Optimized Algebraic Schwarz Methods for strongly heterogeneous and anisotropic layered problems

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Abstract

In this paper we consider unsymmetric elliptic problems of advection-diffusion reaction type, with strongly heterogeneous viscosity coefficients. We build Optimized Schwarz Methods (OSM) on non-overlapping domain decompositions, directly at the algebraic level, in order to guarantee robustness with respect to the heterogeneities in the coefficients. We study new interface conditions where only one or two real parameters have to be chosen along the entire interface. Using one real parameter it is possible to design interface conditions of Robin type, whereas the use of two real parameters and of more general interface conditions allows to better take into account the heterogeneities of the medium. Numerical results validate the proposed interface conditions.

1 Introduction

High fluid pressures within the rock layers of the subsurface are among the biggest problems an oil company has to deal with when drilling. A mathematical model for the prediction of fluid pressures on a geological time scale is based on conservation of mass and Darcy’s law (see for instance [5]). This can be generalized to a time-dependent advection-diffusion equation, where the region also changes in time as rocks are deposited or eroded. An Euler backward method is used for the time integration, and a numerical method such as finite volumes or finite differences is applied at any time step in order to solve the advection-diffusion equation, yielding a linear system of equations.

A further complication of the physical problem is given by the heterogeneities of the underground: the presence of layers with very large differences in permeability yields contrasts up to seven orders of magnitude in the different regions of the computational domain. The widespread availability of parallel computers makes domain decomposition methods a natural candidate to take into account such problems. Such methods are based on the subdivision of the computational domain into several subdomains (which may or may not overlap) and the parallel solution of the local problems. This procedure leads to an iterative method that converges to the solution of the original problem if the solutions in the subdomains are related by means of suitable boundary conditions at the interface. The performance of the method depends drastically on the design of interface conditions, which has been the subject of several works (see e.g. [24, 25, 29] and references therein).

We consider here elliptic problems of advection-diffusion reaction type, with strongly heterogeneous viscosity coefficients. Such problems arise naturally also in several other applications of practical interest, where different materials with different physical properties are present in the computational domain, as in the modeling electrical power networks, semiconductor devices and electromagnetics. These differences may be rather significant and this would reflect into large discontinuities in the coefficients of the problem.

We use here an Optimized Schwarz Method (OSM) with a non-overlapping decomposition. The original

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Schwarz Algorithm uses Dirichlet interface conditions, and overlapping is necessary to ensure convergence. In [23] Robin interface conditions are introduced, ensuring convergence without resorting to overlap. Optimized Schwarz Methods are becoming quite popular and have been introduced at the continuous level in [14, 21, 26] for advection-diffusion problems and then applied to other problems such Helmholtz and Maxwell equations (see for instance [9, 15, 5]), and are based on Fourier analysis. Recently, such methods have been studied directly at the discrete level in [28, 12, 24]. In this paper we design the interface conditions directly at the algebraic level, in order to guarantee robustness with respect to heterogeneities in the coefficients.

The paper is organized as follows. In Section 2 we enlighten the link between an LDU factorization of a matrix \( M \) and the construction of absorbing boundary conditions (ABC) to restrict the underlying differential problem to a part of the computational domain. In Section 3, optimal algebraic interface conditions in domain decomposition are derived for the linear system arising from the discretization of a problem with layered coefficients set on an infinite strip. In Section 4 we describe the Algebraic Schwarz algorithm, and in Section 5 we derive two families of interface conditions depending on one or two real parameters: we address both the cases of the underlying differential operator being symmetric and unsymmetric. Finally, in Section 6 some numerical results are given to validate the proposed interface conditions, in both the cases of advection dominated flows and diffusion dominated flows, with strongly heterogeneous and anisotropic viscosity coefficients. Some numerical tests intended to show the robustness of the interface conditions with respect to the mesh refinement and the mesh heterogeneities conclude the section.

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. As it is well known in domain decomposition literature, such conditions provide optimal interface transmission operators.

Let \( \Omega \in \mathbb{R}^3 \) be a bounded polyedral domain. After a finite element, finite differences or finite volume discretization of a PDE boundary value problem, we obtain a large sparse system of linear equations, given by

\[
B w = g. \tag{2.1}
\]

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 \( N_z \), \( w \in \mathbb{R}^{N_x \times N_y \times N_z} \). If the unknowns are numbered lexicographically, the vector \( w \) is a collection of \( N_x \) sub-vectors \( w_i \in \mathbb{R}^{N_y \times N_z} \), i.e.

\[
w = (w_1^T, \ldots, w_{N_x}^T)^T, \tag{2.2}
\]

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

\[
B = \begin{pmatrix}
D_1 & U_1 \\
L_1 & D_2 & \\
& \ddots & \ddots \\
& & L_{N_x-1} & U_{N_x-1} \\
& & & D_{N_x}
\end{pmatrix}, \tag{2.3}
\]

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

An exact block factorization of the matrix \( B \) defined in (2.3) is given by

\[
B = (L + T)T^{-1}(U + T), \tag{2.4}
\]

where

\[
L = \begin{pmatrix}
0 & & \\
& L_1 & \\
& & \ddots \\
& & & L_{N_x-1}
\end{pmatrix}, \quad
U = \begin{pmatrix}
0 & & \\
& U_1 & \\
& & \ddots \\
& & & U_{N_x-1}
\end{pmatrix}, \quad
T = \begin{pmatrix}
T_1 & & \\
& & \ddots \\
& & & T_{N_x}
\end{pmatrix},
\]

2
the blocks $T_i$ being matrices defined recursively as
\[
T_i = \begin{cases} 
D_i & \text{for } i = 1 \\
D_i - L_{i-1} T_{i-1}^{-1} U_{i-1} & \text{for } 1 \leq i \leq N_x.
\end{cases}
\]

So far, we can give here the algebraic counterpart of absorbing boundary conditions to truncate a part of the computational domain. Assume $g = (0, \ldots, 0, g_{p+1}, \ldots, g_{N_x})$, and let $N_p = N_x - p + 1$. To reduce the size of the problem, we look for a block matrix $K \in (\mathbb{R}^{N_p \times N_p})^{N_p}$, each entry of which is a $N_y \times N_y$ matrix, such that the solution of $K \mathbf{v} = \tilde{g} = (0, g_{p+1}, \ldots, g_{N_x})^T$ satisfies $v_k = w_{k+p-1}$ for $k = 1, \ldots, N_p$. The rows 2 through $N_p$ in the matrix $K$ coincide with the last $N_p - 1$ rows of the original matrix $B$. To identify the first row, which corresponds to the absorbing boundary condition, we take as a right hand side in (2.1) the vector $\mathbf{g} = (0, \ldots, 0, g_{p+1}, \ldots, g_{N_x})$, and, owing to (2.4), we consider the first $p$ rows of the factorized problem
\[
\begin{pmatrix}
T_1 & L_1 & T_2 \\
L_1 & T_2 \\
& & \ddots \\
& & & L_{p-1} & T_p
\end{pmatrix} 
\begin{pmatrix}
T_1^{-1} \\
T_2^{-1} \\
& \ddots \\
& & \ddots & T_p
\end{pmatrix} 
\begin{pmatrix}
T_1 & U_1 & T_2 & U_2 \\
U_1 & T_2 & \ddots & \ddots \\
& & \ddots & T_p \\
& & & T_p & U_p
\end{pmatrix} 
\begin{pmatrix}
w_1 \\
\vdots \\
w_p \\
w_{p+1}
\end{pmatrix} = \begin{pmatrix} 0 \\
\vdots \\
0 \end{pmatrix}.
\]

The first two are $p \times p$ square invertible matrices, so we need to consider only the third one, a rectangular $p \times (p+1)$ matrix: from the last row we get
\[
T_p w_p + U_p w_{p+1} = 0, 
\]
which, identifying $v_1 = w_p$ and $v_2 = w_{p+1}$, provides the first row in matrix $K$.

Assume then $\mathbf{g} = (g_1, g_{p+1}, \ldots, g_{N_x})^T$. A similar procedure can be developed to reduce the size of the problem, by starting the recurrence in the factorization (2.4) from $D_{N_x}$, as
\[
\tilde{T}_i = \begin{cases} 
D_i - L_{i-1} \tilde{T}_{i-1}^{-1} L_i & \text{for } 1 \leq i < N_x \\
D_{N_x} & \text{for } i = N_x,
\end{cases}
\]
and we can easily obtain the equation for the last row in the reduced equation as
\[
L_q w_{q-1} + \tilde{T}_q w_q = 0. 
\]

3 Optimal interface conditions in domain decomposition for an infinite layered domain

Let $\Omega = \mathbb{R} \times Q$, where $Q$ is a bounded domain of $\mathbb{R}^d$, and consider the elliptic PDE of advection-diffusion-reaction type given by
\[
-\text{div} (\epsilon \nabla u) + \text{div} (bu) + \eta u = f \
Bu = g \
\text{in } \Omega \\
\text{on } \mathbb{R} \times \partial Q,
\]
with the additional requirement on the solutions to be bounded at infinity, where the coefficients are layered (i.e. they do not depend on the $x$ variable), where $B$ is a suitable boundary operator. This can be for instance the case of a stratified material, where discontinuities in the coefficients are concentrated in the $y$ and $z$ directions. After a finite element, finite differences or finite volume discretization, we obtain an infinite sparse system of linear equations, given by
\[
A w = f.
\]

Under classical assumptions on the coefficients of the problem (e.g. $\eta - \frac{1}{\epsilon} \text{div} b > 0$ a.e. in $\Omega$) the matrix $A$ in (3.2) is definite positive.

