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Quasi Optimal Interface Conditions in Domain Decomposition Methods. Application to Problems with Extreme Contrasts in the Coefficients.

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Abstract

Interface conditions are crucial in domain decomposition methods and their design has been the subject of many works. We propose in this paper a novel approach where only one or two real parameters have to be chosen for the entire interface. The method relies on van der Sluis' result on a quasi optimal diagonal preconditioner for a symmetric positive definite matrix, see [35]. It is then possible to design Robin interface conditions using only one real parameter for the entire interface. By adding a second real parameter and more general interface conditions, it is possible to take into account highly heterogeneous media. Numerical results are given.

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1 Introduction

The classical Schwarz method is based on Dirichlet boundary conditions. Overlapping subdomains are necessary to ensure convergence. It has been proposed independently in [19] and [24] to use more general interface conditions in order to accelerate the convergence and to allow for non overlapping decomposition. In [19], exact absorbing conditions are used in domain decomposition methods. They are optimal in terms of iteration counts [30] but are practically very difficult to compute or even use. In [24], Robin interface conditions are proposed. These seminal papers have been the basis for many other works: [8], [9], [7], [3], [4], [5], [6] or [15] for Helmholtz and Maxwell problems. The idea to design the interface conditions by solving an optimization problem related to the convergence rate of the domain decomposition method was apparently first raised in [33]. This optimization proved to be difficult. By using the relation between interface conditions in DDM and exact absorbing boundary conditions, the optimization becomes tractable and has been the subject of many works: see e.g. [21], [38], [11], [1], [25], [14], [2] or [13]. Such transmission conditions are essential for evolution equations [12] and for systems of equations, for the Euler equations, see [10] .

The approach in these papers consist in choosing a frozen coefficients approach either at the continuous level and then discretized (see e.g. [15], [13], [29]), or at the discrete level (see e.g. or [16]). See also [34] and [25], [31] for other approaches. In any case, parameters have to be computed at each interface node.

We propose in this paper to use a novel approach where only one or two real parameters have to be chosen for the entire interface. The method relies on van der Sluis' result on a quasi optimal diagonal preconditioner for a symmetric positive definite matrix, see [35]. It is then possible to design Robin interface conditions using only one real parameter for the entire interface, see Theorem 4.1. By adding a second real parameter and more general interface conditions (similar to the optimized of order two interface conditions [21], [1]), it is possible to take into account highly heterogeneous media.

More precisely, in § 2 we define the semi-discrete model problem under study. In § 3 we substructure the domain decomposition method. In § 4 we introduce the Robin interface condition. In § 5, we optimize a two parameter family of interface conditions. In § 6 we show numerical results and we conclude in § 7.

2 Setting of the semi-discrete problem

We consider a model problem set in an infinite tube $\Omega = \mathbb{R} \times \omega$ where ω is some bounded open set of $\mathbb{R}^p$ for some $p \geq 1$. A point in Ω will be denoted by $(x, \mathbf{y})$. Let

$$\mathcal{L} := -\frac{\partial}{\partial x} c(\mathbf{y}) \frac{\partial}{\partial x} + \mathcal{B}(\mathbf{y}) \tag{1}$$

where c is a positive real valued function and $\mathcal{B}$ is a symmetric positive definite operator independent of the variable x. For instance, if $p = 2$ one might think of

$$\mathcal{B} := \eta(y, z) - \left(\frac{\partial}{\partial y} \kappa_y(y, z) \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \kappa_z(y, z) \frac{\partial}{\partial z} \right) \tag{2}$$

with homogeneous Dirichlet boundary conditions and $\eta \geq 0$, $c, \kappa_y, \kappa_z > 0$ are given real-valued functions and $(y, z) \in \omega$.
We want to solve the following problem

$$\begin{aligned} &\mathcal{L}(u) = f \text{ in } \Omega \\ &u = 0 \text{ on } \partial\Omega \end{aligned}$$

by a domain decomposition method. The domain is decomposed into two non overlapping half tubes $\Omega_1 = (-\infty, 0) \times \omega$ and $\Omega_2 = (0, \infty) \times \omega$. The problem can be considered at the continuous level and then discretized (see e.g. [15], [13], [29]), or at the discrete level (see e.g. [25], [31] or [16]). We choose here a semi-discrete approach where only the tangential directions to the interface $x = 0$ are discretized whereas the normal direction x is kept continuous.

We therefore consider a discretization in the tangential directions which leads to

$$\mathcal{L}_h := -\frac{\partial}{\partial x} C \frac{\partial}{\partial x} + B \tag{3}$$

where B and C are symmetric positive matrices of order n where n is the number of discretization points of the open set $\omega \subset \mathbb{R}^p$. For instance if we take $\mathcal{B}$ to be defined as in (2), B may be obtained via a finite volume or finite element discretization of (2) on a given mesh or triangulation of $\omega \subset \mathbb{R}^2$.

We consider a domain decomposition method based on arbitrary interface conditions $\mathcal{Q}_1$ and $\mathcal{Q}_2$. The corresponding additive Schwarz method (ASM) reads:

$$\begin{array}{llll} \mathcal{L}_h(u_1^{n+1}) = f \quad \text{in} \quad \Omega_1 & & \mathcal{L}_h(u_2^{n+1}) = f \quad \text{in} \quad \Omega_2 \\ \mathcal{Q}_1(u_1^{n+1}) = \mathcal{Q}_1(u_2^n) \quad \text{on} \quad \Gamma & & \mathcal{Q}_2(u_2^{n+1}) = \mathcal{Q}_2(u_1^n) \quad \text{on} \quad \Gamma \end{array} \tag{4}$$

where Γ is the interface $x = 0$. It is possible to both increase the robustness of the method and its convergence speed by replacing the above fixed point iterative solver by a Krylov type method. This is made possible by substructuring the algorithm in terms of interface unknowns

$$H_1 = \mathcal{Q}_2(u_1)(0, .) \quad \text{and} \quad H_2 = \mathcal{Q}_1(u_2)(0, .)$$

Let us define the operator

$$\mathbf{T} : H_1,\, H_2,\, f \longrightarrow (\mathcal{Q}_1(v_2)\ \mathcal{Q}_2(v_1))$$

where v_i, $i = 1, 2$ solves

$$\begin{aligned} \mathcal{L}_h(v_i) &= f \quad \text{in} \quad \Omega_i \\ \mathcal{Q}_i(v_i) &= H_i \quad \text{on} \quad \Gamma \end{aligned} \tag{5}$$

