

Robust preconditioners via generalized eigenproblems for hybrid sparse linear solvers

Emmanuel Agullo, Luc Giraud, Louis Poirel

▶ To cite this version:

Emmanuel Agullo, Luc Giraud, Louis Poirel. Robust preconditioners via generalized eigenproblems for hybrid sparse linear solvers. SIAM Journal on Matrix Analysis and Applications, Society for Industrial and Applied Mathematics, 2019, 40 (2), pp.417-439. 10.1137/17M1153765. hal-02074474

HAL Id: hal-02074474 https://hal.inria.fr/hal-02074474

Submitted on 20 Mar 2019

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

1 ROBUST PRECONDITIONERS VIA GENERALIZED EIGENPROBLEMS FOR 2 HYBRID SPARSE LINEAR SOLVERS

E. AGULLO, L. GIRAUD, L. POIREL

Abstract. The solution of large sparse linear systems is one of the most time consuming kernels in many 4 numerical simulations. The domain decomposition community has developed many efficient and robust methods in the last decades. While many of these solvers fall into the abstract Schwarz (aS) framework, their robustness has 6 originally been demonstrated on a case-by-case basis. In this paper, we propose a bound for the condition number 7 of all deflated aS methods provided that the coarse grid consists of the assembly of local components that contain 8 the kernel of some local operators. We show that classical results from the literature on particular instances of 9 10 aS methods can be retrieved from this bound. We then show that such a coarse grid correction can be explicitly 11 obtained algebraically via generalized eigenproblems, leading to a condition number independent of the number of 12 domains. This result can be readily applied to retrieve or improve the bounds previously obtained via generalized 13 eigenproblems in the particular cases of Neumann-Neumann (NN), Additive Schwarz (AS) and optimized Robin but 14also generalizes them when applied with approximate local solvers. Interestingly, the proposed methodology turns 15out to be a comparison of the considered particular aS method with generalized versions of both NN and AS for 16 tackling the lower and upper part of the spectrum, respectively. We furthermore show that the application of the 17 considered grid corrections in an additive fashion is robust in the AS case although it is not robust for aS methods in 18 general. In particular, the proposed framework allows for ensuring the robustness of the AS method applied on the 19 Schur complement (AS/S), either with deflation or additively, and with the freedom of relying on an approximate 20 local Schur complement. Numerical experiments illustrate these statements.

Key words. preconditioning, SPD linear systems, robust, scalable, coarse space, generalized eigenvalue, parallel hybrid (direct/iterative) solver

23 AMS subject classifications. 15A06, 65F08, 65F10, 15A12, 65N55

1. Introduction. Many scientific or engineering applications require at some point the solution of large sparse linear systems in parallel. Once the specific problem has been discretized, the resulting matrix equation can be solved using either an external general purpose linear solver, or a more specific solver tailored to the particular problem. With the first approach, referred to as the algebraic approach, the user can benefit with little integration effort from the developments and optimizations of black-box libraries which perform very well on modern architectures [4, 19].

On the other hand, the second approach often allows additional optimizations that further exploit additional characteristics of the underlying problem and requires a tighter integration of the solver within the application code. A widely used class of methods that fall in this latter category are domain decomposition methods (DDM) [10, 20, 28, 30, 35], which are inherently parallel and provide robust and scalable solvers for a wide range of physical problems.

In this article, we aim at combining the advantages of both these approaches. For that, while remaining as algebraic as possible, we identify some key information to be provided to the solver alongside the matrix. For symmetric positive definite (SPD) problems we show that providing the matrix in a distributed fashion, as a sum of symmetric positive semi-definite (SPSD) matrices, is enough to build a robust and scalable hybrid solver. This is a common situation when applying a finite element method over a partitioned mesh, but the methods presented in this article are not limited to this particular case: for instance, more complex discretizations such as the hybridizable discountinuous Galerkin method [7] can be used instead.

43 The linear system to be solved is

where \mathcal{K} is a $n \times n$ sparse SPD matrix that does not need to be known explicitly. Instead, the parallel application provides \mathcal{K} to the solver as a sum $\mathcal{K} = \sum_{i=1}^{N} \mathcal{K}_{i}^{(g)}$ of N SPSD matrices $\mathcal{K}_{i}^{(g)}$. 46 47 Even though $\mathcal{K}_i^{(g)}$ is of size $n \times n$, in practical applications it has only n_i non-zero rows (and columns), 48 meaning that this matrix represents the interaction of only a subset of the unknowns from the global 49 problem. We define the global domain $\Omega = \{1, \ldots, n\}$ as the set of row (or column) indices in \mathcal{K} , 50 and the subdomain $\Omega_i = \{\omega_1^{(i)}, \omega_2^{(i)}, \dots, \omega_{n_i}^{(i)}\}$ as the set of indices of the non-zero rows and columns in $\mathcal{K}_{i}^{(g)}$ (Ω_{i} is the set of vertices in the adjacency graph of $\mathcal{K}_{i}^{(g)}$). We introduce the $n_{i} \times n$ canonical restriction matrix $\mathcal{R}_{\Omega_{i}}$ from Ω to Ω_{i} , such that for any vector $u = (u_{1}, \ldots, u_{n}) \in \mathbb{R}^{n}$, $\mathcal{R}_{\Omega_{i}} u$ is 52 53 the vector $(u_{\omega_1^{(i)}}, \ldots, u_{\omega_n^{(i)}}) \in \mathbb{R}^{n_i}$. Then, we define the $n_i \times n_i$ SPSD matrix $\mathcal{K}_i = \mathcal{R}_{\Omega_i} \mathcal{K}_i^{(g)} \mathcal{R}_{\Omega_i}^T$, 54referred to as the *local matrix* of subdomain Ω_i , leading to

56 (1.2)
$$\mathcal{K} = \sum_{i=1}^{N} \mathcal{R}_{\Omega_i}^T \, \mathcal{K}_i \, \mathcal{R}_{\Omega_i}.$$

The unknowns in any subdomain Ω_i can be partitioned into an interior $\mathcal{I}_i = \{\omega \in \Omega_i \quad s.t. \quad \forall j \neq 1$ $i, \quad \omega \notin \Omega_j\}$ and an interface $\Gamma_i = \{\omega \in \Omega_i \quad s.t. \quad \exists j \neq i \quad \omega \in \Omega_j\} = \Omega_i \setminus \mathcal{I}_i$. If an unknown $\omega \in \Omega_i$ appears in at least one other subdomain, then $\omega \in \Gamma_i$, otherwise $\omega \in \mathcal{I}_i$. This yields a partition of the global domain $\Omega = \{1, \ldots, n\} = \mathcal{I}_1 \cup \cdots \cup \mathcal{I}_N \cup \Gamma$ where $\Gamma = \Gamma_1 \cup \cdots \cup \Gamma_N$ is the global interface.

⁶³ Then, eliminating in parallel the interior unknowns following for instance [Section 2, 25] the ⁶⁴ original system (1.1) reduces to a Schur problem defined on the interface Γ

65 (1.3)
$$\mathcal{S}u_{\Gamma} = \tilde{f}'_{\Gamma}, \qquad \mathcal{S} = \sum_{i=1}^{N} \mathcal{R}^{T}_{\Gamma_{i}} \, \mathcal{S}_{i} \, \mathcal{R}_{\Gamma_{i}}$$

67 where the global Schur matrix \mathcal{S} is SPD and the local Schur matrices \mathcal{S}_i are SPSD. Using the 68 classical index notation for referring to sub-blocks of matrices and vectors, we have $\mathcal{S} = \mathcal{K}_{\Gamma\Gamma} -$ 69 $\sum_{i=1}^{N} \mathcal{K}_{\Gamma\mathcal{I}_i} \mathcal{K}_{\mathcal{I}_i\mathcal{I}_i}^{-1} \mathcal{K}_{\mathcal{I}_i\Gamma}, \ \widetilde{f}'_{\Gamma} = f_{\Gamma} - \sum_{i=1}^{N} \mathcal{K}_{\Gamma\mathcal{I}_i} \mathcal{K}_{\mathcal{I}_i\mathcal{I}_i}^{-1} f_{\mathcal{I}_i} \text{ and } \mathcal{S}_i = \mathcal{K}_{\Gamma_i\Gamma_i} - \mathcal{K}_{\Gamma_i\mathcal{I}_i} \mathcal{K}_{\mathcal{I}_i\Gamma_i}^{-1} \mathcal{K}_{\mathcal{I}_i\Gamma_i}.$ From the 70 interface solution u_{Γ} , the solution in \mathcal{I}_i can be computed as $u_{\mathcal{I}_i} = \mathcal{K}_{\mathcal{I}_i\mathcal{I}_i}^{-1} (f_{\mathcal{I}_i} - \mathcal{K}_{\mathcal{I}_i\mathcal{I}_i}^{-1} \mathcal{K}_{\mathcal{I}_i\Gamma} u_{\Gamma}).$

