^{br} := M^{br} = -h^2 \begin{bmatrix} 0.2222 & & & & \\ & 0.2015 & & & \\ & & \ddots & & \\ & & & 0.2015 & \\ & & & & 0.2222 \end{bmatrix}. \tag{11}$$

In order to understand to what type of transmission conditions this approximation leads, it is best to look at the corresponding Schur complement approximation $S_{2,\mathrm{app}}$ of $S_{2,\mathrm{opt}}$ from (7), see also [3, Section 4.1], which is also modified only at the bottom right,

$$S_{2,\mathrm{app}}^{br} = A_{22}^{br} - [A_{21} M A_{12}]^{br} = \frac{1}{h^2} T - \frac{1}{h^2} D_{2,\mathrm{app}}^{br} \frac{1}{h^2}. \tag{12}$$

Rearranging this expression into

$$S_{2,\mathrm{app}}^{br} = \frac{1}{h^2} \begin{bmatrix} -2 & 1/2 & & & \\ 1/2 & -2 & 1/2 & & \\ & \ddots & \ddots & \ddots & \\ & & 1/2 & -2 & 1/2 \\ & & & 1/2 & -2 \end{bmatrix} + \frac{1}{2h^2} \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} - \frac{1}{h^2} \begin{bmatrix} 0.7778 & & & & \\ & 0.7895 & & & \\ & & \ddots & & \\ & & & 0.7895 & \\ & & & & 0.7778 \end{bmatrix} \tag{13}$$

and neglecting the fact that the first and last entry from the diagonal SPAI approximation are slightly different from the others, we can interpret this as a second order transmission operator at the continuous level, see [3, Section 4.1],

$$\mathcal{B}_1 = -\frac{\partial u}{\partial n} + \frac{h}{2} \frac{\partial^2 u}{\partial y^2} - \frac{1}{h} 0.7895 u. \tag{14}$$

With the analogous result approximating the Schur complement $S_{1,\mathrm{opt}}$ by SPAI, the corresponding OSM at the continuous level with overlap of one mesh size h would then have in Fourier space the convergence factor (see [3, Section 4.1])

$$\rho_1(k,h) = \left| \frac{|k| - 0.7895 \frac{1}{h} - \frac{h}{2} k^2}{|k| + 0.7895 \frac{1}{h} + \frac{h}{2} k^2} \right| e^{-kh}, \tag{15}$$

where $k > 0$ corresponds to the frequency in Fourier space, which allows us to asses the quality of this approximation theoretically for our model Poisson equation.

Using a tridiagonal SPAI approximation of the term A_{11}^{-1} leads to

$$D_{2,\text{app}}^{br} = -h^2 \begin{bmatrix} 0.2446 & 0.0504 & & & & \\ 0.0552 & 0.2557 & 0.0521 & & & \\ & 0.0516 & 0.2540 & 0.0516 & & \\ & & 0.0516 & 0.2540 & 0.0516 & \\ & & & \ddots & \ddots & \ddots \end{bmatrix}. \tag{16}$$

As observed for the Schur complement in (12), the changes occur only in the bottom right block, which we can rewrite in the form (where we did not specify the slightly different boundary terms for simplicity in the last matrix)

$$S_{2,\text{app}}^{br} = \frac{1}{h^2}\begin{bmatrix} -2 & 1/2 & & & \\ 1/2 & -2 & 1/2 & & \\ & \ddots & \ddots & \ddots & \\ & & 1/2 & -2 & 1/2 \\ & & & 1/2 & -2 \end{bmatrix} + \frac{0.0516}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} - \frac{1}{h^2}\begin{bmatrix} \ddots & & & & \\ & \ddots & & & \\ & & 0.6428 & & \\ & & & \ddots & \\ & & & & \ddots \end{bmatrix}. \tag{17}$$

This can again be interpreted as a second order transmission operator, namely

$$\mathcal{B}_3 = -\frac{\partial u}{\partial n} + 0.0516\, h\frac{\partial^2 u}{\partial y^2} - \frac{1}{h}0.6428u, \tag{18}$$

and the corresponding convergence factor in Fourier space with overlap h is

$$\rho_3(k,h) = \left|\frac{|k| - \frac{1}{h}0.6428 - 0.0516hk^2}{|k| + \frac{1}{h}0.6428 + 0.0516hk^2}\right| e^{-kh}. \tag{19}$$

The two convergence factors ρ_1 from the diagonal SPAI approximation and ρ_3 from the tridiagonal SPAI approximation are very similar, there is no apparent benefit one would expect when going from a diagonal to a tridiagonal approximation, like when going from a zeroth order optimized (OO0) to a second order optimized (OO2) transmission condition [5, Theorem 4.5 and 4.8]. This is also clearly visible in Figure 1 on the left: SPAI(1) and SPAI(3) have a comparable and much larger low frequency (k small) contraction factor than OO0 and OO2.