The substructured problem is obtained by matching the interface conditions on the interface and reads

$$\begin{pmatrix} H_1 \\ H_2 \end{pmatrix} - \mathbf{\Pi} T(H_1,\, H_2,\, 0) = \mathbf{\Pi} T(0, 0,\, f) \tag{6}$$

where $\mathbf{\Pi}$ is the swap operator on the interfaces:

$$\mathbf{\Pi}((H_1\, H_2)^T) = (H_2\, H_1)^T$$

or in block matrix form

$$\mathbf{\Pi} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

3 The substructured problem

The convergence rate of (4) and the spectra of (6) depend on the choice of the interface conditions $\mathcal{Q}_{1,2}$. In order to design an efficient method, we need to have a formula for the substructured problem and so first for the solution to (5) with $f = 0$. An essential tool will the Dirichlet to Neumann map whose symbol is obtained here via a factorization of the operator $\mathcal{L}_h$.

3.1 Semi-continuous factorization

The factorization can be sought in this form where Λ is a SPD matrix of order n.

$$\begin{aligned} \mathcal{L}_h &= (-\frac{\partial}{\partial x} C. + \Lambda) C^{-1} (C \frac{\partial}{\partial x}. + \Lambda) \\ &= -\frac{\partial}{\partial x} C \frac{\partial}{\partial x} - \frac{\partial}{\partial x} \Lambda + \Lambda \frac{\partial}{\partial x} + \Lambda C^{-1} \Lambda \\ &= -\frac{\partial}{\partial x} C \frac{\partial}{\partial x} + \Lambda C^{-1} \Lambda \end{aligned}$$

It is thus necessary to have

$$\Lambda C^{-1}\Lambda = B$$

This equation can be solved easily in the form

$$C^{-1/2}\Lambda C^{-1/2}C^{-1/2}\Lambda C^{-1/2} = C^{-1/2}BC^{-1/2}$$

We have thus

$$\Lambda = C^{1/2}(C^{-1/2}BC^{-1/2})^{1/2}C^{1/2}$$

so that

$$\Lambda = C^{1/2}A^{1/2}C^{1/2} \tag{7}$$

where

$$A := C^{-1/2}BC^{-1/2} \tag{8}$$

Finally, we have the double equality

$$\mathcal{L}_h = (-\frac{\partial}{\partial x}C. + \Lambda)C^{-1}(C\frac{\partial}{\partial x}. + \Lambda) = (\frac{\partial}{\partial x}C. + \Lambda)C^{-1}(-C\frac{\partial}{\partial x}. + \Lambda) \tag{9}$$

3.2 Spectra of the substructured problem

Taking

$$\mathcal{Q}_1 = (C\frac{\partial}{\partial x} + \Lambda) \quad \text{and} \quad \mathcal{Q}_2 = (-C\frac{\partial}{\partial x} + \Lambda)$$

leads to a convergence in two steps of (4), see [30] or [28]. This result is optimal in terms of iteration counts. But, the matrix Λ is a priori a full matrix of order n costly to compute and use. Instead, we will use approximations to it in terms of sparse matrices denoted Λ_{ap}. We substructure in terms of

$$\begin{pmatrix} H_1 \\ H_2 \end{pmatrix} = \begin{pmatrix} (C\frac{\partial}{\partial x} + \Lambda_{ap})(u) \\ (-C\frac{\partial}{\partial x} + \Lambda_{ap})(u) \end{pmatrix}$$

We need to compute $\mathbf{T}(H_1,\, H_2,\, 0)$ for arbitrary vectors $H_1,\, H_2 \in \mathbb{R}^n$. From (9), the solution v_2 to problem (5) has the general following form

$$v_2 = exp(-\frac{1}{C}\Lambda x)(\alpha) + exp(\frac{1}{C}\Lambda x)(\beta)$$

for some $\alpha,\, \beta \in \mathbb{R}^n$. Since the solution has to be bounded as x goes to infinity, we have $\beta \equiv 0$. The boundary condition on Γ yields

$$(\Lambda + \Lambda_{ap})(\alpha) = H_2$$

so that

$$v_2 = exp(-\frac{1}{C}\Lambda x)(\Lambda + \Lambda_{ap})^{-1}(H_2)$$

It is then easy to check that the substructured problem (6) has the following form

$$(\mathbf{I} - \mathbf{\Pi T}(.,.,0)) \begin{pmatrix} H_1 \\ H_2 \end{pmatrix} = G \tag{10}$$

where $\mathbf{T}(.,.,0)$ has the following expression

$$\mathbf{T}(.,.,0) = \begin{pmatrix} (\Lambda - \Lambda_{ap})(\Lambda + \Lambda_{ap})^{-1} & 0 \\ 0 & (\Lambda - \Lambda_{ap})(\Lambda + \Lambda_{ap})^{-1} \end{pmatrix} \tag{11}$$

and

$$G = \mathbf{\Pi T}(0,0,f)$$

We have a first result relating the spectra of the substructured problem to the convergence rate of the additive Schwarz method:

Lemma 3.1 *We assume that Λ_{ap} is a SPD matrix of order n.*
Let $\rho(\Lambda_{ap})$ be the convergence rate of the Schwarz algorithm, i.e. $\rho_{Sc}(\Lambda_{ap}) = \max\{|\mu| \setminus \mu \in Sp((\Lambda - \Lambda_{ap})(\Lambda + \Lambda_{ap})^{-1})\}$.
We have that

$$\rho_{Sc}(\Lambda_{ap}) < 1$$

Moreover, the matrix $Sub(\Lambda_{ap}) := \mathbf{I} - \mathbf{\Pi T}(.,.,0)$ has real eigenvalues in $(0,2)$ symmetric w.r.t one and

$$\kappa(Sub(\Lambda_{ap})) = \frac{1 + \rho_{Sc}(\Lambda_{ap})}{1 - \rho_{Sc}(\Lambda_{ap})}$$

Proof It is then easy to check that any eigenvalue of $(\Lambda - \Lambda_{ap})(\Lambda + \Lambda_{ap})^{-1}$ is real and belongs to $(-1,1)$.
As for the second part of the proof, let (v, μ) be an eigenvector, eigenvalue of $(\Lambda - \Lambda_{ap})(\Lambda + \Lambda_{ap})^{-1}$, then

$$\begin{pmatrix} v \\ v \end{pmatrix}, 1 - \mu$$

and

$$\begin{pmatrix} v \\ -v \end{pmatrix}, 1 + \mu$$

are eigenmodes of $Sub(\Lambda_{ap})$. Let us notice that a very similar result may be found in [16]. ■

Minimizing the condition number is thus equivalent to minimizing the convergence rate of the Schwarz algorithm.