Algebraically, the problems (1.1) and (1.3) are very similar; their only difference is that even 71 when \mathcal{K}_i is sparse, \mathcal{S}_i is in general a dense matrix (as soon as \mathcal{K}_i is irreducible). Although eliminating 72 the interior unknowns is often associated with specific DDM such as BDD [8, 26] or FETI [13], it is in 73 74fact an optional step in the solution of Problem (1.1) and most domain decomposition methods can be applied either directly on \mathcal{K} or, after eliminating the interior unknowns, on \mathcal{S} . This elimination 75step may take time and consume memory, but it allows us to reduce the size and the condition 76 number of the linear system (S) to be solved [5, 27], making it a useful optional preprocessing. 77 Since the theory presented in sections 2 and 3 can be applied to solve either the original problem 78 in (1.1) or the reduced Schur problem in (1.3), we write them in a general form as 79

80 (1.4)
$$\mathcal{A}x = b, \qquad \mathcal{A} = \sum_{i=1}^{N} \mathcal{R}_{i}^{T} \mathcal{A}_{i} \mathcal{R}_{i},$$

where the global SPD matrix \mathcal{A} , the local SPSD matrices \mathcal{A}_i , and the restriction matrices \mathcal{R}_i can represent \mathcal{K} , \mathcal{K}_i and \mathcal{R}_{Ω_i} or \mathcal{S} , \mathcal{S}_i and \mathcal{R}_{Γ_i} when solving (1.1) or (1.3), respectively. When needed, a specific method M will be noted M/\mathcal{K} or M/\mathcal{S} to specify on which problem this method is applied. In both cases, \mathcal{A} is SPD, assuming that the \mathcal{A}_i are assigned to different computing units, Problem (1.4) can be solved in parallel using the preconditioned conjugate gradient method (PCG). A good preconditioner \mathcal{M} for (1.4) should have the two following properties: (1) \mathcal{M} is SPD and *close* to \mathcal{A}^{-1} , in the sense that the condition number $\kappa(\mathcal{M}\mathcal{A})$ should be as small as possible; (2) it is easy to compute $\mathcal{M}u$ for any vector u (at least much easier than $\mathcal{A}^{-1}u$). DDM are often used to build such preconditioners of the form

91 (1.5)
$$\mathcal{M}_{aS} = \sum_{i=1}^{N} \mathcal{R}_{i}^{T} \widehat{\mathcal{A}}_{i}^{\dagger} \mathcal{R}_{i}$$

where $\hat{\mathcal{A}}_i$ is a local problem associated with \mathcal{A} on subdomain i, and [†] represents a pseudo-inverse. These preconditioners have been studied for a long time using the abstract Schwarz (aS) theory (see, e.g., [10, 35] for recent overviews). Two particular cases of preconditioners that fit this description are the Neumann-Neumann (NN) preconditioner [26], with $\hat{\mathcal{A}}_i = D_i^{-1} \mathcal{A}_i D_i^{-1}$, and the Additive Schwarz (AS) preconditioner, with $\hat{\mathcal{A}}_i = \mathcal{R}_i \mathcal{A} \mathcal{R}_i^T$

98 (1.6)
$$\mathcal{M}_{NN} = \sum_{i=1}^{N} \mathcal{R}_{i}^{T} D_{i} \mathcal{A}_{i}^{\dagger} D_{i} \mathcal{R}_{i}, \qquad \mathcal{M}_{AS} = \sum_{i=1}^{N} \mathcal{R}_{i}^{T} \left(\mathcal{R}_{i} \mathcal{A} \mathcal{R}_{i}^{T} \right)^{-1} \mathcal{R}_{i},$$

where $(D_i)_{i=1}^N$ is a partition of unity such that $\sum_{i=1}^N \mathcal{R}_i^T D_i \mathcal{R}_i = I_n$ and I_n is the $n \times n$ identity matrix. These two preconditioners are of particular importance, but any other SPSD matrix can be used as the local preconditioner $\widehat{\mathcal{A}}_i$ in (1.5).

¹⁰³ Unless \mathcal{A}_i perfectly mimics the global action of \mathcal{A} in subdomain Ω_i , $\kappa(\mathcal{M}_{aS}\mathcal{A})$ may significantly ¹⁰⁴ increase with the number N of subdomains, leading to a non scalable numerical method.

Furthermore, if $\widehat{\mathcal{A}}_i$ is singular, the pseudo-inverse is only defined up to an element in its nullspace ker $(\widehat{\mathcal{A}}_i)$. To solve these two problems, a coarse space V_0 such that $\mathcal{R}_i^T \ker(\widehat{\mathcal{A}}_i) \subset V_0$

107 can be introduced, leading to the deflated aS preconditioner

108 (1.7)
$$\mathcal{M}_{aS,D} = V_0 (V_0^T \mathcal{A} V_0)^{\dagger} V_0^T + (I_n - \mathcal{P}_0) \left(\sum_{i=1}^N \mathcal{R}_i^T \widehat{\mathcal{A}}_i^{\dagger} \mathcal{R}_i \right) (I_n - \mathcal{P}_0)^T$$

110 where $\mathcal{P}_0 = V_0 (V_0^T \mathcal{A} V_0)^{\dagger} V_0^T \mathcal{A}$ is the \mathcal{A} -orthogonal projection onto V_0 . A simpler additive two-111 level preconditioner can also be obtained by just adding the coarse component to the one-level 112 preconditioner

113 (1.8)
$$\mathcal{M}_{aS,2} = V_0 (V_0^T \mathcal{A} V_0)^{\dagger} V_0^T + \sum_{i=1}^N \mathcal{R}_i^T \widehat{\mathcal{A}}_i^{\dagger} \mathcal{R}_i.$$

115 While previous works had proposed bounds on the condition number $\kappa(\mathcal{MA})$ on particular 116 numerical cases, often relying on analytical assumptions, Le Tallec and Vidrascu [25] derived an 117 algebraic bound for a new class of preconditioners, relying on the generalized Rayleigh quotient of 118 two local matrices. These preconditioners are called *generalized NN* in the original article; however, 119 because the generalization consists of handling an approximate matrix, we will instead refer to them 120 as *approximate NN* preconditioners in the present article. The approximation is not related to the 121 use of inexact solvers to compute the preconditioner, but to the use of an approximation matrix 122 \mathcal{A} instead of \mathcal{A} in the construction of the preconditioner. The approximate NN preconditioner is 123 in fact an exact algebraic NN preconditioner for $\widetilde{\mathcal{A}}$. Then, this approximate preconditioner is used 124 to accelerate the convergence of PCG applied on the exact matrix \mathcal{A} , guaranteeing a convergence 125 towards the actual solution of Equation (1.4).

This class of approximate NN preconditioners generalizes classical NN but does not cover 126the whole aS class of preconditioners. Note, for instance, that AS cannot be expressed as a NN 127 preconditioner. The first contribution (Section 2) of this article is to extend the result from [25] 128 by using a generic local preconditioner and cover a broader range of aS methods, which we name 129130 approximate deflated aS methods and consist of all deflated aS methods whose coarse grid consists of the assembly of local components that contain the kernel of some local operators (that are formally introduced below, in Definition 1). Interestingly, the bound we exhibit (Theorem 2) highlights the 132key position of NN and AS among other local preconditioners in the Schwarz framework: they 133134 provide two bounds on the spectrum of the preconditioned operator, and the convergence of any aS local preconditioner can be evaluated by comparing it to these two well-known methods. 135

136 This bound depends on generalized Rayleigh quotients which are traditionally estimated using functional analysis. Alternatively, we propose to control these Rayleigh quotients algebraically by 137building the coarse space using eigenvectors of well chosen generalized eigenproblems (Theorem 10). 138 For that, we follow the Generalized Eigenvalue in the Overlap (GenEO) procedure [33]. 139 This second contribution (Section 3) results in an explicit procedure for building a robust coarse space 140 of any approximate deflated aS method leading to a bound on the condition number (hence on 141 the number of iterations of PCG) independent of the number of subdomains. This result can be 142readily applied to retrieve or improve the bounds previously obtained via generalized eigenproblems 143 in the particular cases of AS/ \mathcal{K} [33], NN/ \mathcal{S} [34] and optimized Robin (SORAS/ \mathcal{K}) [18]. It also 144 generalizes these results to the approximate case. The idea of building a coarse space by solving 145 146 local eigenproblems in each subdomain was introduced in [15, 29]; it was successfully applied for other DDM such as FETI-DP [12] or BDDC [9] in [22, 23, 24]. 147

The third contribution (Section 4) of this paper is that the application of the considered coarse grid correction in an additive fashion is robust in the approximate AS case (although it is not robust for aS methods in general). The bound we obtain (Theorem 12) can be applied for retrieving the bound obtained in [33], when the coarse correction is applied additively to the AS method on the original matrix (AS/ \mathcal{K}). When working on the Schur matrix (AS/ \mathcal{S}) [6], the bound is still valid and leads, as commented in [15], to a smaller coarse space compared to AS/ \mathcal{K} .

Numerical experiments illustrate our discussion in Section 5. A high performance implementation of the coarse grid correction of one particular, consistently robust method (AS/S) has furthermore been implemented in the high-performance MaPHyS¹ hybrid (direct/iterative) sparse linear solver [2, 3] to eventually assess its performance on a modern parallel computer (Section 5.5) and make this scalable method available to the scientific community.