We consider a discretization on a uniform grid via a finite volume scheme (see for instance [10]) with an upwind treatment of the advective flux, and a lexicographic numbering of the unknowns. We solve problem
(3.2) by means of an Optimized Schwarz Method: such methods have been introduced at the continuous level in [23], and at the discrete level in [28]. In the following, we design optimized interface conditions directly at the algebraic level, in order to guarantee robustness with respect to heterogeneities in the coefficients. In this order, we firstly extend the absorbing boundary conditions (ABC) of the previous section to the case of infinite domain. Then we introduce optimal interface conditions for a Schwarz method, expressed in terms of ABC.

3.1 Absorbing boundary conditions for an infinite layered domain

The lexicographic numbering of the degrees of freedom entails that the matrix of the discrete problem (3.2) is given by

$$A = \begin{pmatrix} L & D & U \\ L & D & U \\ L & D & U \end{pmatrix}.$$  (3.3)

As the number of columns in (3.3) is infinite, we can define the block

$$T_\infty := D - LT_\infty^{-1}U.$$  (3.4)

Assuming \( f = (\ldots, f_{p+1}, f_{p+2}, \ldots) \), the absorbing boundary condition for the restriction \( v = \{w_k \mid k \geq p\} \), is thus given by

$$T_\infty w_p + U w_{p+1} = 0.$$  (3.5)

Assuming then \( f = (\ldots, f_{q-2}, f_{q-1}, 0, \ldots) \), the absorbing boundary condition for the restriction \( v = \{w_k \mid k \leq q+1\} \), can be obtained, by defining the block

$$\bar{T}_\infty := D - UT_\infty^{-1}L,$$  (3.6)

as

$$L w_{q-1} + \bar{T}_\infty w_q = 0.$$  (3.7)

3.2 Optimal interface conditions in domain decomposition

So far, we consider a two domain decomposition \( \Omega = \Omega_1 \cup \Omega_2 \), \( \Omega_1 \cap \Omega_2 = \emptyset \), where

$$\Omega_1 = \mathbb{R}^- \times Q, \quad \Omega_2 = \mathbb{R}^+ \times Q,$$

and we denote with \( \Gamma = \partial \Omega_1 \cap \partial \Omega_2 \) the common interface of the two subdomains.

The resulting linear system is given by

$$\begin{pmatrix} A_{11} & A_{1\Gamma} & 0 \\ A_{\Gamma 1} & A_{\Gamma \Gamma} & A_{\Gamma 2} \\ 0 & A_{2\Gamma} & A_{22} \end{pmatrix} \begin{pmatrix} w_1 \\ w_\Gamma \\ w_2 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_\Gamma \\ f_2 \end{pmatrix},$$  (3.8)

where \( w_\Gamma \) is the vector of the internal unknowns in domain \( \Omega_i \) \( (i = 1, 2) \), and \( w_\Gamma \) is the vector of interface unknowns. In order to guarantee the conservativity of the finite volume scheme, the vector of interface unknown consists of two sets of variables, \( w_\Gamma = (w_{\Gamma,1}, w_{\Gamma,2})^T \), the first one to express the continuity of the diffusive flux, the second to express the continuity of the advective one.

At the cost of duplicating the interface variables \( w_\Gamma \) into \( w_{\Gamma,1} \) and \( w_{\Gamma,2} \), we can write a Schwarz method by introducing two square matrices \( B_1 \) and \( B_2 \) (acting on the interface variables), in the following way:

$$\begin{pmatrix} A_{11} & A_{1\Gamma} \\ A_{\Gamma 1} & A_{\Gamma \Gamma} + B_1 \end{pmatrix} \begin{pmatrix} w_{1,1}^{k+1} \\ w_{\Gamma,1}^{k+1} \end{pmatrix} = \begin{pmatrix} f_1 \\ f_\Gamma + B_1 w_{\Gamma,2}^{k+1} - A_{\Gamma 2} w_2^{k+1} \end{pmatrix},$$  (3.9)

$$\begin{pmatrix} A_{21} & A_{2\Gamma} \\ A_{\Gamma 2} & A_{\Gamma \Gamma} + B_2 \end{pmatrix} \begin{pmatrix} w_{2,1}^{k+1} \\ w_{\Gamma,2}^{k+1} \end{pmatrix} = \begin{pmatrix} f_2 \\ f_\Gamma + B_2 w_{\Gamma,1}^{k+1} - A_{\Gamma 1} w_1^{k+1} \end{pmatrix},$$  (3.10)
Lemma 3.1 Assume $A_{11}$ and $A_{22}$ are invertible. Then, choosing

$$B_1 = -A_{12}A_{22}^{-1}A_{21}, \quad B_2 = -A_{11}A_{11}^{-1}A_{11}$$

in (3.9)-(3.10) yields convergence in two steps.

Proof The result is well-known in the domain decomposition literature. We report here the proof for sake of completeness. First of all, notice that with this choice of $B_1$ and $B_2$, the bottom right blocks in (3.9) and (3.10) are Schur complements. It is classical that the subproblems in (3.9) and (3.10) are well-posed. To prove convergence it is enough, by linearity, to consider convergence to the zero solution when $(f_1, f_2, f_3)^T = 0$. At step 1 we have from (3.9)

$$A_{11}w_1 + A_{11}w_{1,1} = 0,$$

which is equivalent (applying $A_{11}A_{11}^{-1}$) to

$$A_{11}w_1 + A_{11}A_{11}^{-1}A_{11}w_{1,1} = 0.$$

The right hand side in (3.10) thus vanishes at step 2 and we have convergence to zero in two steps. The same proof holds also for $\Omega_1$. \hfill \square

The matrix $A$ of the coupled problem in (3.8) is given by

$$A = \begin{bmatrix}
  \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
  L_1 & D_1 & U_1 & 0 & 0 & 0 \\
  L_1 & D_{1\Gamma} & U_{1\Gamma} & \mathbb{0} & \mathbb{0} & \mathbb{0} \\
  \mathbb{0} & \mathbb{0} & \mathbb{0} & \mathbb{0} & \mathbb{0} & \mathbb{0} \\
  \mathbb{0} & \mathbb{0} & \mathbb{0} & \mathbb{0} & \mathbb{0} & \mathbb{0} \\
  \mathbb{0} & \mathbb{0} & \mathbb{0} & \mathbb{0} & \mathbb{0} & \mathbb{0} \\
  \mathbb{0} & \mathbb{0} & \mathbb{0} & \mathbb{0} & \mathbb{0} & \mathbb{0} \\
  \end{bmatrix}, \quad (3.11)$$

where the block $D_{1\Gamma}$ is square

$$D_{1\Gamma} = \begin{bmatrix}
  D_{1\Gamma} & 0 \\
  0 & D_{\lambda} \\
  \end{bmatrix},$$

and the blocks $L_{i\Gamma}$, $L_{i\lambda}$ and $U_{i\lambda}$ ($i = 1, 2$) are rectangular and are given by

$$L_{\Gamma 1} = \begin{bmatrix}
  L_{\Gamma 1} \\
  L_{\lambda 1} \\
  \end{bmatrix}, \quad L_{\Gamma 2} = \begin{bmatrix}
  L_{\Gamma 2} & L_{\Gamma \lambda} \\
  \end{bmatrix}, \quad U_{1\Gamma} = \begin{bmatrix}
  U_{1\Gamma} & U_{1\lambda} \\
  \end{bmatrix}, \quad U_{\Gamma 2} = \begin{bmatrix}
  U_{\Gamma 2} \\
  U_{\lambda 2} \\
  \end{bmatrix}.$$

So far, we can prove the following result.