We now give a partial optimality result:

Lemma 3.2 *Let Λ_{ap} be a SPD matrix. Then,*

$$\min_{\beta\in\mathbb{R}} \kappa(Sub(\beta\Lambda_{ap})) = \kappa(Sub(\beta_{opt}\Lambda_{ap})) = \kappa(\Lambda_{ap}^{-1}\Lambda)^{1/2}$$

where

$$\beta_{opt} = (\lambda_{min}(\Lambda_{ap}^{-1}\Lambda)\lambda_{max}(\Lambda_{ap}^{-1}\Lambda))^{1/2}$$

Proof We have

$$\rho_{Sc}(\beta\Lambda_{ap}) = \max_{\lambda\in Sp((\beta\Lambda_{ap})^{-1}\Lambda)} \left|\frac{1-\lambda}{1+\lambda}\right| = \max(\left|\frac{1-\lambda_{min}((\beta\Lambda_{ap})^{-1}\Lambda)}{1+\lambda_{min}((\beta\Lambda_{ap})^{-1}\Lambda)}\right|, \left|\frac{1-\lambda_{max}((\beta\Lambda_{ap})^{-1}\Lambda)}{1+\lambda_{max}((\beta\Lambda_{ap})^{-1}\Lambda)}\right|)$$

This expression is minimized by taking $\beta = \beta_{opt}$ as defined in Lemma 3.2. In that case, we get

$$\rho_{Sc}(\beta_{opt}\Lambda_{ap}) = \frac{1-\gamma}{1+\gamma}$$

where

$$\gamma := \sqrt{\lambda_{min}(\Lambda_{ap}^{-1}\Lambda)/\lambda_{max}(\Lambda_{ap}^{-1}\Lambda)} = \kappa(\Lambda_{ap}^{-1}\Lambda)^{-1/2}$$

Thus, we have (recalling that minimizing the convergence rate of the Schwarz method is equivalent to minimizing the condition number of the symmetrized substructured problem)

$$\min_{\beta\in\mathbb{R}} \kappa(Sub(\beta\Lambda_{ap})) = \kappa(Sub(\beta_{opt}\Lambda_{ap})) = 1/\gamma = \kappa(\Lambda_{ap}^{-1}\Lambda)^{1/2}$$

$\blacksquare$

4 Robin interface conditions

Notation: Consider the largest (resp. smallest) eigenvalue denoted by $\lambda_{Max}(M)$ (resp. $\lambda_{min}(M)$) for any matrix M.

We consider the case where Λ_{ap} is a diagonal matrix. We prove a condition number estimate for the following choice:

$$\Lambda_{ap}^{q-opt} := \beta_{opt0}\; C^{1/2} diag(A)^{1/2} C^{1/2} \tag{12}$$

where

$$\beta_{opt0} = (\lambda_{min}(diag(A)^{-1}A)\,\lambda_{Max}(diag(A)^{-1}A))^{1/4}. \tag{13}$$

More precisely, we have

Theorem 4.1

$$\min_{D \in \mathcal{D}} \kappa(Sub(D)) \leq \kappa(Sub(\Lambda_{ap}^{q-opt}) \leq m^{1/4} \, . \, \min_{D \in \mathcal{D}} \kappa(D^{-1}AD^{-1})^{1/4}$$

where $\mathcal{D} = \{positive\ definite\ diagonal\ matrices\}$ and m is the maximum number of nonzeros in any row of A.

As an example, for a standard finite volume discretization for a three dimensional problem $m = 5$ and $m^{1/4} = 1.49...$

The sequel of the section is devoted to the proof of the theorem. We first give a series of results of linear algebra. The basis for the proof is

Theorem 4.2 (van der Sluis) *If F is SPD matrix, then*

$$\min_{D \in \mathcal{D}} \kappa(D^{-1/2}FD^{-1/2}) \leq \kappa(diag(F)^{-1/2}F diag(F)^{-1/2}) \leq m \, . \, \min_{D \in \mathcal{D}} \kappa(D^{-1/2}FD^{-1/2})$$

where $\mathcal{D} = \{positive\ definite\ diagonal\ matrices\}$ and m is the maximum number of nonzeros in any row of F.

see [35] and for further references [18].

Lemma 4.1 *Let L be a non singular matrix with positive real eigenvalues, then*

$$\kappa(L) = \kappa(L^T L)^{1/2} \geq \frac{\lambda_{Max}(L)}{\lambda_{min}(L)}$$

Proof see [?] ∎

Lemma 4.2 *Let E and F be SPD matrices. Then,*

$$\kappa(E^{-1/4}F^{1/2}E^{-1/4})^2 \leq \kappa(E^{-1/2}FE^{-1/2})$$

Proof Let E and F be any symmetric positive definite matrices. Let us define $L := F^{1/2}E^{-1/2}$. We have by Lemma 4.1,

$$\kappa(E^{-1/2}FE^{-1/2}) \geq \frac{\lambda_{Max}(F^{1/2}E^{-1/2})^2}{\lambda_{min}(F^{1/2}E^{-1/2})^2}$$

The spectrum of $F^{1/2}E^{-1/2}$ is the same as the spectrum of $F^{1/4}E^{-1/2}F^{1/4}$ which is symmetric

$$\kappa(E^{-1/2}FE^{-1/2}) \geq \frac{\lambda_{Max}(E^{-1/4}F^{1/2}E^{-1/4})^2}{\lambda_{min}(E^{-1/4}F^{1/2}E^{-1/4})^2)^2} = \kappa(E^{-1/4}F^{1/2}E^{-1/4})^2$$

■

The proof of theorem 4.1 is now easy. Indeed, by applying successively Lemma 3.2, Lemma 4.2, Theorem 4.2, we have

$$\begin{array}{ll} \kappa(Sub(\Lambda_{ap}^{q-opt})) & \\ & = \kappa((\Lambda_{ap}^{q-opt})^{-1}\Lambda)^{1/2} \\ & \leq \kappa(diag(A)^{-1/2}Adiag(A)^{-1/2})^{-1/4} \\ & \leq m^{1/4}\min_{D\in\mathcal{D}}\kappa(D^{-1/2}A\,D^{-1/2})^{1/4} \end{array}$$

5 Two parameters interface condition

In the previous section, the interface condition is a Robin interface condition which reads for domain Ω_1:

$$C\frac{\partial}{\partial x}+\beta_{opt}C^{1/2}DC^{1/2}$$

where and $D = diag(A)^{1/2}$, see (12). In this section, we want to design more efficient interface conditions by considering more general interface conditions than Robin interface conditions.