The paper is organized as follows. Section 2 introduces a new class of approximate (deflated) aS preconditioners and provides a bound on their condition number, which depends on generalized Rayleigh quotients. Applying the GenEO procedure on two well chosen generalized eigenproblems, Section 3 proposes a procedure to explicitly compute the coarse space while bounding these Rayleigh quotients leading to a bound on the condition number (hence on the number of iterations of PCG) independent of the number of subdomains. Section 4 shows that a similar result (and procedure) can be obtained when the coarse grid correction is additively applied, in the case of approximate

¹See https://gitlab.inria.fr/solverstack/maphys/

AS problems. Numerical experiments illustrate our discussion in Section 5 before concluding in Section 6.

2. Approximate abstract Schwarz preconditioners. In this section, we first define a class of approximate aS preconditioners, which combine a local preconditioner $\hat{\mathcal{A}}_i$, an approximate matrix $\tilde{\mathcal{A}}$ and a coarse space V_0 in Section 2.1. We then provide a bound on the condition number of this class of methods in Section 2.2, whose proof is provided in Section 2.3.

172 **2.1. Context.**

173 DEFINITION 1 (Approximate abstract Schwarz preconditioner $\widetilde{\mathcal{M}}_{aS,D}$).

- In order to build such a preconditioner for Problem (1.4), we need the three following ingredients:
- 175 1. a set of symmetric positive semi-definite (SPSD) local preconditioners $\widehat{\mathcal{A}}_i$,
- 176 2. an approximation $\widehat{\mathcal{A}}$ of \mathcal{A} such that

177 (2.1)
$$\exists (\widetilde{\mathcal{A}}_i)_{i=1}^N, \quad \widetilde{\mathcal{A}} = \sum_{i=1}^N \mathcal{R}_i^T \widetilde{\mathcal{A}}_i \mathcal{R}_i \text{ and } \widetilde{\mathcal{A}}_i \text{ is SPSD},$$

$$\exists \omega_{-}, \omega_{+} > 0, \quad \forall v \in V \quad \omega_{-} \ v^{T} \mathcal{A} v \leq v^{T} \widetilde{\mathcal{A}} v \leq \omega_{+} \ v^{T} \mathcal{A} v,$$

180 3. and a coarse space V_0 such that

181 (2.3)
$$\exists (V_i^0)_{i=1}^N, \quad V_0 = \sum_{i=1}^N \mathcal{R}_i^T V_i^0 \quad with \quad \ker(\widehat{\mathcal{A}}_i) + \ker(\widetilde{\mathcal{A}}_i^{(NN)}) \subset V_i^0,$$
182

183 where $\widetilde{\mathcal{A}}_{i}^{(NN)} = D_{i}^{-1} \widetilde{\mathcal{A}}_{i} D_{i}^{-1}$.

We can then define a coarse matrix $\widetilde{\mathcal{A}}_0 = V_0^T \widetilde{\mathcal{A}} V_0$, a coarse projection $\widetilde{\mathcal{P}}_0 = V_0 \widetilde{\mathcal{A}}_0^{\dagger} V_0^T \widetilde{\mathcal{A}}$ and the approximate as preconditioner is then defined as

186 (2.4)
$$\widetilde{\mathcal{M}}_{aS,D} = V_0 \widetilde{\mathcal{A}}_0^{\dagger} V_0^T + (I_n - \widetilde{\mathcal{P}}_0) \left(\sum_{i=1}^N \mathcal{R}_i^T \widehat{\mathcal{A}}_i^{\dagger} \mathcal{R}_i \right) (I_n - \widetilde{\mathcal{P}}_0)^T.$$
187

Note that the matrix $\widetilde{\mathcal{A}}_{i}^{(NN)}$ introduced in (2.3) is the local matrix in the approximate NN preconditioner $\widetilde{\mathcal{M}}_{NN,D}$ with the algebraic decomposition from (2.1). The matrices D_{i} can be any partition of unity as in (1.6). $\widetilde{\mathcal{A}}_{i}^{(NN)}$ is a scaled version of the local matrix $\widetilde{\mathcal{A}}_{i}$ in the approximation $\widetilde{\mathcal{A}}$ of \mathcal{A} .

When no approximation is used, after a suitable initialization, $\widetilde{\mathcal{M}}_{aS,D}$ can be replaced by $(I_n - \widetilde{\mathcal{P}}_0) \left(\sum_{i=1}^N \mathcal{R}_i^T \widehat{\mathcal{A}}_i^{\dagger} \mathcal{R}_i \right)$ in the PCG iterations, as noted in [26].

2.2. Convergence result for $\widetilde{\mathcal{M}}_{aS,D}$. In each subdomain, we note $N_i = \#\{j \neq i, \mathcal{R}_i \widetilde{\mathcal{A}} \mathcal{R}_j^T \neq 0\}$ 195 0} the number of neighbors through the connectivity graph of $\widetilde{\mathcal{A}}$. We also define two local subspaces \widehat{V}_i^{\perp} and \widetilde{V}_i^{\perp} as the orthogonal spaces of V_i^0 for the inner products inferred by $\widehat{\mathcal{A}}_i$ in range $(\widehat{\mathcal{A}}_i)$ and $\widetilde{\mathcal{A}}_i^{(NN)}$ in range $(\widetilde{\mathcal{A}}_i^{(NN)})$ respectively. Then,

198 (2.5) $\operatorname{range}(\mathcal{R}_i) = \widehat{V}_i^{\perp} \oplus V_i^0 = \widetilde{V}_i^{\perp} \oplus V_i^0,$

$$\forall u \in V_i^0, \ \forall v \in \widehat{V}_i^\perp, \ \forall w \in \widetilde{V}_i^\perp \quad u^T \widehat{\mathcal{A}}_i v = u^T \widetilde{\mathcal{A}}_i^{(NN)} w = 0.$$

Finally, for any SPSD matrix \mathcal{B} and vector u, we note $|u|_{\mathcal{B}} = \sqrt{u^T \mathcal{B} u}$ the \mathcal{B} -seminorm of u; if \mathcal{B} is SPD, we note it $||u||_{\mathcal{B}}$.

- 203 THEOREM 2 (Convergence result for approximate aS).
- 204 The condition number of the preconditioned matrix $\mathcal{M}_{aS,D}\mathcal{A}$ is bounded by

$$\sum_{205} \kappa(\widetilde{\mathcal{M}}_{aS,D}\mathcal{A}) \leq \frac{\omega_+}{\omega_-} \left(1 + \max_{1 \leq i \leq N} \sup_{v \in \widetilde{V}_i^{\perp}} \frac{|v|_{\widehat{\mathcal{A}}_i}^2}{|v|_{\widetilde{\mathcal{A}}_i^{(NN)}}^2} \right) \max\left(1, \max_{1 \leq i \leq N} \frac{(N_i + 1)}{(N_i + 1)} \sup_{v \in \widehat{V}_i^{\perp}} \frac{|v|_{\widetilde{\mathcal{A}}_i^{(AS)}}^2}{|v|_{\widehat{\mathcal{A}}_i}^2} \right)$$

207 where $\widetilde{\mathcal{A}}_{i}^{(NN)} = D_{i}^{-1} \widetilde{\mathcal{A}}_{i} D_{i}^{-1}$ and $\widetilde{\mathcal{A}}_{i}^{(AS)} = \mathcal{R}_{i} \widetilde{\mathcal{A}} \mathcal{R}_{i}^{T}$.

We see three factors in this bound:

208

209

- The first one, with ω_+ and ω_- , controls the quality of the approximation $\widetilde{\mathcal{A}}$. If no approximation is used, then $\widetilde{\mathcal{A}} = \mathcal{A}$ and $\omega_- = \omega_+ = 1$.
- The second one is a generalized Rayleigh quotient between the local preconditioner $\widehat{\mathcal{A}}_i$ and the approximate NN preconditioner $\widetilde{\mathcal{A}}_i^{(NN)} = D_i^{-1} \widetilde{\mathcal{A}}_i D_i^{-1}$ defined in [25].
- The last one is a generalized Rayleigh quotient between the local preconditioner $\widehat{\mathcal{A}}_i$ and an approximate AS preconditioner $\widetilde{\mathcal{A}}_i^{(AS)} = \mathcal{R}_i \widetilde{\mathcal{A}} \mathcal{R}_i^T$.

As for $\widetilde{\mathcal{A}}_{i}^{(NN)}$ above with NN, $\widetilde{\mathcal{A}}_{i}^{(AS)} = \mathcal{R}_{i}\widetilde{\mathcal{A}}\mathcal{R}_{i}^{T}$ is an algebraic generalization of the local matrix in the AS preconditioner in Equation (1.6), built upon the approximation $\widetilde{\mathcal{A}}$ instead of \mathcal{A} .