We thus add further diagonals in the SPAI approximation, and obtain with five diagonals

$$D_{2,\text{app}}^{br} = -h^2 \begin{bmatrix} 0.2302 & 0.0478 & 0.0084 & 0.001 & & \\ 0.0521 & 0.2559 & 0.0570 & 0.0113 & 0.0017 & \\ & 0.0106 & 0.0573 & 0.2577 & 0.0573 & 0.0106 \\ & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}. \tag{20}$$

Proceeding as before, and using the matrix spdiag([1, −4, 6, −4, 1]) which corresponds to a fourth-order derivative, we can show that the resulting transmission

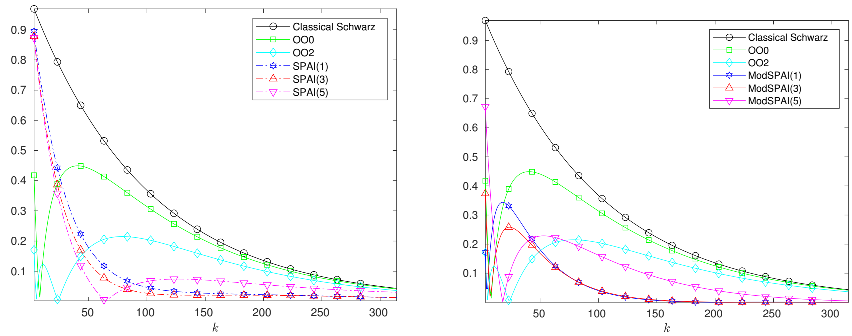

Fig. 1 Comparison of the convergence factors as function of the Fourier frequency k for the classical Schwarz method, algebraic SPAI transmission conditions (left) and the modified SPAI transmission conditions (right).

operator in Fourier space is a fourth-order operator given by

$$\mathcal{B}_5 = -\frac{\partial u}{\partial n} + x_1\, h\frac{\partial^2 u}{\partial y^2} - \frac{p}{h}u + h^3 0.0106\frac{\partial^4 u}{\partial y^4}, \tag{21}$$

where $x_1 = 0.0573 + 4 \times 0.0106$, $x_2 = 0.2577 - 6 \times 0.0106$, and $p = 1 - x_2 - 2x_1$. The corresponding convergence factor in Fourier is

$$\rho_5(k,h) = \left| \frac{|k| - \frac{1}{h}p - x_1 h k^2 - h^3 0.0106 k^4}{|k| - \frac{1}{h}p - x_1 h k^2 - h^3 0.0106 k^4} \right| e^{-kh}. \tag{22}$$

We see in Figure 1 on the left that this approximation now manages to put a zero into the convergence factor, like the OO0 does already with the diagonal approximation, but still the low frequency behavior of the SPAI transmission conditions is much worse than the low frequency behavior of the OO0 and OO2 transmission conditions. It seems that it is not sufficient to just minimize the norms (9) using SPAI approximations to obtain a transmission condition similar in the quality of the OO0 and OO2 transmission conditions.

We therefore now minimize instead the entire norms in (4) using a generic optimization algorithm, namely Nelder Mead, which leads to algebraic transmission conditions and associated AOSMs we call ModSPAI(1), ModSPAI(3), and ModSPAI(5), see Figure 1, right. More specifically, ModSPAI(1) is obtained by minimizing the norms in (4) with respect to the quantity p where $D_i = -pI$, $i = 1, 2$. ModSPAI(3) is obtained by minimizing the corresponding norms w.r.t to quantities p and q such that $D_i = -\text{spdiags}([p, q, p], -1 : 1)$, $i = 1, 2$. Similarly, ModSPAI(5) depends on quantities p, q, and r where $D_i = -\text{spdiags}([p, q, r, q, p], -2 : 2)$, $i = 1, 2$. By introducing these quantities we expect to decrease significantly the corresponding convergence factors. We clearly see that the minimization of the entire product in (4) is essential