Inspired by Higdon's trick for absorbing boundary conditions [20] (see also [15]), we first consider an interface condition of the form

$$\mathcal{Q} := (C\frac{\partial}{\partial x}+\beta_1 C^{1/2}DC^{1/2})(C\frac{\partial}{\partial x}+\beta_2 C^{1/2}DC^{1/2})$$

for some positive parameters β_1, β_2 and D is an invertible matrix not necessarily equal to $diag(A)^{1/2}$. This product yields a second order derivative w.r.t x the normal tangential direction:

$$\mathcal{Q} := C\frac{\partial}{\partial x}(C\frac{\partial}{\partial x})+(\beta_1+\beta_2)C^{1/2}DC^{1/2}C\frac{\partial}{\partial x}+\beta_1\beta_2 C^{1/2}DCDC^{1/2}$$

By using the operator $\mathcal{L}_h$ this second order can be replaced by

$$CB$$

so that condition $\mathcal{Q}$ is equivalent to

$$\mathcal{Q} := CB+(\beta_1+\beta_2)C^{1/2}DC^{1/2}C\frac{\partial}{\partial x}+\beta_1\beta_2 C^{1/2}DCDC^{1/2}.$$

We still have to write this condition in the form

$$C\frac{\partial}{\partial x} + \Lambda_{ap,2}$$

for some operator $\Lambda_{ap,2}$. Since interface conditions are equivalent up to the left composition with any invertible operator acting along the interface, we obtain an equivalent condition $\mathcal{R}$ by left multiplying $\mathcal{Q}$ by the inverse of $(\beta_1+\beta_2)C^{1/2}DC^{1/2}$:

$$\mathcal{R} := C\frac{\partial}{\partial x} + C^{1/2}\frac{D^{-1}A + \beta_1\beta_2 D}{\beta_1+\beta_2}C^{1/2} \tag{14}$$

In other words, we choose to approximate Λ by

$$\Lambda_{ap,\beta_1,\beta_2} := C^{1/2}\frac{D^{-1}A + \beta_1\beta_2 D}{\beta_1+\beta_2}C^{1/2} \tag{15}$$

with $\beta_1, \beta_2 > 0$. Let us notice that

1. If $D = diag(A)^{1/2}$, $D^{-1/2}AD^{-1/2}$ is another approximation to $A^{1/2}$ that is consistant with approximating $A^{1/2}$ by D. Indeed, from $D \simeq A^{1/2}$, we have $D^2 \simeq A$, i.e. $D \simeq D^{-1/2}AD^{-1/2}$, but $A^{1/2} \simeq D$

2. The form (15) is preferred to the simpler form

   $$C^{1/2}(\beta D^{-1}A + \delta D)C^{1/2}$$

   because definition (15) makes optimization easier.

3. If D is any diagonal operator then operators D and $D^{-1/2}AD^{-1/2}$ are linearly independent. Indeed, suppose there exists $a \in \mathbb{R}$ such that

   $$D^{-1/2}AD^{-1/2} = a\,D$$

   then $A = aD^2$. But A is not a diagonal operator.

4. The matrix A may be seen as a discretization matrix of a second order partial differential operator in the tangential directions to the interface. It is thus related to the optimized of order two interface conditions [21], [1].

As in § 4, we have to find the best parameters β_1, β_2 in (15).

Theorem 5.1 *Suppose matrices D and $A^{1/2}$ commute. Let $\lambda_m := \lambda_{min}(D^{-1}A^{1/2})$ and $\lambda_M := \lambda_{max}(D^{-1}A^{1/2})$. The choice*

$$\beta_{1,opt}\beta_{2,opt} = \lambda_m\,\lambda_M \tag{16}$$

$$\beta_{1,opt} + \beta_{2,opt} = \left(\min_{\lambda \in Sp(D^{-1}A^{1/2})} (\lambda + \frac{\lambda_m \lambda_M}{\lambda})\,(\lambda_m + \lambda_M) \right)^{-1/2} \tag{17}$$

is optimal in the sense that:

$$\min_{\beta_1 \in \mathbb{R}^+, \beta_2 \in \mathbb{R}^+} \kappa(Sub(\Lambda_{ap,\beta_1,\beta_2})) = \kappa(Sub(\Lambda_{ap,\beta_{1,opt},\beta_{2,opt}}))$$

We have a bound on the condition number

$$\kappa(Sub(\Lambda_{ap,\beta_{1,opt},\beta_{2,opt}})) \le \frac{1}{\sqrt{2}} \left(\sqrt{\frac{\lambda_M}{\lambda_m}} + \sqrt{\frac{\lambda_m}{\lambda_M}} \right)^{1/2}$$

Remark 1 *The spectrum of the matrix $D^{-1}A^{1/2}$ is discrete. If it is replaced in the above optimization problem by the segment $[\lambda_m, \lambda_M]$, it can be shown, see [15], that it can be reduced to the optimization solved by Wachspress for ADI methods [37] and whose solution is the same than in theorem with $Sp(D^{-1}A^{1/2})$ replaced by $[\lambda_m, \lambda_M]$.*

Proof By Lemma 3.2, we have to minimize

$$\kappa(\Lambda^{-1}_{ap,\beta_1,\beta_2}\Lambda) = \kappa(\Lambda_{ap,\beta_1,\beta_2}\Lambda^{-1})$$