Proof. The proof of Theorem 2 is a direct consequence of lemmas 6 and 8 in Section 2.3, using the definition of

219
220
$$\kappa(\widetilde{\mathcal{M}}_{aS,D}\mathcal{A}) = \frac{\lambda_{\max}(\widetilde{\mathcal{M}}_{aS,D}\mathcal{A})}{\lambda_{\min}(\widetilde{\mathcal{M}}_{aS,D}\mathcal{A})}.$$

221 COROLLARY 3 (Convergence results for approximate AS and approximate NN).

We define the approximate AS and NN preconditioners $\widetilde{\mathcal{M}}_{AS,D}$ and $\widetilde{\mathcal{M}}_{NN,D}$ by replacing $\widehat{\mathcal{A}}_i$ with $\widetilde{\mathcal{A}}_i^{(AS)}$ or $\widetilde{\mathcal{A}}_i^{(NN)}$ respectively in Equation (2.4). We also define $N_c = \max_{1 \le i \le N} (N_i + 1)$.

224 Then, the condition numbers of $\widetilde{\mathcal{M}}_{NN,D}\mathcal{A}$ and $\widetilde{\mathcal{M}}_{AS,D}\mathcal{A}$ are bounded by

225
$$\kappa(\widetilde{\mathcal{M}}_{AS,D}\mathcal{A}) \leq \frac{\omega_{+}}{\omega_{-}} \left(1 + \max_{1 \leq i \leq N} \sup_{v \in \widetilde{V}_{i}^{\perp}} \frac{|v|^{2}_{\widetilde{\mathcal{A}}_{i}^{(AS)}}}{|v|^{2}_{\widetilde{\mathcal{A}}_{i}^{(NN)}}} \right) N_{c}$$

226
$$\kappa(\widetilde{\mathcal{M}}_{NN,D}\mathcal{A}) \leq \frac{\omega_{+}}{\omega_{-}} \max\left(1, \sup_{v \in \widehat{V}_{i}^{\perp}} \frac{|v|_{\widetilde{\mathcal{A}}_{i}^{(AS)}}}{|v|_{\widetilde{\mathcal{A}}_{i}^{(NN)}}}\right) N_{c}.$$

228 Proof. The proof of Corollary 3 is a consequence of lemmas 6 and 7 for AS, and lemmas 5 and 8 229 for NN. $\hfill \Box$

Note that the bound for $\mathcal{M}_{NN,D}$ in Corollary 3 is the same as in [Theorem 1, 25]. This bound is tighter than the bound obtained by setting $\widehat{\mathcal{A}}_i = \widetilde{\mathcal{A}}_i^{(NN)}$ in Theorem 2; this comes from the fact that the bound in Lemma 5 is also tighter than its generalization in Lemma 6.

The similarity of the bounds for AS and NN in Corollary 3 shows that the convergence of these two methods are governed by the same quantity $\sup_{v \in \widetilde{V}_i^{\perp}} |v|^2_{\widetilde{\mathcal{A}}_i^{(AS)}} / |v|^2_{\widetilde{\mathcal{A}}_i^{(NN)}}$. As a result, with

- the same coarse space, we expect the AS/S method [6] to show the same convergence behavior 235as the BDD method (NN/S) [26] or its dual counterpart FETI [13]. Although AS require more 236
- communication than NN (each subdomain *i* has to send the matrix block $\mathcal{R}_j \mathcal{R}_i^T \widetilde{\mathcal{A}}_i \mathcal{R}_i \mathcal{R}_j^T$ to each
- neighbor j) to setup the preconditioner, one advantage of using AS over NN is that the local preconditioner $\widetilde{\mathcal{A}}_i^{(NN)}$ is often singular in some domains while $\widetilde{\mathcal{A}}_i^{(AS)}$ remains SPD, and $\widetilde{\mathcal{A}}_i^{(AS)-1}u_i$ 238
- 239
- is easier and faster to compute than $\widetilde{\mathcal{A}}_{i}^{(NN)\dagger}u_{i}$. 240

2.3. Proof of Theorem 2. To estimate the condition number of $\widetilde{\mathcal{M}}_{aS,D}\mathcal{A}$, we need to bound 241the spectrum of this operator from above and below. The lower bound is a consequence of the 242Stable Decomposition Lemma as stated in [35]. 243

LEMMA 4 (Stable decomposition lemma). 244

If there exists a constant C_0 , local matrices \mathcal{B}_i and extension operators \mathcal{I}_i , such that $\ker(\mathcal{B}_i) \subset$ 245 $\operatorname{ker}(\mathcal{I}_i)$ and every $u \in V$ admits a decomposition 246

247
$$u = \sum_{i=0}^{N} \mathcal{I}_{i} u_{i}, \quad \{u_{i} \in V_{i}, 0 \le i \le N\} \quad that \ satisfies \quad \sum_{i=0}^{N} |u_{i}|_{\mathcal{B}_{i}}^{2} \le C_{0}^{2} \ ||u||_{\mathcal{A}}^{2}.$$

250
$$\lambda_{\min}(\mathcal{MA}) \ge C_0^{-2}, \quad where \quad \mathcal{M} = \sum_{i=0}^N \mathcal{I}_i \mathcal{B}_i^{\dagger} \mathcal{I}_i^T.$$

Proof. see, e.g., Lemma 2.5 in [35]. 252

Then, although it is not directly used in the proof of Theorem 2, we first expose in Lemma 5 253a lower bound for the spectrum of NN $(\widehat{\mathcal{A}}_i = \widetilde{\mathcal{A}}_i^{(NN)})$ as it provides a good insight on the reason behind the Rayleigh quotients in the bound presented in Lemma 6 for the general case. 254255

LEMMA 5 (Lower bound for the approximate Neumann-Neumann preconditioner). 256

257 Let
$$\widetilde{\mathcal{M}}_{NN,D} = V_0 \widetilde{\mathcal{A}}_0^{\dagger} V_0^T + (I_n - \widetilde{\mathcal{P}}_0) \left(\sum_{i=1}^N \mathcal{R}_i^T \widetilde{\mathcal{A}}_i^{(NN)^{\dagger}} \mathcal{R}_i \right) (I_n - \widetilde{\mathcal{P}}_0)^T.$$

Then, 258

259260

$$\lambda_{\min}(\widetilde{\mathcal{M}}_{NN,D}\mathcal{A}) \geq rac{1}{\omega_+}$$

Proof. This is a consequence of Lemma 4 (see Theorem 1 in [25]). 261

If, instead of $\widetilde{\mathcal{A}}_i^{(NN)}$, another local preconditioner $\widehat{\mathcal{A}}_i$ is used, there is no change on the bound 262 if we restrict the operators to the coarse space V_0 since the application of the local preconditioner is preceded and followed by projections $(I_n - \tilde{\mathcal{P}}_0)$ and $(I_n - \tilde{\mathcal{P}}_0)^T$. However, in the orthogonal of 263264the coarse space, the bound has to change and reflect the difference between $\widetilde{\mathcal{A}}_{i}^{(NN)}$ and $\widehat{\mathcal{A}}_{i}$. As is 265proved in Lemma 6, the lower bound on the spectrum of $\widetilde{\mathcal{M}}_{aS,D}\mathcal{A}$ can be deduced from the bound 266for $\widetilde{\mathcal{M}}_{NN,D}\mathcal{A}$ in Lemma 5 by adding a correction related to the generalized Rayleigh quotient 267between $\widetilde{\mathcal{A}}_{i}^{(NN)}$ and $\widehat{\mathcal{A}}_{i}$ in the orthogonal of the coarse space. 268

LEMMA 6 (Lower bound for the approximate abstract Schwarz preconditioner).

270
271
$$\lambda_{\min}(\widetilde{\mathcal{M}}_{aS,D}\mathcal{A}) \ge \frac{1}{\omega_{+}} \left(1 + \max_{1 \le i \le N} \sup_{v \in \widetilde{V}_{i}^{\perp}} \frac{|v|_{\widehat{\mathcal{A}}_{i}}^{2}}{|v|_{\widetilde{\mathcal{A}}_{i}^{(NN)}}^{2}} \right)^{-1}$$

Proof. We want to split u into a sum of local contributions, while being able to uniformly 272control the \mathcal{A}_i -norm of these contributions u_i with the global \mathcal{A} -norm of u to apply Lemma 4. For 273any u and $i \ge 1$, we decompose $D_i \mathcal{R}_i u = u_i^0 + u_i^\perp$ where $u_i^0 \in V_i^0$ and $u_i^\perp \in \tilde{V}_i^\perp$. We then define $u_0 = (V_0^T \tilde{\mathcal{A}} V_0)^\dagger V_0^T \mathcal{A} u$ such that $V_0 u_0 = \tilde{\mathcal{P}}_0 u$. We can use the facts that $\sum_{i=1}^N \mathcal{R}_i^T D_i \mathcal{R}_i = I_n$ and $\sum_{i=0}^N \mathcal{R}_i^T u_i^0 \in V_0 \subset \ker(I_n - \tilde{\mathcal{P}}_0)$ to obtain the decomposition 274275276

277
$$u = \widetilde{\mathcal{P}}_0 u + (I_n - \widetilde{\mathcal{P}}_0) u = V_0 u_0 + (I_n - \widetilde{\mathcal{P}}_0) \sum_{i=1}^N \mathcal{R}_i^T D_i \mathcal{R}_i u$$

