

Optimized algebraic interface conditions in domain decomposition methods for strongly heterogeneous unsymmetric problems

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1.1 Introduction

Let $\Omega = \mathbf{R} \times Q$, where Q is a bounded domain of \mathbf{R}^2 , and consider the elliptic PDE of advection-diffusion-reaction type given by

$$\begin{aligned} -\operatorname{div}(c\nabla u) + \operatorname{div}(\mathbf{b}u) + \eta u &= f && \text{in } \Omega \\ \mathcal{B}u &= g && \text{on } \mathbf{R} \times \partial Q, \end{aligned} \tag{1.1}$$

with the additional requirement on the solutions to be bounded at infinity. After a finite element, finite differences or finite volume discretization, we obtain a large sparse system of linear equations, given by

$$\mathbf{A} \mathbf{w} = \mathbf{f}. \tag{1.2}$$

Under classical assumptions on the coefficients of the problem (*e.g.* $\eta - \frac{1}{2}\operatorname{div} \mathbf{b} > 0$ a.e. in Ω) the matrix \mathbf{A} in (1.2) is definite positive.

We solve problem (1.2) by means of an Optimized Schwarz Method: such methods have been introduced at the continuous level in [4], and at the discrete level in [5]. We design optimized interface conditions directly at the algebraic level, in order to guarantee robustness with respect to heterogeneities in the coefficients.

1.2 LDU factorization and absorbing boundary conditions

In this section we enlighten the link between an LDU factorization of a matrix and the construction of absorbing conditions on the boundary of a domain

(see [1]). As it is well known in domain decomposition literature, such conditions provide exact interface transmission operators. Let then $\tilde{\Omega} \in \mathbf{R}^3$ be a bounded polyedral domain. We assume that the underlying grid is obtained as a deformation of a Cartesian grid on the unit cube, so that for suitable integers N_x , N_y , and N_z , $\mathbf{w} \in \mathbf{R}^{N_x \times N_y \times N_z}$. If the unknowns are numbered lexicographically, the vector \mathbf{w} is a collection of N_x sub-vectors $w_i \in \mathbf{R}^{N_y \times N_z}$, *i.e.*

$$\mathbf{w} = (w_1^T, \dots, w_{N_x}^T)^T. \quad (1.3)$$

From (1.3), the discrete problem in $\tilde{\Omega}$ reads

$$\mathbf{B} \mathbf{w} = \mathbf{g}, \quad (1.4)$$

where $\mathbf{g} = (g_1, \dots, g_{N_x})^T$, each g_i being a $N_y \times N_z$ vector, and where the matrix \mathbf{B} of the discrete problem has a block tri-diagonal structure

$$\mathbf{B} = \begin{pmatrix} D_1 & U_1 & & & \\ L_1 & D_2 & \ddots & & \\ & \ddots & \ddots & U_{N_x-1} & \\ & & L_{N_x-1} & D_{N_x} & \end{pmatrix}, \quad (1.5)$$

where each block is a matrix of order $N_y \times N_z$.

An exact block factorization of the matrix \mathbf{B} defined in (1.5) is given by

$$\mathbf{B} = (\mathbf{L} + \mathbf{T})\mathbf{T}^{-1}(\mathbf{U} + \mathbf{T}), \quad (1.6)$$

where

$$\mathbf{L} = \begin{pmatrix} 0 & & & & \\ L_1 & \ddots & & & \\ & \ddots & \ddots & & \\ & & \ddots & L_{N_x-1} & 0 \end{pmatrix} \quad \mathbf{U} = \begin{pmatrix} 0 & U_1 & & & \\ & \ddots & \ddots & & \\ & & \ddots & U_{N_x-1} & \\ & & & 0 & \end{pmatrix},$$

while \mathbf{T} is a block-diagonal matrix whose nonzero entries are the blocks T_i defined recursively as

$$T_i = \begin{cases} D_1 & \text{for } i = 1 \\ D_i - L_{i-1}T_{i-1}^{-1}U_{i-1} & \text{for } 1 < i \leq N_x. \end{cases}$$

So far, we can give here the algebraic counterpart of absorbing boundary conditions. Assume $\mathbf{g} = (0, \dots, 0, g_{p+1}, \dots, g_{N_x})$, and let $N_p = N_x - p + 1$. To reduce the size of the problem, we look for a block matrix $\mathbf{K} \in (\mathbf{R}^{N_y \times N_z})^{N_p}$, each entry of which is a $N_y \times N_z$ matrix, such that the solution of $\mathbf{K}\mathbf{v} = \tilde{\mathbf{g}} = (0, g_{p+1}, \dots, g_{N_x})^T$ satisfies $v_k = w_{k+p-1}$ for $k = 1, \dots, N_p$. The rows 2 through N_p in the matrix \mathbf{K} coincide with the last $N_p - 1$ rows of the original matrix \mathbf{B} . To identify the first row, which corresponds to the absorbing boundary condition,