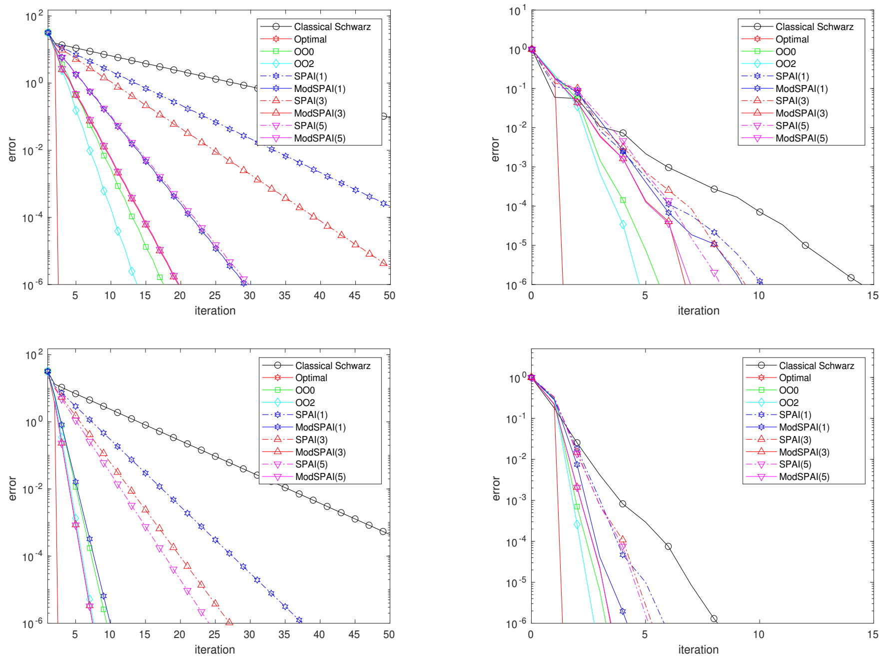

Fig. 2 Convergence history of SPAI based AOSMs compared to the optimal choice of transmission blocks and OO0 and OO2. Left: iterative methods; Right: GMRES. Top: additive; Bottom: multiplicative.

to obtain AOSMs which have similar performance as OO0 and OO2. It is therefore important to develop an adapted nonlinear SPAI technique to make the norms (4) small, since the generic optimization we used here is too costly in practice, requiring the knowledge of the entire Schur complements to be performed.

4 Numerical experiments

To illustrate the performance of the new SPAI AOSMs we consider the advection-reaction-diffusion equation, $\eta u - \nabla \cdot (a \nabla u) + b \cdot \nabla u = f$, where $a = a(x, y) > 0$, $b = [b_1(x, y), b_2(x, y)]^T$, $\eta = \eta(x, y) \geq 0$, with $b_1 = y - \frac{1}{2}$, $b_2 = -x + \frac{1}{2}$, $\eta = x^2 \cos(x + y)^2$, $a = 1 + (x + y)^2 e^{x-y}$. We perform the experiments on the unit square domain $\Omega = (0, 1) \times (0, 1)$, which we decompose into two subdomains $\Omega_1 = (0, \beta) \times (0, 1)$ and $\Omega_2 = (\alpha, 1) \times (0, 1)$, where $0 < \alpha \leq \beta < 1$. After discretization with a finite difference method, the corresponding matrix A is of size 1024×1024, with a decomposition into two subdomains where the blocks A_{11}, A_{12}, A_{21}, and A_{22} are of size 480×480, 480×32, 32×480, and 32×32 respectively. The parameter of OO0 is evaluated numerically and is given by $p = 51.72$. Similarly, the parameters of OO2 are given numerically by $p = 7.9515$ and $q = 0.3786$. In Figure 2, we present the evolution of the 2-norm of the error as a function of the number of iterations for our methods used as iterative solvers (left) and as preconditioners (right). We mention that the proposed technique can be applied to different type of equations and discretizations.

Concluding Remarks

We proposed a new SPAI approach which permits the inexpensive computation of transmission conditions in algebraic optimized Schwarz methods. Our analysis for a model Poisson problem showed that in order to completely capture optimized transmission conditions, it is either necessary to increase the bandwidth in the new SPAI approach, or to also include a second term in the optimization, for which a new nonlinear SPAI technique would need to be developed.

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