278
$$= V_0 u_0 + (I_n - \widetilde{\mathcal{P}}_0) \sum_{i=1}^N \mathcal{R}_i^T (u_i^0 + u_i^\perp) = V_0 u_0 + (I_n - \widetilde{\mathcal{P}}_0) \sum_{i=1}^N \mathcal{R}_i^T u_i^\perp$$

279
$$= \sum_{i=0}^{N} \mathcal{I}_{i} u_{i} \quad \text{where} \quad \mathcal{I}_{0} = V_{0}, \quad \mathcal{I}_{i} = (I_{n} - \widetilde{\mathcal{P}}_{0}) \mathcal{R}_{i} \quad \text{and} \quad u_{i} = u_{i}^{\perp}$$
280

Since $\widetilde{\mathcal{P}}_0$ is a $\widetilde{\mathcal{A}}$ -orthogonal projection, it holds that: 281

$$|u_0|^2_{\tilde{\mathcal{A}}_0} = |u_0|^2_{V_0^T \tilde{\mathcal{A}} V_0} = |V_0 u_0|^2_{\tilde{\mathcal{A}}} = |\tilde{\mathcal{P}}_0 u|^2_{\tilde{\mathcal{A}}} \le |u|^2_{\tilde{\mathcal{A}}}$$

284

Let

$$C = \max_{1 \le i \le N} \sup_{v \in \widetilde{V}_i^{\perp}} \frac{|v|^2_{\widehat{\mathcal{A}}_i}}{|v|^2_{\widehat{\mathcal{A}}_i^{(NN)}}} = \max_{1 \le i \le N} \sup_{v \in \widetilde{V}_i^{\perp}} \frac{|v|^2_{\widehat{\mathcal{A}}_i}}{|v|^2_{D_i^{-1}\widetilde{\mathcal{A}}_i D_i^{-1}}}.$$

We can then use equations (2.6), (2.1) and (2.7): 286

287
$$|u_i^{\perp}|_{\widehat{\mathcal{A}}_i}^2 \le C|u_i^{\perp}|_{D_i^{-1}\widetilde{\mathcal{A}}_i D_i^{-1}}^2 \le C|u_i^{\perp} + u_i^0|_{D_i^{-1}\widetilde{\mathcal{A}}_i D_i^{-1}}^2 = C|\mathcal{R}_i u|_{\widetilde{\mathcal{A}}_i}^2$$

288 (2.8)
$$\sum_{i=1}^{N} |u_i^{\perp}|_{\widehat{\mathcal{A}}_i}^2 \leq C \sum_{i=1}^{N} |\mathcal{R}_i u|_{\widetilde{\mathcal{A}}_i}^2 = C |u|_{\sum_{i=1}^{N}}^2 \mathcal{R}_i^T \widetilde{\mathcal{A}}_i \mathcal{R}_i}^2 = C |u|_{\widetilde{\mathcal{A}}}^2,$$

289
290
290
$$|u_0|_{\tilde{\mathcal{A}}_0}^2 + \sum_{i=1}^N |u_i^{\perp}|_{\hat{\mathcal{A}}_i}^2 \le (1+C) |u|_{\tilde{\mathcal{A}}}^2 \le \omega_+ (1+C) |u|_{\mathcal{A}}^2,$$

291and the local norms are controlled by the global norm. Then, applying Lemma 4, we get

292
293
$$\lambda_{\min}(\widetilde{\mathcal{M}}_{aS,D}\mathcal{A}) \geq \frac{1}{\omega_{+}} \left(1 + \max_{1 \leq i \leq N} \sup_{v \in \widetilde{V}_{i}^{\perp}} \frac{|v|_{\widehat{\mathcal{A}}_{i}}^{2}}{|v|_{\widetilde{\mathcal{A}}_{i}^{(NN)}}^{2}} \right)^{-1}.$$

Now that we proved a lower bound for the spectrum of $\widetilde{\mathcal{M}}_{NN,D}\mathcal{A}$, we will prove an upper 294 bound in Lemma 8. We first recall a classic upper bound for AS preconditioners in Lemma 7 since 295it explains the origin of the Rayleigh quotient in the bound for the general case. 296

297 LEMMA 7 (Upper bound for the approximate Additive Schwarz preconditioner).

Let
$$\widetilde{\mathcal{M}}_{AS,D} = V_0 \widetilde{\mathcal{A}}_0^{\dagger} V_0^T + (I_n - \widetilde{\mathcal{P}}_0) \left(\sum_{i=1}^N \mathcal{R}_i^T \widetilde{\mathcal{A}}_i^{(AS)^{-1}} \mathcal{R}_i \right) (I_n - \widetilde{\mathcal{P}}_0)^T.$$

Then,

299 300

303 304

298

$$\lambda_{\max}(\widetilde{\mathcal{M}}_{AS,D}\mathcal{A}) \leq \frac{1}{\omega_{-}} \max_{1 \leq i \leq N} (N_i + 1)$$

301 *Proof.* This lemma is a particular case of Lemma 8 which is proven below.

302 LEMMA 8 (Upper bound for the approximate abstract Schwarz preconditioner).

$$\lambda_{\max}(\widetilde{\mathcal{M}}_{aS,D}\mathcal{A}) \leq \frac{1}{\omega_{-}} \max\left(1, \max_{1 \leq i \leq N} (N_i + 1) \sup_{v \in \widehat{V}_i^{\perp}} \frac{|v|_{\widetilde{\mathcal{A}}_i^{(AS)}}^2}{|v|_{\widehat{\mathcal{A}}_i}^2}\right).$$

305 *Proof.* First, let us remark that

$$\widetilde{\mathcal{M}}_{aS,D}\widetilde{\mathcal{A}}u = V_0\widetilde{\mathcal{A}}_0^{\dagger}V_0^T\widetilde{\mathcal{A}}u + (I_n - \widetilde{\mathcal{P}}_0)\sum_{i=1}^N \mathcal{R}_i^T\widehat{\mathcal{A}}_i^{\dagger}\mathcal{R}_i(I_n - \widetilde{\mathcal{P}}_0)^T\widetilde{\mathcal{A}}u = u_0 + (I_n - \widetilde{\mathcal{P}}_0)\sum_{i=1}^N \mathcal{R}_i^T u_i$$

where $u_0 = \widetilde{\mathcal{P}}_0 u$ and u_i is the orthogonal projection of $\widehat{\mathcal{A}}_i^{\dagger} \mathcal{R}_i (I_n - \widetilde{\mathcal{P}}_0)^T \widetilde{\mathcal{A}} u$ onto range $(\widehat{\mathcal{A}}_i)$ along ker $(\widehat{\mathcal{A}}_i) \subset V_i^0 \subset \ker \left[(I_n - \widetilde{\mathcal{P}}_0) \mathcal{R}_i^T \right].$

310 As a consequence,
$$u_i \in \widehat{V}_i^{\perp}$$
:

$$\underset{312}{\overset{311}{312}} \qquad \qquad u_i^T \widehat{\mathcal{A}}_i V_i^0 = u^T \widetilde{\mathcal{A}}(I_n - \widetilde{\mathcal{P}}_0) \mathcal{R}_i^T \widehat{\mathcal{A}}_i^{\dagger} \widehat{\mathcal{A}}_i V_i^0 = u^T \widetilde{\mathcal{A}}(I_n - \widetilde{\mathcal{P}}_0) \mathcal{R}_i^T V_i^0 = 0.$$

313 Then,

314
$$|\widetilde{\mathcal{M}}_{aS,D}\widetilde{\mathcal{A}}u|_{\widetilde{\mathcal{A}}}^2 = |u_0|_{\widetilde{\mathcal{A}}}^2 + |(I_n - \widetilde{\mathcal{P}}_0)\sum_{i=1}^N \mathcal{R}_i^T u_i|_{\widetilde{\mathcal{A}}}^2 \le |u_0|_{\widetilde{\mathcal{A}}}^2 + |\sum_{i=1}^N \mathcal{R}_i^T u_i|_{\widetilde{\mathcal{A}}}^2$$

$$\leq |u_0|_{\widetilde{\mathcal{A}}}^2 + \sum_{i=1}^N (N_i + 1) |\mathcal{R}_i^T u_i|_{\widetilde{\mathcal{A}}}^2 = |u_0|_{\widetilde{\mathcal{A}}}^2 + \sum_{i=1}^N (N_i + 1) |u_i|_{\mathcal{R}_i \widetilde{\mathcal{A}} \mathcal{R}_i^T}^2$$