Lemma 3.2 Let $A$ be the matrix defined in (3.11), and let $T_{1,\infty}$ and $T_{2,\infty}$ be such that

$$T_{1,\infty} = D_1 - L_1T_{1,\infty}^{-1}U_1, \quad T_{2,\infty} = D_2 - U_2T_{2,\infty}^{-1}L_2. \quad (3.12)$$

We then have

$$A_{11}^{-1}A_{11}^{-1} = L_{\Gamma 1} \left( D_{1\Gamma} - L_1T_{1,\infty}^{-1}U_1 \right)^{-1}U_{1\Gamma} \quad A_{22}^{-1}A_{22}^{-1} = U_{\Gamma 2} \left( D_{2\Gamma} - U_2T_{2,\infty}^{-1}L_2 \right)^{-1}L_{2\Gamma}.$$

Proof Let us consider $\Omega_1$ and let $V$ be a block vector defined as

$$V_\Gamma = A_{11}^{-1}A_{11}^{-1} = A_{11}^{-1} \begin{bmatrix}
  \vdots \\
  0 \\
  \end{bmatrix},$$

which can be rewritten as

$$V_{\Gamma} = \begin{bmatrix}
  0 \\
  \vdots \\
  \end{bmatrix} = \begin{bmatrix}
  L_1 & D_1 & U_1 \\
  \end{bmatrix} \begin{bmatrix}
  \vdots \\
  \end{bmatrix}.$$
The last row reads
\[ \mathbf{U}_{1\Gamma} = \mathbf{L}_1 \mathbf{V}_{-2} + D_{1\Gamma} \mathbf{V}_{-1}. \]  
(3.13)

Since the matrix \( \mathbf{A}_{11} \) is infinite, equation (3.5) allows to express \( \mathbf{V}_{-2} \) in terms of \( \mathbf{V}_{-1} \), as
\[ \mathbf{V}_{-2} = -T^{-1}_{1,\infty} \mathbf{U}_1 \mathbf{V}_{-1}, \]
where \( T_{1,\infty} = D_1 - L_1 T^{-1}_{1,\infty} U_1 \). Substituting into (3.13), we get
\[ \mathbf{U}_{1\Gamma} = \left( D_{1\Gamma} - L_1 T^{-1}_{1,\infty} U_1 \right) \mathbf{V}_{-1}. \]

So far, we can express the block \( \mathbf{V}_{-1} \) in terms of the block \( \mathbf{U}_{1\Gamma} \), as
\[ \mathbf{V}_{-1} = \left( D_{1\Gamma} - L_1 T^{-1}_{1,\infty} U_1 \right)^{-1} \mathbf{U}_{1\Gamma}. \]

Now, multiplying \( \mathbf{A}^{-1}_{11} \mathbf{A}_{1\Gamma} \) on the left by \( \mathbf{A}_{\Gamma 1} \) we obtain
\[ \mathbf{A}_{\Gamma 1} \mathbf{A}^{-1}_{11} \mathbf{A}_{1\Gamma} = \begin{bmatrix} \cdots & 0 & \mathbf{L}_{\Gamma 1} \\ \vdots & \vdots & \vdots \\ \mathbf{V}_{-2} & \mathbf{V}_{-1} \end{bmatrix} \]

It is therefore immediate to see that
\[ \mathbf{A}_{\Gamma 1} \mathbf{A}^{-1}_{11} \mathbf{A}_{1\Gamma} = \mathbf{L}_{\Gamma 1} \left( D_{1\Gamma} - L_1 T^{-1}_{1,\infty} U_1 \right)^{-1} \mathbf{U}_{1\Gamma}. \]

It is not difficult to see that a similar argument within \( \Omega_2 \) completes the proof. \( \square \)

We can thus rewrite the optimal Schwarz algorithm (3.9)-(3.10) as
\[ \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{1\Gamma} \\ \mathbf{A}_{\Gamma 1} & \mathbf{M}_{2} \end{pmatrix} \begin{pmatrix} w_{1}^{k+1} \\ w_{r,1}^{k+1} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_{\Gamma} + (\mathbf{M}_{2} - \mathbf{D}_{\Gamma \Gamma}) w_{r,2}^{k} - \mathbf{A}_{\Gamma 2} w_{1}^{k} \end{pmatrix} \]
\[ \begin{pmatrix} \mathbf{A}_{21} & \mathbf{A}_{2\Gamma} \\ \mathbf{A}_{\Gamma 2} & \mathbf{M}_{1} \end{pmatrix} \begin{pmatrix} w_{1}^{k+1} \\ w_{r,2}^{k+1} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_{\Gamma} + (\mathbf{M}_{1} - \mathbf{D}_{\Gamma \Gamma}) w_{r,1}^{k} - \mathbf{A}_{\Gamma 1} w_{2}^{k} \end{pmatrix} \]  
(3.14)

where we have set
\[ \mathbf{M}_{1} = \mathbf{D}_{\Gamma \Gamma} - \mathbf{L}_{\Gamma 1} \left( D_{1\Gamma} - L_1 T^{-1}_{1,\infty} U_1 \right)^{-1} \mathbf{U}_{1\Gamma} \quad \mathbf{M}_{2} = \mathbf{D}_{\Gamma \Gamma} - \mathbf{U}_{1\Gamma} \left( D_{2\Gamma} - U_2 T^{-1}_{2,\infty} L_2 \right)^{-1} \mathbf{L}_{2\Gamma}. \]

(3.15)

4 An algebraic non-overlapping Schwarz method

The optimal Schwarz algorithm (3.14) cannot be used in practice, due to the lack of sparsity of the matrices \( \mathbf{M}_{1} \) and \( \mathbf{M}_{2} \) in (3.15). Let thus \( \mathbf{M}_{1}^{\text{app}} \) and \( \mathbf{M}_{2}^{\text{app}} \) be suitable approximations of \( \mathbf{M}_{1} \) and \( \mathbf{M}_{2} \), respectively, and consider the following algorithm.

The method is defined directly at the algebraic level, and reads
\[ \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{1\Gamma}^{\text{app}} \\ \mathbf{A}_{\Gamma 1} & \mathbf{M}_{1}^{\text{app}} \end{pmatrix} \begin{pmatrix} \mathbf{v}_{1}^{k+1} \\ \mathbf{v}_{r,1}^{k+1} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_{\Gamma} + (\mathbf{M}_{1}^{\text{app}} - \mathbf{D}_{\Gamma \Gamma}) \mathbf{v}_{r,2}^{k} - \mathbf{A}_{\Gamma 2} \mathbf{v}_{1}^{k} \end{pmatrix} \]
\[ \begin{pmatrix} \mathbf{A}_{21} & \mathbf{A}_{2\Gamma}^{\text{app}} \\ \mathbf{A}_{\Gamma 2} & \mathbf{M}_{2}^{\text{app}} \end{pmatrix} \begin{pmatrix} \mathbf{v}_{1}^{k+1} \\ \mathbf{v}_{r,2}^{k+1} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_{\Gamma} + (\mathbf{M}_{2}^{\text{app}} - \mathbf{D}_{\Gamma \Gamma}) \mathbf{v}_{r,1}^{k} - \mathbf{A}_{\Gamma 1} \mathbf{v}_{2}^{k} \end{pmatrix} \]  
(4.1)

We can prove the following result.

**Lemma 4.1** Assume that the matrix \( (\mathbf{M}_{1}^{\text{app}} + \mathbf{M}_{2}^{\text{app}} - \mathbf{D}_{\Gamma \Gamma}) \) is invertible. Then, if the Schwarz algorithm (4.1) converges, it does to the solution to problem (3.8).
Proof We have to prove that, at convergence
\[ v_i = w_i \quad \text{for } i \neq 0 \quad v_{r,1} = v_{r,2} = w_r. \]
It is easy to see that, once convergence is achieved, we have
\[
\begin{align*}
L_{r1} v_{r,1} + M^{ppp}_{2} v_{r,1} &= -U_{r2} v_{r,1} + M^{ppp}_{2} v_{r,2} + f_r - D_{r1} v_{r,2} \\
U_{r2} v_{r,2} + M^{ppp}_{1} v_{r,2} &= -L_{r1} v_{r,1} + M^{ppp}_{1} v_{r,1} + f_r - D_{r1} v_{r,1}
\end{align*}
\]
Summing up the two equations above we get
\[
(M^{ppp}_1 + M^{ppp}_2 - D_{r1}) v_{r,1} = (M^{ppp}_1 + M^{ppp}_2 - D_{r1}) v_{r,2},
\]
which entails the continuity of the block variable \( v_r := v_{r,1} = v_{r,2} \). A simple algebra provides
\[
L_{r1} v_{r,1} + D_{r1} v_{r} + U_{r2} v_{r,1} = f_r.
\]
Thus, \( v \) and \( w \) satisfy the same equations, and this concludes the proof. \( \square \)