Since D and $A^{1/2}$ are supposed to commute, all powers of each of these matrices commute. Therefore, we have

$$\Lambda^{-1}\Lambda_{ap,\beta_1,\beta_2} = C^{-1/2}\frac{D^{-1}A^{1/2} + \beta_1\beta_2 D A^{-1/2}}{\beta_1 + \beta_2}C^{1/2}$$

whose condition number is independent of $\beta_1 + \beta_2$ and reads

$$\kappa(\Lambda_{ap,\beta_1,\beta_2}\Lambda^{-1}) = \frac{\max_{\lambda \in Sp(D^{-1}A^{1/2})} \lambda + \frac{\beta_1\beta_2}{\lambda}}{\min_{\lambda \in Sp(D^{-1}A^{1/2})} \lambda + \frac{\beta_1\beta_2}{\lambda}}$$

We prove

Lemma 5.1 *A necessary optimality condition is that*

$$\lambda_m + \frac{\beta_{1,opt}\beta_{2,opt}}{\lambda_m} = \lambda_M + \frac{\beta_{1,opt}\beta_{2,opt}}{\lambda_M}$$

or equivalently that

$$\beta_{1,opt}\beta_{2,opt} = \lambda_m \, \lambda_M$$

Proof [lemma] Suppose this is not the case, for instance that

$$\lambda_m + \frac{\beta_1\beta_2}{\lambda_m} < \lambda_M + \frac{\beta_1\beta_2}{\lambda_M}$$

The function $x \to x + \frac{\beta_1\beta_2}{x}$ being convex, its maximum over $[\lambda_m, \lambda_M]$ is reached at λ_m or λ_M which belong both to $Sp(D^{-1}A^{1/2})$. In our case, it has to be at λ_M. The minimum of $x + \frac{\beta_1\beta_2}{x}$ over $Sp(D^{-1}A^{1/2})$ is reached at some eigenvalue $y \neq \lambda_M$. Let us introduce $f : \mathbb{R}^+ \to \mathbb{R}^+$ with

$$f(\beta) = \frac{\lambda_M + \dfrac{\beta}{\lambda_M}}{y + \dfrac{\beta}{y}}$$

For small enough variations of β_1 and of β_2, λ_M and y are still the location of the extremal values of $x + \frac{\beta_1\beta_2}{x}$ over $Sp(D^{-1}A^{1/2})$ which is a discrete space. The condition number is thus given by $f(\beta_1\beta_2)$ for small enough variations of β_1 and of β_2. Moreover, we have

$$sgn(\frac{df}{d\beta}) = sgn(1/\lambda_M(y + \frac{\beta}{y}) - 1/y(\lambda_M + \frac{\beta}{\lambda_M})) = sgn(\lambda_M^2 - y^2) > 0$$

Then, decreasing $\beta_1\beta_2$, would improve the condition number. ■

Let us notice that we have then

$$\max_{\lambda \in Sp(D^{-1}A^{1/2})} \lambda + \frac{\beta_1\beta_2}{\lambda} = \lambda_m + \lambda_M$$

Now that the optimal value for $\beta_1\beta_2$ has been found, we know the optimal approximation to Λ up to the multiplicative constant $(\beta_1 + \beta_2)^{-1}$. By applying Lemma 3.2, we have

$$(\beta_{1,opt} + \beta_{2,opt})^{-1} = (\min_{\lambda \in Sp(D^{-1}A^{1/2})} (\lambda + \frac{\beta_{1,opt}\beta_{2,opt}}{\lambda}) \, (\lambda_m + \lambda_M))^{1/2}$$

and

$$\kappa(Sub(\Lambda_{ap,\beta_{1,opt},\beta_{2,opt}})) = \left(\frac{\lambda_m + \lambda_M}{\min\limits_{\lambda \in Sp(D^{-1}A^{1/2})} \lambda + \dfrac{\beta_1\beta_2}{\lambda}} \right)^{1/2}$$

The denominator depends on the repartition of the eigenvalues of $D^{-1}A^{1/2}$. It can be estimated from below since the function $x \to x + \beta_{1,opt}\beta_{2,opt}/x$ admits $2\sqrt{\lambda_m\lambda_M}$ for minimal value over $[\lambda_m, \lambda_M]$. We have thus the following bound

$$\kappa(Sub(\Lambda_{ap,\beta_{1,opt},\beta_{2,opt}})) \le \left(\frac{\lambda_m + \lambda_M}{2\sqrt{\lambda_m\lambda_M}} \right)^{1/2} = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{\lambda_M}{\lambda_m}} + \sqrt{\frac{\lambda_m}{\lambda_M}} \right)^{1/2}$$

■

6 Numerical results

In this section, we test various interface conditions and algorithms in the semi-continuous framework of the previous sections. More precisely, we work in 2D on the infinite tube $\Omega = \mathbb{R} \times (0,1)$ and consider the operator

$$\mathcal{L} = -\frac{\partial}{\partial x} c(y) \frac{\partial}{\partial x} + \eta(y) - \frac{\partial}{\partial y} \kappa(y) \frac{\partial}{\partial y} \tag{18}$$

along with Dirichlet boundary condition at the bottom and a Neumann boundary condition at the top. We use a finite volume discretization of the operator in the y direction which yields a tridiagonal matrix B of order ny. It is then possible to form the matrices of the substructured problems (10) for various interface conditions and study their spectra. We either plot the spectra or give in the tables the ratio of the largest norm of the eigenvalues of the substructured matrix over its smallest real part. We also give iteration counts (#iter in the tables) corresponding to the solving of equation (10) by a gmres algorithm [32] with a random right hand-side G. The stopping criterion is a reduction of the residual by a factor 10^{-6}. Although we don't consider a discretization in the x direction, the results are a good indication of what would happen in the corresponding fully discrete computations.

We now define more precisely the names written in the tables and corresponding to the various domain decomposition methods which have been tested: opt0, opt2, noprec, diagprec

opt0 The interface condition is the one studied in section 4.

opt2 The interface condition is given by formula (14) where $D = diag(A)^{1/2}$ and β_1, β_2 are given by formulas (16) and

$$\beta_1 + \beta_2 = (2\sqrt{\lambda_m \lambda_M}(\lambda_m + \lambda_M))^{-1/2} \tag{19}$$

This last formula corresponds to formula (17) where the discrete spectrum of $D^{-1}\Lambda$ is replaced by the segment of its extremal values. Moreover, by Lemma 4.2, λ_m and λ_M are easily computed by taking the square root of the extremal eigenvalues of $diag(A)^{-1}A$. It should be noted that although matrices D and Λ do not commute in general, the computation of the parameters β_1, β_2 is based on Theorem 5.1.

noprec The conjugate gradient is applied to the substructured system

$$\Lambda(u) = G$$

which corresponds to a Schur type method without preconditioner.

diagprec The above system is preconditioned by its diagonal.