1.4 Optimized algebraic interface conditions for a non-overlapping Schwarz method

The lack of sparsity of the matrices \mathbf{T}_1^{ex} and \mathbf{T}_2^{ex} in (1.12), make them not suitable to be used in practice. Thus we choose for \mathbf{T}_1 and \mathbf{T}_2 in (1.11) two suitable approximations of \mathbf{T}_1^{ex} and \mathbf{T}_2^{ex} , respectively.

At the cost of enlarging the size of the interface problem, we choose $\mathbf{T}_1^{\text{app}}$ and $\mathbf{T}_2^{\text{app}}$ defined as follows:

$$\begin{aligned}\mathbf{T}_1^{\text{app}} &= \mathbf{D}_{\Gamma\Gamma} - \mathbf{L}_{1\Gamma} [D_{1\Gamma} - L_1 (T_{1,\infty}^{\text{app}})^{-1} U_1]^{-1} \mathbf{U}_{1\Gamma} \\ \mathbf{T}_2^{\text{app}} &= \mathbf{D}_{\Gamma\Gamma} - \mathbf{U}_{2\Gamma} [D_{2\Gamma} - U_2 (T_{2,\infty}^{\text{app}})^{-1} L_2]^{-1} \mathbf{L}_{2\Gamma},\end{aligned}\quad (1.13)$$

where $T_{1,\infty}^{\text{app}}$ and $T_{2,\infty}^{\text{app}}$ are suitable sparse approximations of $T_{1,\infty}$ and $T_{2,\infty}$, respectively. The most natural choice would be to take their diagonals, but, in order to have a usable condition, we avoid the computation of both $T_{1,\infty}$ and $T_{2,\infty}$, which is too costly. Notice that if D_j , L_j , and U_j ($j = 1, 2$) were all diagonal matrices the same would hold also for $T_{j,\infty}$. Moreover, if all the matrices involved commute, or if $L_j = U_j^T$, we would have

$$T_{1,\infty} = \frac{D_1}{2} + \sqrt{\frac{(-L_1)^{1/2} D_1 (-U_1)^{-1/2} (-L_1)^{-1/2} D_1 (-U_1)^{1/2}}{4} - L_1 U_1}.$$

and a similar formula holds for $T_{2,\infty}$, with the roles of L_2 and U_2 exchanged. These considerations have led us to consider the following approximations of $T_{1,\infty}$ and $T_{2,\infty}$.

Let d_j , l_j , and u_j be the diagonals of D_j , L_j and U_j , respectively.

Robin: We choose in (1.13)

$$T_{1,\infty}^{\text{app}} = \frac{D_1}{2} + \alpha_1^{\text{opt}} \mathcal{D}_1,$$

where $\mathcal{D}_1 = \text{diag} \left(\frac{\sqrt{d_1^2 - 4l_1 u_1}}{2} \right)$, and where the optimized parameter is given by

$$(\alpha_1^{\text{opt}})^2 = \max \left\{ \sqrt{r_1^2 + I_1^2}, \sqrt{r_1 R_1 - I_1^2} \right\}, \quad (1.14)$$

where we have set $r_1 := \min \text{Re } \lambda$, $R_1 := \max \text{Re } \lambda$, and $I_1 := \max \text{Im } \lambda$, $\lambda \in \sigma \left(\frac{(-L_1)^{1/2} D_1 (-U_1)^{-1/2} (-L_1)^{-1/2} D_1 (-U_1)^{1/2}}{4} - L_1 U_1 \right) \text{diag} \left(\frac{\sqrt{d_1^2 - 4l_1 u_1}}{2} \right)^{-2}$,

whereas a similar formula holds for $T_{2,\infty}^{\text{app}}$.