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
\[
h_1 = (M^{ppp}_2 - D_{r1}) v_{r,2} - A_{r2} v_2, \quad h_2 = (M^{ppp}_1 - D_{r1}) v_{r,1} - A_{r1} v_1,
\]
and we define the interface operator \( \mathcal{K} \)
\[
\mathcal{K} : \begin{pmatrix} h_1 \\ h_2 \\ f \end{pmatrix} \mapsto \begin{pmatrix} -A_{r1} v_1 + (M^{ppp}_2 - D_{r1}) v_{r,1} \\ (M^{ppp}_1 - D_{r1}) v_{r,2} - A_{r2} v_2 \end{pmatrix}
\]
where \( f = (f_1, f_r, f_2)^T \), whereas \( (v_1, v_{r,1}) \) and \( (v_2, v_{r,2}) \) are the solutions of
\[
\begin{pmatrix} A_{11} & A_{1r} \\ A_{r1} & M^{ppp}_2 \end{pmatrix} \begin{pmatrix} v_1 \\ v_{r,1} \end{pmatrix} = \begin{pmatrix} f_1 \\ f_r + h_1 \end{pmatrix} \tag{4.2}
\]
and
\[
\begin{pmatrix} A_{22} & A_{2r} \\ A_{r2} & M^{ppp}_1 \end{pmatrix} \begin{pmatrix} v_2 \\ v_{r,2} \end{pmatrix} = \begin{pmatrix} f_2 \\ f_r + h_2 \end{pmatrix} \tag{4.3}
\]
So far, the substructuring operator is obtained simply by matching the conditions on the interface, and reads
\[
\begin{pmatrix} h_1 \\ h_2 \end{pmatrix} = \Pi \mathcal{K}(h_1, h_2, 0) = \Pi \mathcal{K}(0, 0, f) \tag{4.4}
\]
where \( \Pi \) is the swap operator on the interface, having the block form
\[
\Pi = \begin{pmatrix} 0 & \text{Id} \\ \text{Id} & 0 \end{pmatrix}.
\]
Problem (4.4) can be rewritten in the matrix form
\[
\left( \text{Id} - \Pi \mathcal{K} \right) (h_1, h_2)^T = F, \tag{4.5}
\]
where \( F = \Pi T_k(0, 0, f) \), and where the matrix \( \mathcal{K} \) is given in the following lemma.
Lemma 4.2 The matrix \( K \) in (4.5) is given by

\[
K = \begin{pmatrix}
(M_1^{\text{eff}} - M_1) (M_1 + M_2^{\text{eff}} - D_{\text{rr}})^{-1} & 0 \\
0 & (M_2^{\text{eff}} - M_2) (M_2 + M_1^{\text{eff}} - D_{\text{rr}})^{-1}
\end{pmatrix}
\]

Proof: We have to express \( K(h_1, h_2, 0) \) for arbitrary vectors \( h_1, h_2 \in \mathbb{R}^N \). Owing to (4.2) we have within \( \Omega_1 \):

\[
h_1 = M_2^{\text{eff}} v_{r,1} + A_{r1} v_1 = [M_2^{\text{eff}} - A_{r1} A_r^{-1} A_{1r}] v_{r,1}
\]

the last equality being justified by Lemma 3.2 and formula (3.15). We thus have

\[
\begin{cases}
    v_{r,1} = (M_1 + M_2^{\text{eff}} - D_{\text{rr}})^{-1} h_1 \\
v_1 = -A_r^{-1} A_{1r} (M_1 + M_2^{\text{eff}} - D_{\text{rr}})^{-1} h_1,
\end{cases}
\]

and we easily get

\[
[K(h_1, h_2, 0)]_1 = -A_{r1} v_1 + (M_1^{\text{eff}} - D_{\text{rr}}) v_{r,1}
\]

\[
= [A_{r1} A_r^{-1} A_{1r} + M_2^{\text{eff}} - D_{\text{rr}}] (M_1 + M_2^{\text{eff}} - D_{\text{rr}})^{-1} h_1
\]

\[
= (M_1^{\text{eff}} - M_1) (M_1 + M_2^{\text{eff}} - D_{\text{rr}})^{-1} h_1.
\]

A similar argument within \( \Omega_2 \) provides

\[
[K(h_1, h_2, 0)]_2 = (M_2^{\text{eff}} - M_2) (M_2 + M_1^{\text{eff}} - D_{\text{rr}})^{-1} h_2.
\]

\[\square\]

The convergence properties of the Schwarz algorithm depend clearly on the choice of the approximated matrices \( T_{1,1}^{\text{eff}} \) and \( T_{2,2}^{\text{eff}} \) in the interface condition. The following sections are dedicated to their choice.

5 Approximation of the exact interface conditions

In this section we design interface conditions depending on real parameters, and we look for sparse approximations of the exact interface conditions given in (3.15). At the cost of enlarging the interface problem, we approximate \( M_1 \) and \( M_2 \) by

\[
M_1^{\text{eff}} = D_{\text{rr}} - L_{r1} [D_{1r} - L_1 (T_{1,1}^{\text{app}})^{-1} L_{1r}]^{-1} U_{1r} \quad (5.1)
\]

and

\[
M_2^{\text{eff}} = D_{\text{rr}} - U_{2r} [D_{2r} - U_2 (T_{2,2}^{\text{app}})^{-1} L_{2r}]^{-1} L_{2r} \quad (5.2)
\]

where \( T_{1,1}^{\text{app}} \) and \( T_{2,2}^{\text{app}} \) are suitable sparse approximations of \( T_{1,1} \) and \( T_{2,2} \) respectively, which are optimized to concentrate at maximum around 1 the spatial distribution of the spectrum of the substructured matrix. The optimization procedure is carried out in the case where the underlying differential operator is the same in both subdomains, and the decomposition has a minimal overlap of one cell. In this case there is no need to introduce the interface variables \( w_r \), the unknowns of the cell in the overlap are duplicated and the matrix of the coupled problem is

\[
M = \begin{pmatrix}
\begin{array}{ccc|ccc}
1 & \cdots & L & D & U & 0 \\
\vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
L & D & U & 0 & 0 & \cdots \\
0 & 0 & \cdots & 0 & 0 & \cdots \\
0 & 0 & \cdots & 0 & 0 & \cdots \\
0 & 0 & \cdots & 0 & 0 & \cdots \\
\end{array}
& \begin{array}{ccc}
1 & \cdots & L & T_2 \\
\vdots & \ddots & \vdots & \vdots \\
L & T_2 & -T_2 + D & U \\
0 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 \\
\end{array}
& \begin{array}{ccc}
1 & \cdots & L & D & U \\
\vdots & \ddots & \vdots & \vdots & \vdots \\
L & D & U & 0 & 0 & \cdots \\
0 & 0 & \cdots & 0 & 0 & \cdots \\
0 & 0 & \cdots & 0 & 0 & \cdots \\
\end{array}
\end{pmatrix},
\end{pmatrix}
\]

(5.3)
where $T_1$ and $T_2$ are suitable approximations of $T_{1,\infty}$ and $T_{2,\infty}$, respectively.
A direct computation similar to that of Section 4.1 yield the substructured matrix $M = \Id - \II K$, the matrix $K$ being given by

$$
K = \begin{pmatrix}
(T_1 - T_{1,\infty})(T_2 + T_{1,\infty})^{-1} & 0 \\
0 & (T_2 - T_{2,\infty})(T_1 + T_{2,\infty})^{-1}
\end{pmatrix}.
$$

(5.4)

One may argue that the optimization of the parameters has been done for a different problem with respect to (4.5): however, owing to (5.1) and (5.2), we optimize the approximation of the inner operators $T_{j,\infty}$ ($j = 1, 2$), rather than that of $M_1$ and $M_2$. Since they are the only matrices not sparse in (5.1) and (5.2), a good approximation of $T_{j,\infty}$ ($j = 1, 2$) entails a good approximation of the exact interface conditions. The numerical tests of the next section validate this approach. The main feature is that the so designed interface conditions are built directly at the algebraic level and are easy to implement. Clearly, they rely on the approximation of the Schur complement and, if on one hand the extension to a decomposition into stripes 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.

In the following we firstly give an explicit formula for the computation of $T_{j,\infty}$, in both the cases of a symmetric and, relying on a commutativity assumption, a non-symmetric operator. Then we design optimized interface conditions depending on one or two real parameters.

The symmetric case

If the elliptic operator is symmetric, $L_j = L_j^T = U_j$, we have

$$
T_{j,\infty} := D_j - L_j T_{j,\infty}^{-1} L_j,
$$

and we can prove the following result.

**Lemma 5.1** Assume that $-L_j = -L_j^T$ and $K_j = \begin{pmatrix} \ddots & \ddots & \ddots & \ddots \\ L_j & D_j & L_j & \ddots \\
\ddots & \ddots & \ddots & \ddots \\
\ddots & \ddots & \ddots & \ddots \\
\ddots & \ddots & \ddots & \ddots \end{pmatrix}$ are symmetric positive definite (SPD) matrices. Then,

$$
T_{j,\infty} = \frac{1}{2} D_j + \Lambda_j
$$

where

$$
\Lambda_j = (-L_j)^{-1/2} \sqrt{\frac{1}{4} (-L_j)^{-1/2} D_j (-L_j)^{-1} D_j (-L_j)^{-1/2} - \Id (-L_j)^{-1/2}}.
$$

(5.6)

is a SPD matrix.