6.1 Constant coefficients

The operator $\mathcal{L}$ is the Laplace operator. The diagonal of the matrix Λ is constant (except for the entries corresponding to $y = 0$ or $y = 1$). Preconditioning by the diagonal is hardly efficient. Therefore iterations counts corresponding to *diagprec* and *noprec* are given in the same line.

Table 1: Results for constant coefficients problems

ny		10	20	40	80	160
(opt0)	#iter	10	13	16	20	24
	$\lvert\lambda\rvert_{max}/real(\lambda)_{min}$	3.2	4.5	6.5	9.24	13.1
(opt2)	#iter	6	7	8	9	10
	$\lvert\lambda\rvert_{max}/real(\lambda)_{min}$	1.4	1.7	2.0	2.4	2.88
(diag/no prec)	#iter	10	15	23	35	50
	$\lambda_{max}/\lambda_{min}$	10.2	21.0	42.7	86.4	1.74e+02

6.2 Rapidly varying coefficients

For this series of tests, $\eta = 1.e{-}9$, $c = exp(-2y^2)$ and $\kappa = 5sin(2y^2)$. Except for *noprec*, iterations counts are very similar to the constant coefficient case.

Table 2: Results for rapidly varying coefficients

ny		10	20	40	80	160
(opt0)	#iter	10	12	15	18	22
	$\lvert\lambda\rvert_{max}/real(\lambda)_{min}$	2.6	3.8	5.3	7.5	10.6
(opt2)	#iter	6	7	8	9	10
	$\lvert\lambda\rvert_{max}/real(\lambda)_{min}$	1.2	1.4	1.6	1.9	2.3
(noprec)	#iter	10	20	34	55	82
	$\lambda_{max}/\lambda_{min}$	13.4	28.4	5.8e+01	1.2e+02	2.4e+02
(diagprec)	#iter	10	15	23	34	48
	$\lambda_{max}/\lambda_{min}$	6.5	13.3	2.6e+01	5.3e+01	1.1e+02

6.3 Highly heterogeneous problems

The diffusion coefficients are highly heterogeneous: $c(y) = \kappa(y) = val([10y])$ where [ ] is the integer part function and *val* is the vector val=[a d a b a b a b a b] where $a = 1.e4$, $b = 1.e0$ and $d = 1.e2$. We have $\eta = 1e - 9$. Iteration counts are larger than in the previous cases.

Table 3: Results for highly heterogeneous problems

ny		10	20	40	80	160
(opt0)	#iter	11	17	22	28	37
	$\|\lambda\|_{max}/real(\lambda)_{min}$	6.8	31.4	48.8	71.9	1.1e+02
(opt2)	#iter	9	11	15	17	18
	$\|\lambda\|_{max}/real(\lambda)_{min}$	1.8	3.8	4.9	5.9	7.2
(noprec)	#iter	10	22	61	136	320
	$\lambda_{max}/\lambda_{min}$	7.3e+02	1.1e+04	2.5e+04	5.3e+04	1.1e+05
(diagprec)	#iter	7	17	27	42	64
	$\lambda_{max}/\lambda_{min}$	42.7	1.1e+03	2.4e+03	5.1e+03	1.1e+04

6.4 Different Subdomains

In the above cases, by symmetry of the problem w.r.t. the interface, a Neumann-Neumann or FETI algorithm would give convergence in one iteration. In this section, we compare the optimized interface conditions approach developed so far to these algorithms when the operators in domains Ω_1 and Ω_2 are not the same. The model problem reads:

$$\begin{aligned} &\mathcal{L}_{1,h}(u) = f \quad \text{in} \quad \Omega_1 \\ &C_1 \frac{\partial u_1}{\partial x} = C_2 \frac{\partial u_2}{\partial x} \quad \text{on} \quad \Gamma \end{aligned} \qquad \begin{aligned} &\mathcal{L}_{2,h}(u_2) = f \quad \text{in} \quad \Omega_2 \\ &u_2 = u_1 \quad \text{on} \quad \Gamma \end{aligned} \tag{20}$$

where $\mathcal{L}_{i,h}$, $i = 1, 2$ is a finite volume discretization of

$$\mathcal{L}_{i,h} = -\frac{\partial}{\partial x} c_i(y) \frac{\partial}{\partial x} + \eta_i(y) - \frac{\partial}{\partial y} \kappa_i(y) \frac{\partial}{\partial y} \tag{21}$$

This problem is solved by a domain decomposition method. The additive Schwarz method is

$$\begin{aligned} \mathcal{L}_{1,h}(u_1^{n+1}) &= f \quad \text{in} \quad \Omega_1 \\ (C_1 \frac{\partial}{\partial x} + \Lambda_{ap,2})(u_1^{n+1}) &= (C_2 \frac{\partial}{\partial x} + \Lambda_{ap,2})(u_2^n) \quad \text{on} \quad \Gamma \end{aligned} \tag{22}$$

$$\begin{aligned} \mathcal{L}_h(u_2^{n+1}) &= f \quad \text{in} \quad \Omega_2 \\ (-C_2 \frac{\partial}{\partial x} + \Lambda_{ap,1})(u_2^{n+1}) &= (-C_2 \frac{\partial}{\partial x} + \Lambda_{ap,1})(u_1^n) \quad \text{on} \quad \Gamma \end{aligned} \tag{23}$$

where $\Lambda_{ap,i}$, $i = 1, 2$ are matrices approximating the discrete Dirichlet to Neumann map of domain Ω_i

$$\Lambda_i = C_i^{1/2} (C_i^{-1/2} B_i C_i^{-1/2})^{1/2} C_i^{1/2}$$

where B_i is the finite volume discretization matrix of

$$\mathcal{B}_i = \eta_i(y) - \frac{\partial}{\partial y} \kappa_i(y) \frac{\partial}{\partial y}$$

As explained in § 3, the ASM is a fixed point method that can be accelerated by substructuring the problem and using a Krylov method. In our case, we use the gmres algorithm.

We now define more precisely the names written in the tables and corresponding to the various domain decomposition methods which have been tested: opt0, opt2, NeumannKappa and NeumannMatKappa

opt0 and **opt2** in both cases, matrices $\Lambda_{ap,i}$, $i = 1, 2$ are built separately as in section 6. These approximations don't take into account the fact they are used in a domain decomposition in which now operators vary from one domain to the other. Numerical results show that for opt2 iteration counts are still good.