Order 2: This condition is obtained by blending together two first order approximations, and we have

$$T_{1,\infty}^{\text{app}} = L_1 \left([\tilde{\mathcal{D}}_1, \mathcal{L}_1] + (\alpha_1 + \alpha_2) \mathcal{L}_1 \right)^{-1} \left(\tilde{\mathcal{D}}_1^2 + (\alpha_1 + \alpha_2) \tilde{\mathcal{D}}_1 + \alpha_1 \alpha_2 Id - \mathcal{L}_1 U_1 \right)$$

where $[\cdot, \cdot]$ is the Lie bracket, where $\tilde{\mathcal{D}}_1 = \frac{\mathcal{D}_1^{-1} D_1}{2}$, $\mathcal{L}_1 = \mathcal{D}_1^{-1} L_1$, $\mathcal{U}_1 = \mathcal{D}_1^{-1} U_1$, and where

$$(\alpha_1 \alpha_2)^2 = r_1 R_1 \quad (\alpha_1 + \alpha_2)^2 = \sqrt{2(r_1 + R_1)} \sqrt{r_1 R_1}, \quad (1.15)$$

r_1 and R_1 being defined as before.

The tuning of the optimized parameters for both conditions can be found in [2], and a more exhaustive presentation of the construction of interface conditions and of the numerical tests will be given in a forthcoming paper [3]. The proposed interface conditions are built directly at the algebraic level, and are easy to implement. However, they rely heavily on the approximation of the Schur complement and, if on one hand the extension to a decomposition in strips appears quite straightforward, on the other hand further work needs to be done in order to analyse their scalability to an arbitrary decomposition of the computational domain.

Finally, it is easy to prove the following result (see [3]).

Lemma 2. *The Schwarz algorithm*

$$\begin{aligned} \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{1\Gamma} \\ \mathbf{A}_{\Gamma 1} & \mathbf{T}_2^{\text{app}} \end{pmatrix} \begin{pmatrix} \mathbf{v}_1^{k+1} \\ \mathbf{v}_{\Gamma,1}^{k+1} \end{pmatrix} &= \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_\Gamma + (\mathbf{T}_2^{\text{app}} - \mathbf{D}_{\Gamma\Gamma}) \mathbf{v}_{\Gamma,2}^k - \mathbf{A}_{\Gamma 2} \mathbf{v}_2^k \end{pmatrix} \\ \begin{pmatrix} \mathbf{A}_{22} & \mathbf{A}_{2\Gamma} \\ \mathbf{A}_{\Gamma 2} & \mathbf{T}_1^{\text{app}} \end{pmatrix} \begin{pmatrix} \mathbf{v}_2^{k+1} \\ \mathbf{v}_{\Gamma,2}^{k+1} \end{pmatrix} &= \begin{pmatrix} \mathbf{f}_2 \\ \mathbf{f}_\Gamma + (\mathbf{T}_1^{\text{app}} - \mathbf{D}_{\Gamma\Gamma}) \mathbf{v}_{\Gamma,1}^k - \mathbf{A}_{\Gamma 1} \mathbf{v}_1^k \end{pmatrix}. \end{aligned}$$

converges to the solution to problem (1.9). ■

1.4.1 Substructuring

The iterative method can be substructured in order to use a Krylov type method and speed up the convergence. We introduce the auxiliary variables

$$\mathbf{h}_1 = (\mathbf{T}_2^{\text{app}} - \mathbf{D}_{\Gamma\Gamma}) \mathbf{v}_{\Gamma,2} - \mathbf{A}_{\Gamma 2} \mathbf{v}_2, \quad \mathbf{h}_2 = -\mathbf{A}_{\Gamma 1} \mathbf{v}_1 + (\mathbf{T}_1^{\text{app}} - \mathbf{D}_{\Gamma\Gamma}) \mathbf{v}_{\Gamma,1},$$

and we define the interface operator T_h

$$T_h : \begin{pmatrix} \mathbf{h}_1 \\ \mathbf{h}_2 \\ \mathbf{f} \end{pmatrix} \mapsto \begin{pmatrix} -\mathbf{A}_{\Gamma 1} \mathbf{v}_1 + (\mathbf{T}_1^{\text{app}} - \mathbf{D}_{\Gamma\Gamma}) \mathbf{v}_{\Gamma,1} \\ (\mathbf{T}_2^{\text{app}} - \mathbf{D}_{\Gamma\Gamma}) \mathbf{v}_{\Gamma,2} - \mathbf{A}_{\Gamma 2} \mathbf{v}_2 \end{pmatrix}$$

where $\mathbf{f} = (\mathbf{f}_1, \mathbf{f}_\Gamma, \mathbf{f}_2)^T$, whereas $(\mathbf{v}_1, \mathbf{v}_{\Gamma,1})$ and $(\mathbf{v}_2, \mathbf{v}_{\Gamma,2})$ are the solutions of

$$\begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{1\Gamma} \\ \mathbf{A}_{\Gamma 1} & \mathbf{T}_2^{\text{app}} \end{pmatrix} \begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_{\Gamma,1} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_\Gamma + \mathbf{h}_1 \end{pmatrix}$$

and

$$\begin{pmatrix} \mathbf{A}_{22} & \mathbf{A}_{2\Gamma} \\ \mathbf{A}_{\Gamma 2} & \mathbf{T}_1^{\text{app}} \end{pmatrix} \begin{pmatrix} \mathbf{v}_2 \\ \mathbf{v}_{\Gamma,2} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_2 \\ \mathbf{f}_\Gamma + \mathbf{h}_2 \end{pmatrix}.$$