**Proof** First of all, since $K_j$ is a SPD, both $D_j$ and $D_j + 2L_j$ are SPD matrices. Let

$$
\tilde{T}_j = (-L_j)^{-1/2} T_{j,\infty} (-L_j)^{-1/2} \text{ and } \tilde{D}_j = (-L_j)^{-1/2} D_j (-L_j)^{-1/2}.
$$

We have that $\tilde{D}_j \geq 2 \Id$ and then $\tilde{D}_j^2 \geq 4 \Id$. With these notations, we have

$$
\frac{1}{4} (-L_j)^{-1/2} D_j (-L_j)^{-1} D_j (-L_j)^{-1/2} - \Id = \frac{1}{4} \tilde{D}_j^2 - \Id.
$$

Therefore, $\frac{1}{4} \tilde{D}_j^2 - \Id$ is a SPD matrix and formula (5.5) makes sense. From (5.5), we have

$$
\tilde{T}_j = \frac{1}{2} \tilde{D}_j + \sqrt{\frac{1}{4} \tilde{D}_j^2 - \Id}.
$$

Therefore, we get

$$
\tilde{T}_j^2 = \frac{1}{2} (\tilde{D}_j \tilde{T}_j + \tilde{T}_j \tilde{D}_j) + \frac{1}{4} \tilde{D}_j^2 = \frac{1}{4} \tilde{D}_j^2 - \Id.
$$
Using that $\tilde{D}_j$ and $\tilde{T}_j$ commute, we have
\[
\tilde{T}_j^2 - \tilde{D}_j \tilde{T}_j = -\text{Id}
\]
or equivalently,
\[
\tilde{D}_j = \tilde{T}_j + \tilde{T}_j^{-1}
\]
It means that $T_{j,\infty}$ is a solution to the matrix equation
\[
D_j = T_{j,\infty} + L_j T_{j,\infty}^{-1} L_j
\]

The unsymmetric case

In the unsymmetric case, $L_j \neq U_j$, and an explicit formula for $T_{j,\infty}$ ($j = 1, 2$) cannot be derived unless the matrices $L_j$, $D_j$, and $U_j$ commute. In this case, we can prove the following result.

**Lemma 5.2** Assume that, for $j = 1, 2$, $L_j D_j = D_j L_j$, $U_j D_j = D_j U_j$, and $L_j U_j = U_j L_j$. Then

\[
T_{j,\infty} = \frac{1}{2} D_j + \Lambda_j
\]

where

\[
\Lambda_1 = (-L_1)^{-1/2} \sqrt{\frac{1}{4} (-L_1)^{-1/2} D_1 (-U_1)^{-1/2} (L_1)^{-1/2} D_1 (-U_1)^{-1/2} - \text{Id} (-U_1)^{-1/2}},
\]

and

\[
\Lambda_2 = (-U_2)^{-1/2} \sqrt{\frac{1}{4} (-U_2)^{-1/2} D_2 (-L_2)^{-1/2} (U_2)^{-1/2} D_2 (-L_2)^{-1/2} - \text{Id} (-L_2)^{-1/2}}.
\]

**Proof** By multiplying the first equation in (3.12) on the left by $(-L_1)^{-1/2}$ and on the right by $(-U_1)^{-1/2}$ we get

\[
(-L_1)^{-1/2} T_{1,\infty} (-U_1)^{-1/2} = (-L_1)^{-1/2} D_1 (-U_1)^{-1/2} - (-L_1)^{-1/2} T_{1,\infty}^{-1} (-U_1)^{-1/2}.
\]

So far, we set $X = (-L_1)^{-1/2} T_{1,\infty} (-U_1)^{-1/2}$, $A = (-L_1)^{-1/2} D_1 (-U_1)^{-1/2}$, and, relying on the commutativity assumption, we can rewrite the above equation as $X + X^{-1} = A$. Multiplying by $X$ once on the left and once on the right, and summing up we obtain the equation

\[
\left( X - \frac{A}{2} \right)^2 = \frac{A^2}{4} - \text{Id},
\]

whose positive solution provides

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

By a similar argument on the second equation in (3.12), it can be easily seen that the following formula holds for $T_{2,\infty}$

\[
T_{2,\infty} = \frac{D_2}{2} + (-U_2)^{1/2} \sqrt{\frac{1}{4} (-U_2)^{-1/2} D_2 (-L_2)^{-1/2} (U_2)^{-1/2} D_2 (-L_2)^{-1/2} - \text{Id} (-L_2)^{-1/2}}.
\]
5.1 One parameter interface conditions

Owing to the results of the previous section, we choose to approximate \( T_{j,\infty} \) \(( j = 1, 2)\) as

\[ T_1 = \frac{D_1}{2} + \Lambda_1^{app}, \quad T_2 = \frac{D_2}{2} + \Lambda_2^{app}. \]

A first opportunity consists in choosing a diagonal approximation of \( \Lambda_1 \) and \( \Lambda_2 \). We take

\[ \Lambda_1^{app} = \alpha_1^{opt} D_1, \quad \Lambda_2^{app} = \alpha_2^{opt} D_2 \]

(5.11)

where \( D_j \) \(( j = 1, 2)\) are diagonal matrices and the parameters \( \alpha_j^{opt} \) \(( j = 1, 2)\) are optimized in the following.

5.1.1 The symmetric case

If the differential operator is symmetric, we have \( T_{1,\infty} = T_{2,\infty} = \frac{D}{2} + \Lambda \). Choosing

\[ T_1 = T_2 = \frac{D}{2} + \beta D, \]

where \( \beta \in \mathbb{R} \) and \( D \) is a diagonal matrix, we get

\[ K_{\beta} = \begin{pmatrix}
(\beta D - \Lambda)(\beta D + \Lambda)^{-1} & 0 \\
0 & (\beta D - \Lambda)(\beta D + \Lambda)^{-1}
\end{pmatrix}. \]

We can prove the following result.

**Lemma 5.3** Let \( \Lambda \) and \( D \) be symmetric positive definite matrix, let \( \beta \in \mathbb{R} \), and let \( M_\beta = \text{Id} - \Pi K_\beta \). Then

\[ \min_{\beta \in \mathbb{R}} \kappa_{eff}(M_\beta) = \kappa_{eff}(M_{\beta^{opt}}) = \kappa_{eff}(D^{-1}\Lambda)^{1/2} \]

where

\[ \beta^{opt} = (\lambda_{min}(D^{-1}\Lambda)\lambda_{max}(D^{-1}\Lambda))^{1/2}, \]

(5.12)

and where \( \kappa_{eff}(M) \) denotes the ratio of the largest eigenvalue of a matrix \( M \) over its smallest one.

**Proof** Let \( \sigma(M) \) denote the spectrum of a matrix \( M \), and let \( \rho(M) \) be its spectral radius. We have

\[ \rho(K_{\beta}) = \max_{\lambda \in \sigma((\beta D)^{-1}\Lambda)} \left| \frac{1 - \lambda}{1 + \lambda} \right| \]

This expression is minimized by taking \( \beta = \beta_{opt} \) as defined in (5.12). In that case, we get

\[ \rho(K_{\beta_{opt}}) = \frac{1 - \gamma}{1 + \gamma} \]

where

\[ \gamma := \sqrt{\lambda_{min}(D^{-1}\Lambda)/\lambda_{max}(D^{-1}\Lambda)} = \kappa(D^{-1}\Lambda)^{-1/2} \]

Thus, we have

\[ \min_{\beta \in \mathbb{R}} \kappa_{eff}(M_{\beta}) = \kappa_{eff}(M_{\beta_{opt}}) = 1/\gamma = \kappa_{eff}(D^{-1}\Lambda)^{1/2} \]

If the operator is symmetric, owing to the following result by Van der Sluis, (see [30, 19])

**Theorem 5.1 (Van der Sluis)** If \( F \) is symmetric positive definite matrix, then

\[ \min_{\beta \in \mathbb{R}} \kappa(D^{-1/2}FD^{-1/2}) \leq \kappa(\text{diag}(F)^{-1/2}F\text{diag}(F)^{-1/2}) \leq m \cdot \min_{D \in \mathcal{D}} \kappa(D^{-1/2}FD^{-1/2}) \]

where \( D = \{ \text{positive definite diagonal matrices} \} \) and \( m \) is the maximum number of nonzeros in any row of \( F \).
we choose in the interface operators (5.11)
\[ D_j = \text{diag}(\Lambda_j), \]
for \( j = 1, 2, \) and
\[ \alpha^{opt}_j = (\lambda_{\min}(\text{diag}(\Lambda_j))^{-1}\Lambda_j)\lambda_{\max}(\text{diag}(\Lambda_j))^{-1}\Lambda_j)^{1/2}. \]

### 5.1.2 The unsymmetric case

If the differential operator is not symmetric, we have
\[ T_{1,\infty} = \frac{D}{2} + \Lambda_1, \quad T_{2,\infty} = \frac{D}{2} + \Lambda_2, \]
and choosing
\[ T_1 = T_2 = \frac{D}{2} + \beta D, \]
we obtain the matrix
\[
\begin{pmatrix}
(\beta D - \Lambda_1)(\beta D + \Lambda_1)^{-1} & 0 \\
0 & (\beta D - \Lambda_2)(\beta D + \Lambda_2)^{-1}
\end{pmatrix}.
\]

Let \( \Sigma_1 = (\beta D - \Lambda_1)(\beta D + \Lambda_1)^{-1}, \) and \( \Sigma_2 = (\beta D - \Lambda_2)(\beta D + \Lambda_2)^{-1}. \) Then, the following result can be easily proved (see [18]).