NeumannKappa This corresponds to a a Neumann-Neumann algorithm. The conjugate gradient algorithm is applied to the substructured problem

$$\Lambda_1 + \Lambda_2(u) = G$$

preconditioned by

$$w_1 \Lambda_1^{-1} w_1 + w_2 \Lambda_2^{-1} w_2$$

with $w_i = \frac{C_1}{C_1 + C_2}$, $i = 1, 2$.

NeumannMatKappa The same as above except that the weights in the preconditioner come from the discretization matrix w_i is the diagonal of the discretization matrix of the problem.

For these last two methods, one iteration consists in solving a Dirichlet and a Neumann boundary value problem in each subdomain. In the tables, we report the number of subdomain solves, one per iteration for opt0 or opt2 and two per iteration for NeumannKappa and NeumannMatKappa. In table 4, $\eta_1 = 1e + 4$, $\eta_2 = c_1 = c_2 = \kappa_1 = \kappa_2 = 1$.

Table 4: Results for highly heterogeneous problems

ny		10	20	40	80	160	320
(opt0)	#subdom. solves	4	5	7	9	12	15
(opt2)	#subdom. solves	2	3	3	5	6	7
(NeumannKappa)	#subdom. solves	16	20	22	22	22	22
(NeumannMatKappa)	#subdom. solves	8	10	14	20	22	22

In Table 5, we consider a highly heterogeneous case: $\eta_{1,2} = 1.e - 9$, $c_1(y) = val1([10y])$ and *val1* is the vector
val1=[b d b a b a b b d b] where $a = 1.e4$, $b = 1.e0$ and $d = 1.e2$, $\kappa_1(y) = val2([10y])$ and *val2* is the vector
val2=[b a b a d a b b e b] where $a = 1.e4$, $b = 1.e0$, $d = 1.e2$ and $e = 1.e3$, $c_2(y) = val3([10y])$ and *val3* is the vector
val3=[a b a g b b a g a b] where $a = 1.e4$, $b = 1.e0$ and $g = 1.e2$ and $\kappa_2(y) = val4([10y])$ and *val4* is the vector
val4=[b a d a b a a a d b] where $a = 1.e0$, $b = 1.e4$ and $d = 1.e2$

Table 5: Results for highly heterogeneous problems

ny		10	20	40	80	160	320
(opt0)	#subdom. solves	8	22	32	40	48	56
	$\|\lambda\|_{max}/real(\lambda)_{min}$	1.9	25.6	43.5	65.1	94.1	1.3e+2
(opt2)	#subdom. solves	8	11	13	15	15	16
	$\|\lambda\|_{max}/real(\lambda)_{min}$	7.6	3.6	4.6	5.7	6.8	8.2
(diagprec)	#subdom. solves	9	20	33	51	77	111
	$\lambda_{max}/\lambda_{min}$	3.5	8.5e+2	2.0e+3	4.4e+3	9.1e+3	1.8e+4
(NeumannKappa)	#subdom. solves	12	18	24	28	32	32
	$\lambda_{max}/\lambda_{min}$	22.1	31.9	35.6	40.7	47.8	59.7
(NeumannMatKappa)	#subdom. solves	10	18	24	24	24	28
	$\lambda_{max}/\lambda_{min}$	1.9	2.2e+2	3.0e+2	4.2e+2	6.2e+2	9.6e+2

Iteration counts for opt0 are significantly higher than in Table 3. Whereas, the interface conditions opt2 are quite insensitive to the fact that operators are not the same in the subdomains. As expected from the theory for Neumann-Neumann or FETI method (see [26], [23] or [22] and references herein), the iteration counts are bounded from above as the mesh size goes to zero.

6.5 Playing with the parameters in the interface conditions

In this section, both subdomains have the same equations. We investigate the influence of the parameters β for interface conditions

$$C\frac{\partial}{\partial n} + \beta_0 C^{1/2} diag(A)^{1/2} C^{1/2} \tag{24}$$

(see 12) and for the ones of the form (14). In both cases, a key factor is the eigenvalues $eigM$ of $M := D^{-1}A^{1/2}$ where $D = diag(A)^{1/2}$. As an example, we take $ny = 40$, $\eta = 0$ and

$$c(y) = \kappa(y) = \begin{cases} 1 \quad \text{for} \quad 0 \le y \le 0.3 \\ 1.e+4 \quad \text{for} \quad 0.3 \le y \le 0.6 \\ 1 \quad \text{for} \quad 0.6 \le y \le 1 \end{cases} \tag{25}$$

The eigenvalues of M are given in Table 6

Table 6: Eigenvalues of matrix M: eigM

5.329469058781055e-04	9.648973328110511e-02
1.385298394166431e-01	2.012580286542583e-01
2.752235067980078e-01	2.871934245780574e-01
3.983838575345311e-01	4.082391320897262e-01
4.710395757370086e-01	5.355974308332332e-01
5.874669548248144e-01	6.433877730503701e-01
6.555459008079766e-01	7.643136997314994e-01
7.665800132401215e-01	7.998197268509604e-01
8.669683088526792e-01	9.260333944553774e-01
9.377196074715888e-01	9.577729169492986e-01
1.040514795453881e+00	1.058622660707454e+00
1.068860211792659e+00	1.117302981041904e+00
1.166314024840675e+00	1.188425463923074e+00
1.189884266810325e+00	1.253099984811212e+00
1.259385633350359e+00	1.286422394468029e+00
1.308867981151973e+00	1.333462304712622e+00
1.354009162092570e+00	1.356941524921361e+00
1.384745441183732e+00	1.387174113550929e+00
1.399819704784228e+00	1.407412336023526e+00
1.410918045589941e+00	1.414213461952472e+00