317 where we used the fact that

$$318 \qquad 0 \leq \sum_{\substack{1 \leq i,j \leq N \\ \mathcal{R}_{i}^{T} \widetilde{\mathcal{A}} \mathcal{R}_{j} \neq 0}} |\mathcal{R}_{i}^{T} u_{i} - \mathcal{R}_{j}^{T} u_{j}|_{\widetilde{\mathcal{A}}}^{2} = 2 \left(\sum_{\substack{1 \leq i,j \leq N \\ \mathcal{R}_{i}^{T} \widetilde{\mathcal{A}} \mathcal{R}_{j} \neq 0}} |\mathcal{R}_{i}^{T} u_{i}|_{\widetilde{\mathcal{A}}}^{2} - \sum_{\substack{1 \leq i,j \leq N \\ \mathcal{R}_{i}^{T} \widetilde{\mathcal{A}} \mathcal{R}_{j} \neq 0}} u_{i}^{T} \mathcal{R}_{i} \widetilde{\mathcal{A}} \mathcal{R}_{j}^{T} u_{j} \right)$$

$$319 \qquad (2.9) \qquad \leq 2 \left(\sum_{i=1}^{N} (N_{i} + 1) |\mathcal{R}_{i}^{T} u_{i}|_{\widetilde{\mathcal{A}}}^{2} - |\sum_{i=1}^{N} \mathcal{R}_{i}^{T} u_{i}|_{\widetilde{\mathcal{A}}}^{2} \right).$$

322
$$C = \max\left(1, \max_{1 \le i \le N} (N_i + 1) \sup_{v \in \widehat{V}_i^{\perp}} \frac{|v|^2_{\widehat{\mathcal{A}}_i^{(AS)}}}{|v|^2_{\widehat{\mathcal{A}}_i}}\right) = \max\left(1, \max_{1 \le i \le N} (N_i + 1) \sup_{v \in \widehat{V}_i^{\perp}} \frac{|v|^2_{\mathcal{R}_i \widetilde{\mathcal{A}} \mathcal{R}_i^T}}{|v|^2_{\widehat{\mathcal{A}}_i}}\right)$$
9

We can now write 323

324
$$|\widetilde{\mathcal{M}}_{aS,D}\widetilde{\mathcal{A}}u|_{\widetilde{\mathcal{A}}}^{2} \leq C|u_{0}|_{\widetilde{\mathcal{A}}}^{2} + C\sum_{i=1}^{N}|u_{i}|_{\widehat{\mathcal{A}}_{i}}^{2} = Cu^{T}\widetilde{\mathcal{P}}_{0}^{T}\widetilde{\mathcal{A}}u_{0} + C\sum_{i=1}^{N}u^{T}\widetilde{\mathcal{A}}(I_{n} - \widetilde{\mathcal{P}}_{0})\mathcal{R}_{i}^{T}\widehat{\mathcal{A}}_{i}^{\dagger}\widehat{\mathcal{A}}_{i}u_{0}^{\dagger}$$

$$325 = Cu^{T}\widetilde{\mathcal{A}}\widetilde{\mathcal{M}}_{aS,D}\widetilde{\mathcal{A}}u \leq C|u|_{\widetilde{\mathcal{A}}}|\widetilde{\mathcal{M}}_{aS,D}\widetilde{\mathcal{A}}u|_{\widetilde{\mathcal{A}}}$$

325

$$\widetilde{\mathcal{M}}_{aS,D}\widetilde{\mathcal{A}}u|_{\widetilde{\mathcal{A}}} \leq C|u|_{\widetilde{\mathcal{A}}},$$

and use the same strategy as in [25] to obtain our result: 328

329
$$\lambda_{\max}(\widetilde{\mathcal{M}}_{aS,D}\mathcal{A}) = \max_{v \in V} \frac{|v|_{\mathcal{A}}^2}{|v|_{\widetilde{\mathcal{M}}_{aS,D}^{-1}}^2} \le \max_{v \in V} \frac{1}{\omega_-} \frac{|v|_{\widetilde{\mathcal{A}}}^2}{|v|_{\widetilde{\mathcal{M}}_{aS,D}^{-1}}^2} \le \max_{v \in V} \frac{1}{\omega_-} \frac{|\widetilde{\mathcal{M}}_{aS,D}\widetilde{\mathcal{A}}v|_{\widetilde{\mathcal{A}}}}{|v|_{\widetilde{\mathcal{A}}}} \le \frac{C}{\omega_-},$$

$$\lambda_{\max}(\widetilde{\mathcal{M}}_{aS,D}\mathcal{A}) \leq \frac{1}{\omega_{-}} \max\left(1, \max_{1 \leq i \leq N} (N_i + 1) \sup_{v \in \widehat{V}_i^{\perp}} \frac{|v|^2_{\widetilde{\mathcal{A}}_i^{(AS)}}}{|v|^2_{\widehat{\mathcal{A}}_i}}\right).$$

3. Building the coarse space via generalized eigenproblems. The bound in Theorem 2 332 has originally been estimated through functional analysis after a coarse space has been chosen. A 333 more algebraic approach is to build the coarse space V_0 by solving a generalized eigenproblem in 334 each subdomain in order to control the Rayleigh quotient as proposed by [33, 34] for AS/K and 335 NN/S, respectively. This approach has also been successfully applied to other aS variants such 336 as the SORAS method [18], in which case two eigenproblems are needed. The case where the 337 correction is applied additively as in [11, 15, 33] for AS is treated in Section 4. 338

The connection between the GenEO method and Theorem 2 comes from the following lemma: 339

341 Let
$$\mathcal{B}$$
 be a SPSD matrix, \mathcal{C} a SPD matrix and $\eta > 0$ be a parameter

If $V_{\eta} = span(\{p, \quad \mathcal{B}p = \lambda \mathcal{C}p, \quad \lambda \leq \eta\})$ and $V_{\eta}^{\perp_{\mathcal{B}}} = \{u \in range(\mathcal{B}), \forall v \in V_{\eta}, u^{T}\mathcal{B}v = 0\},$ 342

343
$$\qquad \qquad then \ \sup_{u \in V_n^{\perp_{\mathcal{B}}}} \frac{|u|_{\mathcal{C}}^2}{|u|_{\mathcal{B}}^2} \le \frac{1}{\eta}$$

Proof. Since C is SPD, the generalized eigenproblem $\mathcal{B}p = \lambda Cp$ has solutions (λ_k, p_k) with 344 $p_k^T \mathcal{C} p_l = \delta_{kl}$ and $p_k^T \mathcal{B} p_l = \lambda_k \delta_{kl}$. 345

346

Now, let $u \in V_{\eta}^{\perp_{\mathcal{B}}}$. We can project u on the basis $(p_k)_k$: $u = \sum_k \alpha_k p_k$. If k is such that $\lambda_k \leq \eta$, then $p_k \in V_{\eta}$ and $0 = u^T \mathcal{B} p_k = \lambda_k \alpha_k$. As a consequence, $\alpha_k = 0$ because if $\lambda_k = 0$, $p_k \in \ker(\mathcal{B}) = (\operatorname{range}(\mathcal{B}))^{\perp} \perp u$ and $\alpha_k = u^T p_k = 0$. This leads to 347 348

$$\frac{|u|_{\mathcal{C}}^2}{350} = \frac{\sum_{\lambda_k > \eta} \alpha_k^2}{\sum_{\lambda_k > \eta} \lambda_k \alpha_k^2} \le \frac{1}{\eta}.$$

Following the GenEO methodology, we propose to build the coarse space V_0 by solving two gen-351 eralized eigenproblems to control the condition number of approximate aS preconditioners through 352 two parameters $\alpha > 0$ and $\beta > 1$. 353

THEOREM 10 (Condition number of aS preconditioners). If $\hat{\mathcal{A}}_i$ is SPD and the coarse space is defined as $V_0 = \sum_{i=1}^N \mathcal{R}_i^T V_i^0$ with

356
$$V_i^0 = span\{\{p_k^i, \quad \widetilde{\mathcal{A}}_i^{(NN)}p_k^i = \lambda_k^i \widehat{\mathcal{A}}_i p_k^i, \quad \lambda_k^i \le \alpha^{-1}\}$$

$$= \{p_k^i, \quad \widehat{\mathcal{A}}_i p_k^i = \lambda_k^i \widetilde{\mathcal{A}}_i^{(AS)} p_k^i, \quad \lambda_k^i \le (N_i + 1)\beta^{-1}\}$$

359 then, we can bound the condition number

$$\kappa(\widetilde{\mathcal{M}}_{aS,D}\mathcal{A}) \leq \frac{\omega_{+}}{\omega_{-}} \left(1 + \alpha\right) \beta$$

³⁶¹ Proof. Using Lemma 9 and the definition of \widetilde{V}_i^{\perp} and \widehat{V}_i^{\perp} in 2.2, we can bound the Rayleigh ³⁶² quotients

$$\sup_{\substack{363\\364}} \sup_{v \in \widetilde{V}_i^\perp} \frac{|v|_{\widehat{\mathcal{A}}_i}^2}{|v|_{\widetilde{\mathcal{A}}_i^{(NN)}}^2} \le \alpha, \qquad \qquad \sup_{v \in \widehat{V}_i^\perp} \frac{|v|_{\widetilde{\mathcal{A}}_i^{(AS)}}^2}{|v|_{\widehat{\mathcal{A}}_i}^2} \le \frac{\beta}{N_i + 1}.$$

365 Replacing these bounds in Theorem 2 gives the result.

366 COROLLARY 11. In the NN or AS cases, for any $\alpha \ge 1$, we can define

$$\Im \{ \widetilde{\mathcal{A}}_{i}^{0} = span \left(\{ p_{k}^{i}, \quad \widetilde{\mathcal{A}}_{i}^{(NN)} p_{k}^{i} = \lambda_{k}^{i} \widetilde{\mathcal{A}}_{i}^{(AS)} p_{k}^{i}, \quad \lambda_{k}^{i} \leq \alpha^{-1} \} \right).$$

369 Then, Corollary 3 and Lemma 9 give

$$\kappa(\widetilde{\mathcal{M}}_{AS,D}\mathcal{A}) \leq \frac{\omega_{+}}{\omega_{-}} (1+\alpha) \ N_{c}, \qquad \qquad \kappa(\widetilde{\mathcal{M}}_{NN,D}\mathcal{A}) \leq \frac{\omega_{+}}{\omega_{-}} \alpha \ N_{c}.$$

If $\alpha^{-1} = \min_{\lambda_k^i \neq 0}(\lambda_k^i)$, then $V_i^0 = \ker(\widetilde{\mathcal{A}}_i^{(NN)}) = D_i \ker(\widetilde{\mathcal{A}}_i)$ and the resulting coarse space for NN is exactly the same as in the BDD algorithm.