**Lemma 5.4** Let \( M_\beta = \text{Id} - \Pi K_\beta. \) Then
\[ \gamma \in \sigma(M_\beta) \Rightarrow (1 - \gamma)^2 \in \sigma(S_1S_2); \quad \mu \in \sigma(S_1S_2) \Rightarrow (1 \pm \sqrt{\mu}) \in \sigma(M_\beta). \]

The previous Lemma states that the eigenvalues of the substructured problem are located in a disc of the complex plane centered in 1 and with radius at most \( \rho(S_1S_2), \) the spectral radius of the product \( S_1S_2. \) We then minimize at once the spectral radii of both \( S_1 \) and \( S_2. \) We set, for \( \beta \in \mathbb{R}, \)
\[ \zeta(\beta) := \max_{\lambda \in \sigma(\Lambda_jD^{-1})} \left| \frac{\lambda - \beta^2}{\lambda + \beta} \right|, \]
and we minimize it with respect to \( \beta. \) The solution is given in the following Lemma (for proof see [18]).

**Lemma 5.5** Let
\[ r := \min_{\lambda \in \sigma(\Lambda_jD^{-1})} \text{Re}\lambda, \quad R := \max_{\lambda \in \sigma(\Lambda_jD^{-1})} \text{Re}\lambda, \quad I := \max_{\lambda \in \sigma(\Lambda_jD^{-1})} \text{Im}\lambda. \]
The solution \( \beta^{opt} \) to problem
\[ \zeta(\beta^{opt}) = \min_{\beta \in \mathbb{R}} \zeta(\beta) \]
is given by
\[ \beta^{opt} = \max \left\{ \sqrt{r^2 + I^2}, \sqrt{rR - I^2} \right\}. \]
(5.13)

Thus, if the differential operator is nonsymmetric, we choose in the interface operators (5.11)
\[ D_j = \text{diag}(\Lambda_j), \]
for \( j = 1, 2, \) and
\[ \alpha^{opt}_j = \max \left\{ \sqrt{r_j^2 + I_j^2}, \sqrt{r_jR_j - I_j^2} \right\}, \]
(5.14)
where we have set, for \( j = 1, 2, \)
\[ r_j := \min_{\lambda \in \sigma(\Lambda_jD_j^{-1})} \text{Re}\lambda, \quad R_j := \max_{\lambda \in \sigma(\Lambda_jD_j^{-1})} \text{Re}\lambda, \quad I_j := \max_{\lambda \in \sigma(\Lambda_jD_j^{-1})} \text{Im}\lambda. \]
(5.15)
5.2 Two parameters interface conditions

We can improve the approximate interface conditions by blending together two diagonal approximations of $\Lambda_1$ and $\Lambda_2$, and using an algebraic counterpart of Higdon’s trick for absorbing boundary conditions (see [20]).

5.2.1 The symmetric case

Using a standard stencil notation, consider now two interface conditions for the Schwarz algorithm as

$$
\begin{bmatrix}
L & \frac{D}{2} + \beta_1 D \\
\end{bmatrix}
\quad \text{and} \quad
\begin{bmatrix}
L & \frac{D}{2} + \beta_2 D \\
\end{bmatrix}
$$

where $\beta_1$ and $\beta_2$ are two parameters to be chosen, and consider their product

$$
Q = \begin{bmatrix}
L & \frac{D}{2} + \beta_1 D \\
\end{bmatrix}
\times
\begin{bmatrix}
L & \frac{D}{2} + \beta_2 D \\
\end{bmatrix}.
$$

The product is a three column stencil:

$$
Q = \begin{bmatrix}
L^2 & L \left( \frac{D}{2} + \beta_2 D \right) + \left( \frac{D}{2} + \beta_1 D \right) L & \frac{D}{2} + \beta_1 D \left( \frac{D}{2} + \beta_2 D \right)
\end{bmatrix}
$$

The three column stencil may be reduced to a two column stencil using the interior equations, given by the three column stencil

$$
\begin{bmatrix}
L & D & L
\end{bmatrix}
$$

Left multiplying this last stencil by $L$ and subtracting it to $Q$, we get

$$
\begin{bmatrix}
M_{-1} & M_0
\end{bmatrix}
$$

where

$$
M_{-1} = \frac{1}{2}(DL - LD) + \beta_1 LD + \beta_1 DL \quad M_0 = \left( \frac{D}{2} + \beta_1 D \right) \left( \frac{D}{2} + \beta_2 D \right) - L^2
$$

We assume that $M_{-1}$ is invertible and we left multiply by $LM_{-1}^{-1}$ to get an equivalent interface condition

$$
\begin{bmatrix}
L & LM_{-1}^{-1} M_0
\end{bmatrix}
$$

This amounts to approximate $\Lambda$ by

$$
\Lambda^{ref} = LM_{-1}^{-1} M_0 - \frac{D}{2}.
$$

The optimization is carried out under a commutativity assumption. In this case, in fact, we have

$$
M_{-1} = (\beta_1 + \beta_2) DL \quad M_0 = \frac{D^2}{4} + \frac{\beta_1 + \beta_2}{2} DD + \beta_1 \beta_2 D - L^2
$$

and, owing to (5.16)

$$
\Lambda^{ref} = \frac{1}{\beta_1 + \beta_2} \left( \frac{D^2}{4} - L^2 \right) + \beta_1 \beta_2 D.
$$

Owing to (5.6), we have $\left[ \frac{D^2}{4} - L^2 \right] = \Lambda^2$, and the substructured problem uses the matrix

$$
K_{\beta_1, \beta_2} =
\begin{pmatrix}
\left( \Lambda - \frac{D^2}{\beta_1 + \beta_2} \right) \left( \Lambda + \frac{D^2}{\beta_1 + \beta_2} \right)^{-1} & 0 \\
0 & \left( \Lambda - \frac{D^2}{\beta_1 + \beta_2} \right) \left( \Lambda + \frac{D^2}{\beta_1 + \beta_2} \right)^{-1}
\end{pmatrix}.
$$

The optimal parameters $\beta_1$ and $\beta_2$ are thus the ones that minimize the norm of the nonzero entries in the matrix $K_{\beta_1, \beta_2}$. Each nonzero entry in the matrix $K_{\beta_1, \beta_2}$ can be easily seen to admit the factorization

$$
\left( \Lambda - \frac{D^2}{\beta_1 + \beta_2} \right) \left( \Lambda + \frac{D^2}{\beta_1 + \beta_2} \right)^{-1} = \left( \Lambda - \beta_1 D \right) \left( \Lambda - \beta_2 D \right)
$$

and the following result holds (for proof see [13, 11])

13
Lemma 5.6 Let $M_{\beta_1,\beta_2} = \text{Id} - \Pi K_{\beta_1,\beta_2}$. Then, the solution to the minimization problem
$$\kappa_{eff}(M_{\beta_1,\beta_2}) = \min_{\beta_1 \in \mathbb{R}^+, \beta_2 \in \mathbb{R}^+} \kappa_{eff}(M_{\beta_1,\beta_2}),$$
is given by $(\beta_1, \beta_2)$ such that
$$\beta_1^{pt}, \beta_2^{pt} = (\lambda_m \lambda_M)^{1/2}$$
$$\beta_1^{pt} + \beta_2^{pt} = \sqrt{2(\lambda_m + \lambda_M)} \sqrt{\lambda_m \lambda_M}$$
(5.17)
where we have set
$$\lambda_m = \min\{ \lambda \in \sigma(D^{-1}A) \} \quad \lambda_M = \max\{ \lambda \in \sigma(D^{-1}A) \}.$$
We therefore choose the approximate interface conditions (5.16), where $D_j = \text{diag}(\Lambda_j)$, and $\beta_1$ and $\beta_2$ are defined in (5.17).