Applying formula (13) for interface conditions opt0, we get $\beta_{0,opt} = 2.74e-02$. Applying formulas (16) and (19) for interface conditions opt2, we have $\beta_1 = 3.8e-01$ and $\beta_2 = 1.9e-03$. Other choices are possible. Indeed, looking at Table 6, we see that the eigenvalues are regularly spaced between 1.41 and 9.648e-02 except for the smallest one $5.329e-04$. This is in agreement with results on the number of very small eigenvalues of a diagonal ([17]) or of an Incomplete Choleski (IC) preconditioner ([36]) for such problems with extreme contrasts in the coefficients. It seems then of interest to use a Robin interface condition that will take into account all the eigenvalues of M except for the smallest one. The interface condition will be better than opt0 except for the smallest eigenvalue that will be left to the Krylov method. This yields $\beta_0 = \sqrt{eigM(2)eigM(ny)} = 3.6e-1$ in (24). This choice will be referred to as bid0. Using the two parameters approach as defined in (19), we can improve over bid0 and hopefully over opt2 by taking $\beta_1 = \beta_0$ and $\beta_2 = eigM(1) = 9.648e-02$ in order to have a uniform approximation to Λ. This choice will be referred to as bid2. The

performances are given in Table 7 and on figure 1 of the eigenvalues of the corresponding substructured problems. This figure corresponds well to the motivation for the choice of the parameter β. The eigenvalues for bid0 are close to one except for two which are close to 0 and 2 respectively. The fact that we have two (and not one) such eigenvalues correspond to the symmetry of the spectrum as stated in Lemma 3.1. The eigenvalues for bid2 are closer to one than for opt2. This does not contradict Theorem 5.1 which assumes that $A^{1/2}$ and D commute which is not the case here.
This kind of optimization is impossible using a frozen coefficients approach where a discontinuity can not be taken into account. Another way to address the problem of the few very small eigenvalues is to use deflation, see [16] or [27] in the context of domain decomposition method. The drawback is that all small eigenvalues and corresponding eigenvectors are then needed.

Table 7: Results for highly heterogeneous problems

Interface Cond.	opt0	opt2	bid0	bid2
#iterations	28	14	18	12
$\lvert\lambda\rvert_{max}/real(\lambda)_{min}$	51.4	5.0	6.97e+2	3.8

The convergence curves of the gmres algorithm for the various interface conditions are given in figure 2. The interface condition bid0 yields a plateau in the convergence curve corresponding to the smallest eigenvalue which is not taken into account. The iteration count is better than for opt0 although the convergence of the latter is more regular. Interface conditions opt2 and bid2 perform similarly well.

7 Conclusion

We proposed a way to compute quasi optimal interface conditions for domain decomposition methods for symmetric positive definite equations. Numerical results in the two-subdomains case and at the semi-continuous level show that the approach is efficient and robust even with highly discontinuous coefficients both across and inside subdomains. Numerical tests for arbitrary decompositions and at the discrete level are necessary to fully assess the method. The extension of this work to a purely algebraic setting is in preparation. The non-symmetric case is under study.

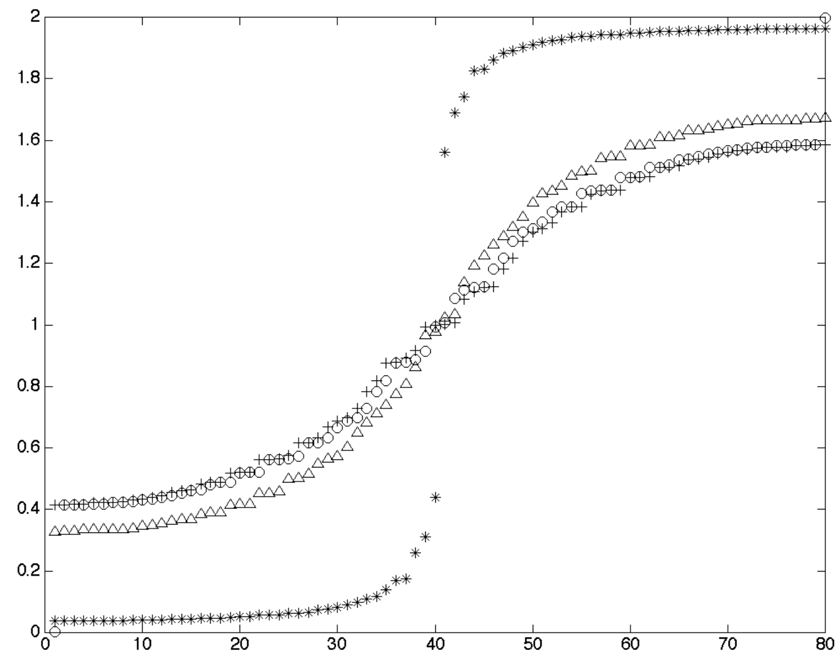

Figure 1: Eigenvalues of the substructured problem for various interface conditions: star: opt0, triangle: opt2, circle: bid0, cross: bid2

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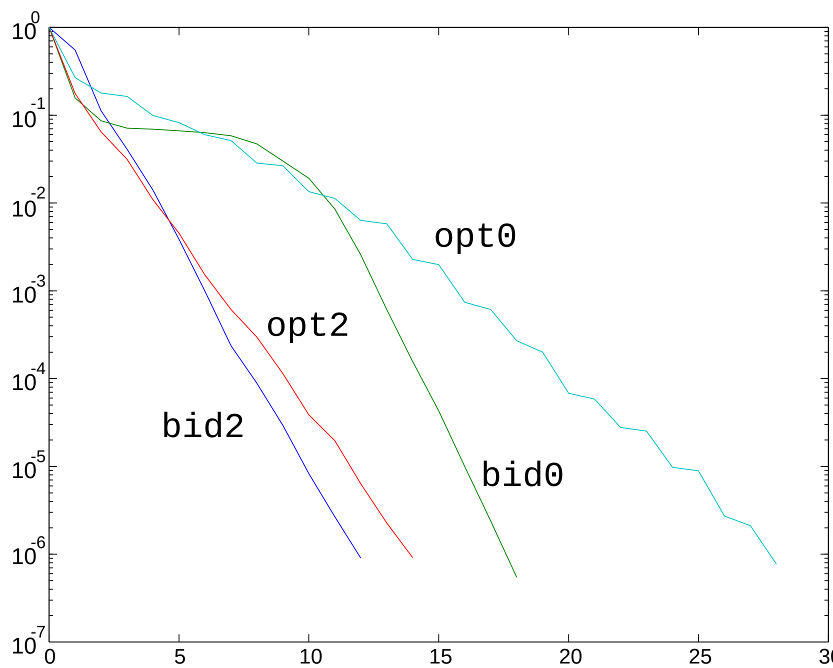

Figure 2: Relative residual vs. iteration number for the gmres algorithm and various interface conditions

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