With small variations in the generalized eigenproblems considered, Theorem 10 and Corollary 11 retrieve or improve previous GenEO results and generalize them to the approximate case: AS/K[32, 33], NN/S [34] and SORAS [18].

377 4. Additive Coarse Correction.

4.1. Context. The preconditioner $\mathcal{M}_{aS,D}$ separates the part of the solution that is in V_0 378(on which a direct coarse solve is performed through $\widetilde{\mathcal{A}}_0^{\dagger}$), from its $\widetilde{\mathcal{A}}$ -orthogonal part (on which 379 the local preconditioner $\mathcal{M}_{aS} = \sum_{i=1}^{N} \mathcal{R}_i^T \hat{\mathcal{A}}_i^{\dagger} \mathcal{R}_i$ is used to accelerate convergence). Eigenvalues or Rayleigh quotients λ corresponding to vectors in the coarse space V_0 are shifted to 1 by the 380 381 coarse solve, and to 0 by the projection steps $(I_n - \widetilde{\mathcal{P}}_0)$ and $(I_n - \widetilde{\mathcal{P}}_0)^T$, so the overall effect of the 382 deflated preconditioner is to shift them to 1 exactly. If we skip these projection steps, we obtain an 383 approximate additive two-level preconditioner $\mathcal{M}_{aS,2}$ similar to $\mathcal{M}_{aS,2}$ presented in Equation (1.8). 384 In this case, without the projection steps eigenvalues are shifted to $1 + \lambda$. As a result, this coarse 385 correction applied on big eigenvalues only makes them bigger, thus hampering convergence. This 386 additive coarse correction can only be effective to tackle the lower part of the spectrum since small 387 eigenvalues $\lambda \ll 1$ are shifted to $1 + \lambda \approx 1$. 388

 \Box

The one-level AS method has already an upper bound on the spectrum (see Lemma 7), and only the lower bound needs to be recovered, making it an ideal candidate for an additive coarse correction. In this section, we show that in the approximate AS case, when $\hat{\mathcal{A}}_i = \tilde{\mathcal{A}}_i^{(AS)} = \mathcal{R}_i \tilde{\mathcal{A}} \mathcal{R}_i^T$, the projection steps can be removed without losing robustness. Namely, we still have a bound for the condition number of the additive two-level AS method independent of the number of subdomains.

394 THEOREM 12 (Condition number of the 2-level approximate AS preconditioner).

395 Let
$$\mathcal{M}_{AS,2} = V_0 \widetilde{\mathcal{A}}_0^{\dagger} V_0^T + \sum_{i=1}^N \mathcal{R}_i^T \widetilde{\mathcal{A}}_i^{(AS)-1} \mathcal{R}_i \text{ and } N_c = \max_{1 \le i \le N} (N_i + 1).$$

396 Then, we can bound the condition number

397
398
$$\kappa(\mathcal{M}_{AS,2}\mathcal{A}) \leq \frac{\omega_{+}}{\omega_{-}} \left[N_{c} + 1 + (N_{c} + 2) \max_{1 \leq i \leq N} \sup_{v \in \widetilde{V}_{i}^{\perp}} \frac{|v|^{2}_{\widetilde{\mathcal{A}}_{i}^{(AS)}}}{|v|^{2}_{\widetilde{\mathcal{A}}_{i}^{(NN)}}} \right] (N_{c} + 1).$$

399 For any $\alpha > 0$, if we choose

$$400 V_i^0 = span\big(\{p_k^i, \quad \widetilde{\mathcal{A}}_i^{(NN)}p_k^i = \lambda_k^i \widetilde{\mathcal{A}}_i^{(AS)}p_k^i, \quad \lambda_k^i \le \alpha^{-1}\}\big),$$

402 it holds that

403
404
$$\kappa(\mathcal{M}_{AS,2}\mathcal{A}) \leq \frac{\omega_+}{\omega_-} \left[N_c + 1 + \alpha(N_c + 2)\right] (N_c + 1).$$

Theorem 12 generalizes [Theorem 4.40, 33] to the approximate case, while improving the bound.

407 A spectral coarse space composed of eigenvectors of a generalized eigenproblem was earlier 408 proposed in [11, 15]. In those studies, the authors also discuss the analytical and numerical interest 409 of using AS,2/S instead of the more traditional AS,2/K to reduce the size of the coarse space. In 410 comparison, our method is more algebraic in the sense that it does not need a stable interpolation 411 operator, nor the mass matrix.

412 *Proof.* If we apply Lemma 7 without a coarse space and consider V_0 as another subdomain in 413 the decomposition, we get

414
$$\lambda_{\max}(\mathcal{M}_{AS,2}\mathcal{A}) \leq \frac{1}{\omega_{-}}(N_{c}+1).$$

The lower bound is a consequence of Lemma 4. We define $u_i^0 \in V_i^0$ and $u_i^{\perp} \in \widetilde{V}_i^{\perp}$ such that $D_i \mathcal{R}_i u = u_i^0 + u_i^{\perp}$ as in the proof of Lemma 6. We now introduce u_0 such that $V_0 u_0 = \sum_{i=1}^N \mathcal{R}_i^T u_i^0$, and $u = V_0 u_0 + \sum_{i=1}^N \mathcal{R}_i^T u_i^{\perp}$.

418 We get from Equation (2.8) that

419
$$\sum_{i=1}^{N} |u_i^{\perp}|^2_{\tilde{\mathcal{A}}_i^{(AS)}} = \sum_{i=1}^{N} |u_i^{\perp}|^2_{\hat{\mathcal{A}}_i} \le C |u|^2_{\tilde{\mathcal{A}}} \quad \text{with} \quad C = \max_{1 \le i \le N} \sup_{v \in \tilde{V}_i^{\perp}} \frac{|v|^2_{\tilde{\mathcal{A}}_i^{(AS)}}}{|v|^2_{\tilde{\mathcal{A}}_i^{(NN)}}} = \frac{|v|^2_{\mathcal{R}_i \tilde{\mathcal{A}} \mathcal{R}_i^T}}{|v|^2_{D_i^{-1} \tilde{\mathcal{A}}_i D_i^{-1}}}.$$

421 Then, we can use the same method as in Equation (2.9):

422
$$|u_0|_{\widetilde{\mathcal{A}}}^2 = |u - \sum_{i=1}^N \mathcal{R}_i^T u_i^\perp|_{\widetilde{\mathcal{A}}}^2 \le (N_c + 1) \left(|u|_{\widetilde{\mathcal{A}}}^2 + \sum_{i=1}^N |\mathcal{R}_i^T u_i^\perp|_{\widetilde{\mathcal{A}}}^2 \right)$$

423

$$= (N_c+1)\left(|u|_{\widetilde{\mathcal{A}}}^2 + \sum_{i=1}^N |u_i^{\perp}|_{\mathcal{R}_i \widetilde{\mathcal{A}} \mathcal{R}_i^T}^2\right) \le (N_c+1)(1+C)|u|_{\widetilde{\mathcal{A}}}^2$$

424
425
$$|u_0|_{\widetilde{\mathcal{A}}}^2 + \sum_{i=1}^{N} |u_i^{\perp}|_{\mathcal{R}_i \widetilde{\mathcal{A}} \mathcal{R}_i^T}^2 \le [N_c + 1 + (N_c + 2)C] |u|_{\widetilde{\mathcal{A}}}^2 \le \omega_+ [N_c + 1 + (N_c + 2)C] |u|_{\mathcal{A}}^2.$$

426 We then use Lemma 4 with $\mathcal{I}_0 = V_0$, $\mathcal{I}_i = \mathcal{R}_i^T$ and $\mathcal{B}_i = \mathcal{I}_i^T \widetilde{\mathcal{A}} \mathcal{I}_i$ to get the bound