5.2.2 The unsymmetric case
A similar procedure to the one of the previous section can be carried out in the unsymmetric case. By using standard stencil notations, the coefficients in the approximate interface conditions can be rewritten as
$$\begin{bmatrix} D_1^{-1}L_1 & D_2^{-1}D_1 + \alpha Id \end{bmatrix} \quad \begin{bmatrix} D_2^{-1}D_2 + \beta Id \\ D_2^{-1}U_2 \end{bmatrix},$$
in $\Omega_1$ and $\Omega_2$ respectively.
Let us focus on $\Omega_1$, and consider two interface conditions based on two different real parameters $\alpha_1$ and $\alpha_2$. The product of such interface conditions yields a three column stencil
$$Q_1 = \begin{bmatrix} D_1^{-1}L_1 & D_2^{-1}D_1 + \alpha_1 Id \end{bmatrix} \times \begin{bmatrix} D_2^{-1}D_2 + \alpha_2 Id \end{bmatrix}$$
$$= \begin{bmatrix} L_1^2 \quad L_1^1 \quad (L_1 + \alpha_2 Id) \quad (L_1 + \alpha_1 Id) \quad (L_1 + \alpha_1 Id) \quad (L_1 + \alpha_2 Id) \end{bmatrix}.$$
where we have set, for sake of simplicity in notations, $D_1 = D_1^{-1}D_1$, and $L_1 = D_1^{-1}L_1$. So far, we can use the interior equation to reduce $Q_1$ to a two column stencil. This can be obtained by multiplying the stencil of the interior equation,
$$\begin{bmatrix} L_1 \quad D_1 \quad U_1 \end{bmatrix}$$
on the left by $D_1^{-1}L_1D_1^{-1}$ and subtracting it to $Q_1$.
We therefore get
$$\begin{bmatrix} A_{-1} \quad A_0 \end{bmatrix},$$
where
$$A_{-1} = [\bar{D}_1, L_1] + (\alpha_1 + \alpha_2)L_1 \quad A_0 = \bar{D}_1^2 + (\alpha_1 + \alpha_2)\bar{D}_1 + \alpha_1 \alpha_2 Id - L_1 \otimes I_1,$$
[\ldots] being the Lie bracket, and $U_1 = D_1^{-1}U_1$.
Assuming that $A_{-1}$ is invertible, we multiply on the left by $L_1 A_{-1}^{-1}$ and we get the equivalent stencil
$$\begin{bmatrix} L_1 \quad L_1 A_{-1}^{-1}A_0 \end{bmatrix}.$$ 
This amounts to approximate $T_{1,\infty}$ by
$$T_1 = L_1 \left( [\bar{D}_1, L_1] + (\alpha_1 + \alpha_2)L_1 \right)^{-1} \left( \bar{D}_1^2 + (\alpha_1 + \alpha_2)\bar{D}_1 + \alpha_1 \alpha_2 Id - L_1 \otimes I_1 \right)$$
where we take $D_1 = \text{diag}(\Lambda_1)$, and, following the choice done in the symmetric case,
$$\alpha_1 \alpha_2 = r_1 R_1 \quad \alpha_1 + \alpha_2 = \sqrt{2(r_1 + R_1)} \sqrt{r_1 R_1},$$
(5.18)
14
$r_1$ and $R_1$ being defined as

$$r_1 := \min_{\lambda \in \sigma(A_1 \Omega^D)} \Re \lambda \quad R_1 := \max_{\lambda \in \sigma(A_1 \Gamma^D)} \Re \lambda,$$

It is then easy to see that, in a similar way, we get for $\Omega_2$ the approximate interface condition

$$\begin{bmatrix}
U_2 \mathcal{B}_1^{-1} \mathcal{B}_0 & U_1 \nabla
\end{bmatrix},$$

where, letting $D_2 = \mathcal{D}_2^{-1} \mathcal{D}_2$, $L_2 = \mathcal{D}_2^{-1} L_2$, and $U_2 = \mathcal{D}_2^{-1} U_2$, we have

$$\mathcal{B}_0 = D_2^2 + (\beta_1 + \beta_2)D_2 + \beta_1 \beta_2 Id - U_2 L_2 \quad \mathcal{B}_1 = [D_2, U_2] + (\beta_1 + \beta_2)U_2.$$

We therefore approximate $T_{2,\infty}$ by

$$T_2 = U_2 \left( [D_2, U_2] + (\beta_1 + \beta_2)U_2 \right)^{-1} \left( D_2^2 + (\beta_1 + \beta_2)D_2 + \beta_1 \beta_2 Id - U_2 L_2 \right),$$

where $D_2 = \text{diag}(\Lambda_2)$, and

$$\beta_1 \beta_2 = r_2 R_2 \quad \beta_1 + \beta_2 = \sqrt{2 (r_2 + R_2) \sqrt{r_2 R_2}},$$

$r_2$ and $R_2$ being again defined as

$$r_2 := \min_{\lambda \in \sigma(A_2 \Omega^D)} \Re \lambda \quad R_2 := \max_{\lambda \in \sigma(A_2 \Gamma^D)} \Re \lambda.$$

6 Numerical Results

In this section we test the proposed interface conditions: we deal with an infinite tube in 2D, $\Omega = \mathbb{R} \times (0, 1)$, and consider the operator

$$L := - \left( \frac{\partial}{\partial x}(y) \frac{\partial}{\partial x} + \frac{\partial}{\partial y}(y) \frac{\partial}{\partial y} \right) + p(y) \frac{\partial}{\partial x} + q(y) \frac{\partial}{\partial y} + \eta(y)$$

with Dirichlet boundary conditions at the bottom and a Neumann boundary condition on the top. We use a finite volume discretization of the operator 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, in both the coefficients and the mesh parameters.

We consider a constant reaction term $\eta = 1$ and two different velocity fields:

- $p = q = 10$: the velocity is diagonal with respect to the interface and is constant.
- $p = \sin(8 \pi y), \quad q = 10(1 + y^2)$: the velocity is variable and changes sign along the interface.

The numerical tests are performed with MATLAB® 6.5, and the interface conditions use the operators $\mathcal{M}_1^{\text{pp}}$ and $\mathcal{M}_2^{\text{pp}}$ defined in (5.1) and (5.2). We list hereafter the different choices of $\Lambda_1^{\text{pp}}$ and $\Lambda_2^{\text{pp}}$ used in the numerical tests.

**One parameter interface conditions**

- $A_1$: we choose $D_1 = \text{diag}(\Lambda_1), \ D_2 = \text{diag}(\Lambda_2)$, and the optimal parameters are the ones given in (5.14).

This choice can be seen as an up tological one parameter approximation, since the computation of $\Lambda_1$ and $\Lambda_2$ is too costly to be performed in practical problems.
Robin: in order to have a usable condition, we avoid the computation of both $\Lambda_1$ and $\Lambda_2$. Observing that, if $D_j$, $L_j$, and $U_j$ ($j = 1, 2$) were all diagonal matrices the same would hold also for $T_{j,\infty}$, let $d_j$, $l_j$, and $u_j$ be their diagonals, respectively. We choose

$$D_1 = \text{diag} \left( \frac{\sqrt{d_1^2 - 4l_1u_1}}{2} \right) \quad D_2 = \text{diag} \left( \frac{\sqrt{d_2^2 - 4l_2u_2}}{2} \right).$$

We can then calculate the square of the optimal parameter $a_1^{\text{opt}}$ from formula (5.14) where, owing to (5.10) we replace $\Lambda_1 D_1^{-1}$ with

$$\left( \frac{(-L_1)^{1/2} D_1 (-U_1)^{-1/2} (-L_1)^{-1/2} D_1 (-U_1)^{1/2}}{4} - L_1 U_1 \right) D_1^{-2}. \quad (6.1)$$

In a similar way, we can calculate the square of the optimal parameter $a_2^{\text{opt}}$ from formula (5.14) where we replace $\Lambda_2 D_2^{-1}$ with

$$\left( \frac{(-U_2)^{1/2} D_2 (-L_2)^{-1/2} (-U_2)^{-1/2} D_2 (-L_2)^{1/2}}{4} - U_2 L_2 \right) D_2^{-2}. \quad (6.2)$$

Two parameters interface conditions

- **O2U**: we choose $D_1 = \text{diag}(\Lambda_1)$, $D_2 = \text{diag}(\Lambda_2)$, and the optimal parameters are the ones given in (5.18) and (5.19). Also this choice can be seen as an utopical two parameters approximation, as in the case of the $\Lambda_1$ approximation.

- **Order 2**: we choose again

$$D_1 = \text{diag} \left( \frac{\sqrt{d_1^2 - 4l_1u_1}}{2} \right) \quad D_2 = \text{diag} \left( \frac{\sqrt{d_2^2 - 4l_2u_2}}{2} \right),$$

and the squares of the optimal parameters are given by (5.18) and (5.19), where we have replaced the matrices $\Lambda_1 D_1^{-1}$ and $\Lambda_2 D_2^{-1}$ by the expressions in (6.1) and (6.2), respectively.