So far, the substructuring operator is obtained simply by matching the conditions on the interface, and in matrix form reads

$$\left(\mathbf{Id} - \mathbf{\Pi T}_h \right) (\mathbf{h}_1, \mathbf{h}_2)^T = \mathbf{F}, \quad (1.16)$$

where $\mathbf{\Pi}$ is the swap operator on the interface, where $\mathbf{F} = \mathbf{\Pi T}_h(0, 0, \mathbf{f})$, and where the matrix \mathbf{T}_h is given in the following lemma (for proof see [3]).

Lemma 3. *The matrix \mathbf{T}_h in (1.16) is given by*

$$\begin{pmatrix} (\mathbf{T}_1^{\text{app}} - \mathbf{T}_1^{\text{ex}})(\mathbf{T}_1^{\text{ex}} + \mathbf{T}_2^{\text{app}} - \mathbf{D}_{\Gamma\Gamma})^{-1} & 0 \\ 0 & (\mathbf{T}_2^{\text{app}} - \mathbf{T}_2^{\text{ex}})(\mathbf{T}_2^{\text{ex}} + \mathbf{T}_1^{\text{app}} - \mathbf{D}_{\Gamma\Gamma})^{-1} \end{pmatrix}.$$

1.5 Numerical Results

We consider problem (1.1) in $\Omega = \mathbf{R} \times (0, 1)$, with Dirichlet boundary conditions at the bottom and a Neumann boundary condition on the top. We use a finite volume discretization with an upwind scheme for the advective term. We build the matrices of the substructured problem for various interface conditions and we study their spectra. We give in the tables the iteration counts corresponding to the solution of the substructured problem by a GMRES algorithm with a random right hand side G , and the ratio of the largest modulus of the eigenvalues over the smallest real part. The stopping criterion for the GMRES algorithm is a reduction of the residual by a factor 10^{-10} . We consider both advection dominated and diffusion dominated flows, and different kind of heterogeneities. We report here the results for three different test cases.

Test 1: the flow is advection dominated, the viscosity coefficients are layered, and the subdomains are symmetric with respect to the interface.

Test 2: the flow is diffusion dominated, the viscosity coefficients are layered, but are not symmetric with respect to the interface.

Test 3: the flow is diffusion dominated, the viscosity coefficients are layered, non symmetric w.r.t. the interface, and anisotropic, with an anisotropy ratio up to order 10^4 .

The velocity field is diagonal with respect to the interface and constant. The numerical tests are performed with MATLAB[®] 6.1. A more detailed description of the test cases as well as further numerical results can be found in a forthcoming paper [3].

Both conditions perform fairly well, in both terms of iteration counts and conditioning of the substructured problem, especially for the second order conditions, that show a good scalability with respect to the mesh size.

$p = q = 10$	ny		10	20	40	80	160	320
Test 1	iter	Robin	4	6	8	11	16	23
		Order 2	4	5	6	8	9	10
	cond	Robin	1.05	1.25	1.68	3.27	6.57	13.51
		Order 2	1.01	1.02	1.14	1.34	1.61	1.92
Test 2	iter	Robin	7	10	13	16	19	21
		Order 2	6	6	8	11	15	19
	cond	Robin	1.61	1.83	2.59	3.52	3.94	4.12
		Order 2	1.21	1.26	1.30	1.83	2.76	3.68
Test 3	iter	Robin	9	17	27	35	42	47
		Order 2	7	10	14	16	19	21
	cond	Robin	5.42	18.27	24.75	31.04	38.32	47.29
		Order 2	1.54	2.75	4.48	5.92	6.32	6.86

Table 1.1. Iteration counts and condition number for the substructured problem in Tests 1-3

1.6 Conclusions

We proposed two kind of algebraic interface conditions for unsymmetric elliptic problem, which appear to be very efficient and robust in term of iteration counts and conditioning of the problem with respect to the mesh size and the heterogeneities in the viscosity coefficients.

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