6.1 Advection dominated flows

In this first series of tests we consider advection dominated flows, which are characterized by a large ratio between the velocity and the diffusion coefficients. The grid is uniform ($hx = hy$), and the subdomains are heterogeneous in the $y$ direction, but they are symmetric with respect to the interface.

**Test 1: Symmetric Subdomains**

The domain $\Omega = \mathbb{R} \times [0, 1)$ is divided into ten slabs of height $hy = .1$, where the viscosity coefficients are constant. The ratio of the viscosities in two neighboring slabs can be of order $10^4$. The viscosity coefficients in the $i$-th slab is given by $c = d = \nu(i)$, the latter being the $i$-th component of the vector $\nu = [x, \beta, \gamma, \beta, \beta, \alpha, \gamma, \alpha]$, where $\alpha = 1e0$, $\beta = 1e-4$, and $\gamma = 1e-2$. We report the results in Table 1: all the interface conditions appear robust with respect to both the mesh size and the velocity field, in terms of iteration counts and conditioning of the problem. The best results are obtained with the two parameter interface conditions O2U and Order2, which appear almost insensitive to the mesh refinement and to the advective field.

6.2 Diffusion dominated flows

In this series of tests we consider diffusion dominated flows, which are characterized by a small ratio between the velocity and the diffusion coefficients. The grid is uniform ($hx = hy$).
\[\begin{array}{|c|c|c|c|c|c|c|}
\hline
\text{Velocity} & 1/hy & 10 & 20 & 40 & 80 & 160 & 320 \\
\hline
p = q = 10 & \text{iter} & \Lambda_j & 4 & 6 & 8 & 9 & 13 & 19 \\
& & Robin & 4 & 6 & 8 & 11 & 16 & 23 \\
& & O2U & 4 & 5 & 6 & 7 & 9 & 10 \\
& & Order 2 & 4 & 5 & 6 & 8 & 9 & 10 \\
\hline
p = \sin(8\pi y) & \text{cond} & \Lambda_j & 1.05 & 1.25 & 1.67 & 2.25 & 4.14 & 8.88 \\
& & Robin & 1.05 & 1.25 & 1.68 & 3.27 & 6.57 & 13.31 \\
& & O2U & 1.01 & 1.02 & 1.11 & 1.30 & 1.54 & 1.83 \\
& & Order 2 & 1.01 & 1.02 & 1.14 & 1.34 & 1.61 & 1.92 \\
\hline
q = 10(1 + y^2) & \text{iter} & \Lambda_j & 3 & 4 & 6 & 8 & 12 & 16 \\
& & Robin & 3 & 4 & 6 & 10 & 13 & 18 \\
& & O2U & 5 & 4 & 6 & 7 & 8 & 9 \\
& & Order 2 & 5 & 4 & 6 & 6 & 8 & 9 \\
\hline
\end{array}\]

Table 1: Test 1: Advection dominated flows, symmetric subdomains

**Test 2: Unsymmetric Subdomains**

In this test the viscosity coefficients are heterogeneous in both the \(x\) and the \(y\) direction. The subdomains \(\Omega_1\) and \(\Omega_2\) are again divided into ten slabs of height \(hy = 1\), where the viscosity coefficients are constant. Let \(\alpha = 1.e4, \beta = 1.e2,\) and \(\gamma = 1.e0\). The viscosity coefficients in the \(i\)-th slab of \(\Omega_1\) is given by \(c_1 = d_1 = \nu_1(i)\), the latter being the \(i\)-th component of the vector \(\nu_1 = [\alpha, \alpha, \beta, \alpha, \alpha, \alpha, \alpha, \alpha, \gamma, \alpha]\), whereas the viscosity coefficients in the \(i\)-th slab of \(\Omega_2\) is given by \(c_2 = d_2 = \nu_2(i)\), the latter being the \(i\)-th component of the vector \(\nu_2 = [\gamma, \alpha, \alpha, \alpha, \alpha, \alpha, \alpha, \alpha, \alpha, \alpha]\). We report the results in Table 2. The interface conditions are robust in terms of both iteration counts and conditioning with respect to the mesh refinement. Moreover, they are almost insensitive to the velocity field in terms of iteration counts. The one parameter interface conditions \(\Lambda\) and \(\text{Robin}\) are a little sensitive to the velocity field in terms of conditioning but this latter remains reasonable. The best performances are again obtained with the two parameters interface conditions \(\text{O2U}\) and \(\text{Order2}\).

**Test 3: Anisotropic Coefficients**

In this test the viscosity coefficients show strong discontinuities in the \(x\) and \(y\) direction, and are also anisotropic. The subdomains \(\Omega_1\) and \(\Omega_2\) are again divided into ten slabs of height \(hy = 1\), where the viscosity coefficients are constant. Let \(\alpha = 1.e4, \beta = 1.e0,\) and \(\gamma = 1.e2\). The viscosity coefficients in the \(i\)-th slab of \(\Omega_1\) are given, in the \(x\) direction, by \(c_1 = \nu_1(i)\), and in the \(y\) direction by \(d_1 = \mu_1(i)\) the latter being the \(i\)-th components of the vectors \(\nu_1 = [\beta, \alpha, \beta, \alpha, \gamma, \alpha, \beta, \gamma, \beta, \gamma]\) and \(\mu_1 = [\gamma, \alpha, \gamma, \alpha, \beta, \alpha, \gamma, \gamma, \beta, \gamma]\), respectively. Similarly, the viscosity coefficients in the \(i\)-th slab of \(\Omega_2\) are given, in the \(x\) direction, by \(c_2 = \nu_2(i)\), and in the \(y\) direction by \(d_2 = \mu_2(i)\) the latter being the \(i\)-th components of the vectors \(\nu_2 = [\gamma, \alpha, \beta, \alpha, \gamma, \alpha, \alpha, \beta, \gamma, \gamma]\) and \(\mu_2 = [\beta, \alpha, \beta, \alpha, \gamma, \alpha, \beta, \gamma, \beta, \gamma]\), respectively. We report the results in Table 3. The interface conditions appear very little sensitive to the velocity fields and the mesh refinement in terms of iteration counts. In terms of condition number the \(\text{Robin}\) interface condition shows an increase with the mesh refinement, differently from the other interface conditions. Again, the best results are obtained with the two parameters interface conditions \(\text{O2U}\) and \(\text{Order2}\).
<table>
<thead>
<tr>
<th>Velocity</th>
<th>$1/h_y$</th>
<th>10</th>
<th>20</th>
<th>40</th>
<th>80</th>
<th>160</th>
<th>320</th>
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<td>16</td>
<td>19</td>
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<td>11</td>
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<td>2.08</td>
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Table 2: Test 2: Diffusion dominated flows, unsymmetric subdomains

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<tr>
<th>Velocity</th>
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<th>20</th>
<th>40</th>
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</table>

Table 3: Test 3: Diffusion dominated flows, anisotropic coefficients

6.3 Influence of the mesh anisotropy

In this last series of tests we study the robustness of the proposed interface conditions with respect to the mesh anisotropy, for both advection and diffusion dominated flows. We consider the velocity field $p = \sin(8\pi y)$, $q = 10(1 + y^2)$, and the viscosity coefficients as described in Test 2, where $\alpha = 1.e0$, $\beta = 1.e-4$, and $\gamma = 1.e-2$ in the advection dominated case, whereas $\alpha = 1.e4$, $\beta = 1.e2$, and $\gamma = 1.e0$ in the diffusion dominated one. We take $h_y = 1/80$ (thus the size of the interface problem remains unchanged), and we either coarsen or refine the mesh in the $x$ direction, allowing different levels of refinement in the two different subdomains. We report the results in Table 4. We observe that when the mesh is coarsened in
the $x$ direction all the interface conditions perform better for both flows, in terms of both iteration counts and conditioning of the problem. This is not surprising, since the underlying finite volume scheme seeks for information at the center of adjacent cells, thus it introduces a virtual overlap: the coarsening of the mesh in the $x$ direction can be interpreted as an increase of the overlap size. In general, however, the interface conditions appear quite robust with respect to the refinement in the $x$ direction. The efficiency of the Robin interface condition decays more remarkably for diffusion dominated flows, nevertheless both the iteration counts and the conditioning remain reasonable. The best results are again obtained with the two parameters interface conditions O2U and Order2; moreover, there is no appreciable difference between their performances.

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Table 4: Influence of the mesh anisotropy for advection (top) and diffusion (bottom) dominated flows

7 Conclusions

We proposed here a way to build optimized interface conditions in a domain decomposition method for advection-diffusion-reaction problems based only on algebraic considerations on the discrete problem. Numerical experiments show that the proposed interface conditions appear to be robust with respect to the velocity field and the mesh size, also in the presence of highly discontinuous coefficients both inside the subdomains and across the interfaces, and anisotropies in both the viscosity coefficients and the discretization grid.

References