427
428
$$\lambda_{\min}(\mathcal{M}_{AS,2}\mathcal{A}) \geq \frac{1}{\omega_{+}} \left[N_{c} + 1 + (N_{c} + 2) \max_{1 \leq i \leq N} \sup_{v \in \widetilde{V}_{i}^{\perp}} \frac{|v|_{\mathcal{R}_{i}\widetilde{\mathcal{A}}\mathcal{R}_{i}^{T}}}{|v|_{\widetilde{\mathcal{A}}_{i}^{(NN)}}^{2}} \right]^{-1}$$

429 We can then conclude with Lemma 9.

430 **5. Numerical experiments.**

5.1. Experimental setup. The methods introduced in sections 2, 3 and 4 are tested on a 431 problem similar to what is presented in [33]. We use the Finite Element Method (FEM) with Q1 432 elements to solve a heterogeneous diffusion equation $\nabla \cdot (k\nabla u) = 1$ in a 3D stratified medium. The 433domain $[0, N] \times [0, 6] \times [0, 1]$ is discretized on a regular mesh of $(5N + 1) \times 31 \times 6$ nodes. The 434 domain is divided into N identical subdomains along the first axis. Along the second axis, it is 435divided into 10 layers (of $5N \times 3 \times 5$ elements each) of alternating conductivity k = 1 and k = K436 (K is a heterogeneity parameter). A Dirichlet boundary condition is applied on the left of the 437 domain (x = 0), a Neumann condition on every other boundary. Using a FEM discretization on 438 each subdomain gives rise naturally to a set of local SPSD matrices and a global matrix that is 439 SPD. The geometry and 1D partitioning of this test case are chosen so as to emphasize the effects of 440 using a coarse grid correction: indeed, without a coarse correction, the number of iterations grows 441 as $O(N^{1/d})$ where d is the dimension of the partitioning. Using a 3D partitioning of the global 442domain, one would need more than 7M subdomains (192^3) to illustrate the same effect as in the 443 experiments presented here with a 1D partitioning and 192 subdomains. The layered structure of 444 the domain is introduced to deteriorate the condition number of the local subproblems. Since all 445subdomains (except the first and last ones) are identical, the bound on the condition number of the 446 method in Theorem 2 is independent of N if at least the kernels of $\widetilde{\mathcal{A}}_i^{(NN)}$ and $\widehat{\mathcal{A}}_i$ are included in V_i^0 ; 447 a coarse space that only includes these kernels (as in BDD for instance) thus yields a method that 448 can be considered as robust in this regard, while being considerably simpler to compute than the 449coarse space proposed in this article. However, the condition number still depends on the inverse 450of the smallest eigenvalues not included in the coarse space, which can be quite close to 0 if the 451 local problems are ill-conditioned (*i.e.*, if K is big). As a result, the condition number, although 452453independent of N, can still be too large for the iterative solver to converge in a reasonable number of iterations. Building the coarse space by solving the generalized eigenproblems as proposed in 454 Section 3 yields a more robust method in the sense that the condition number of the method can 455be controlled independently of both N, K, and the particular choice of a local preconditioner. We 456consider three aS methods: the AS and NN preconditioners introduced in Equation (1.6) and a 457

Shifted (Sh) preconditioner whose local matrix is obtained by shifting the diagonal of $\widetilde{\mathcal{A}}_i$ by 1 to 458remove its potential singularity: $\widetilde{\mathcal{M}}_{Sh} = \sum_{i=1}^{N} \mathcal{R}_{i}^{T} (\widetilde{\mathcal{A}}_{i} + I_{n_{i}})^{\dagger} \mathcal{R}_{i}$ where $I_{n_{i}}$ is the identity matrix 459of same size as \mathcal{A}_i . If built on the Schur matrix, $\widetilde{\mathcal{M}}_{Sh}$ is a (non-optimized) Robin preconditioner. 460 461 The optimization of the Robin condition as proposed in [16] is not considered here as it is out of the scope of this paper. It is introduced as an example of a more generic aS preconditioner than 462 AS and NN; as such, two generalized eigenproblems need to be solved to compute the coarse space 463 for Sh as opposed to only one for AS and NN. Each of these method is assessed with $\mathcal{A} = \mathcal{K}$ or 464 $\mathcal{A} = \mathcal{S}$. Equation (1.4) can therefore either result from: 465

- 466 467
- the FEM discretization (1.1) of the global problem, in which case the preconditioner is said to be applied on the original matrix \mathcal{K} and the abstract Schwarz method is noted aS/ \mathcal{K} ;
- 468 469 470
- or the substructuring system (1.3) obtained by eliminating the interior variables from Equation (1.1), in which case the preconditioner is said to be applied on the Schur matrix S and the method is noted aS/S.

471 We study the numerical behaviour of these methods under the constraint of a bounded condition 472 number or an imposed coarse space size in sections 5.2 and 5.3, respectively. We then study 473 the approximate case with an empirical approach in Section 5.4, using a so-called *sparsification* 474 technique. Our numerical results overall confirm [11, 15] regarding the numerical interest of using 475 AS,2/S instead of the more traditional AS,2/K method to reduce the size of the coarse space. 476 Section 5.5 eventually illustrates the parallel behavior of that promising variant.

The partition of unity D_i is computed using the diagonal values of \mathcal{A}_i . The condition numbers of the preconditioned matrices are estimated using the eigenvalues of the tridiagonal Lanczos matrix computed during the PCG iterations (see, e.g., [14]). The stopping criterion is based on the normwise backward error $||b - \mathcal{A}x_k||/||b|| \leq 10^{-6}$.

481 **5.2.** Imposing an *a priori* bound on the condition number. We proved in Section 3 that 482 it is possible to control the condition number $\kappa(\widetilde{\mathcal{M}}_{aS,D}\mathcal{A})$ of aS methods through some parameters 483 α and β . For now, we do not use any approximation (whose effects are the object of Section 5.4), 484 hence $\widetilde{\mathcal{A}}_i = \mathcal{A}_i$ and $\omega_- = \omega_+ = 1$. In order to compare the three methods, we first choose a bound 485 χ and then we choose α and β such that $\kappa \leq \chi$:

486

487

• for AS (resp. NN), Corollary 11 states that $\kappa \leq (1 + \alpha)N_c$ (resp. $\kappa \leq \alpha N_c$). We choose $\alpha = \chi/N_c - 1$ (resp. $\alpha = \chi/N_c$).

488 489 • for Sh (or any other aS preconditioner), Theorem 10 states that $\kappa \leq (1+\alpha)\beta$ and we choose $\alpha = \sqrt{1/4 + \chi} - 1/2$ and $\beta = \sqrt{1/4 + \chi} + 1/2$.

When we do not impose an upper bound ($\chi = \infty$), no coarse space is used and results are 490presented only for AS and Sh. We observe (Figure 1) that the condition number κ grows quadrat-491 ically with the number of subdomains N and that the number of iterations to reach convergence 492 (Figure 2) is proportional to the number of subdomains (note the log scale for the \$x\$-axis). This 493lack of scalability is the main motivation for using a two-level method. We also note that, with-494out a coarse space, our AS preconditioner outperforms the Sh preconditioner, especially when the 495heterogeneity K is high: the AS preconditioner performs a more appropriate local solve than the 496very basic Sh preconditioner. As expected, the condition number is also lower when working on the 497498Schur matrix \mathcal{S} instead of \mathcal{K} , since all the interior unknowns are solved using a direct method and do not appear anymore in the iterative process. 499

500 When we impose an upper bound on the condition number ($\chi = 10,000$ or $\chi = 100$), we observe 501 that the condition number κ does indeed drop below the prescribed bound χ , independently of the 502 number of subdomains N, the local preconditioner AS, NN or Sh, the heterogeneity K and the

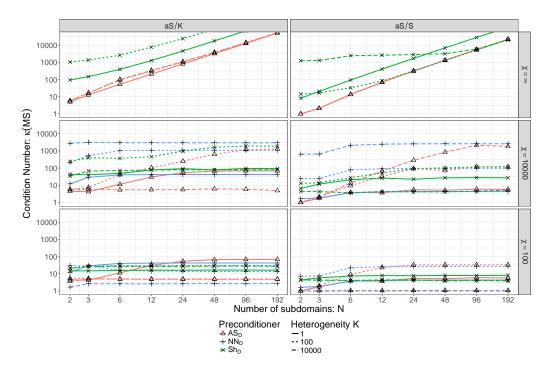


FIG. 1. Imposing an a priori bound χ on the condition number using deflation. Whatever the chosen target χ , we ensure that the condition number of the iterative problem $\kappa(\mathcal{MA})$ remains below χ . Each preconditioner (AS, NN, Sh) can be applied either on the original matrix \mathcal{K} (aS/ \mathcal{K}), left, or in a substructuring context on \mathcal{S} (aS/ \mathcal{S}), right.

choice of operating on \mathcal{K} or \mathcal{S} . However, this *a priori* control on the condition number comes at 503the expense of having to use a direct solve on a coarse space V_0 whose dimension can be quite 504large. Each subdomain computes a local coarse space V_i^0 of dimension $n_v^{(i)}$ (Figure 3) and the size 505of the global coarse space therefore grows linearly with the number of subdomains. Since without 506 deflation $(\chi = \infty)$ the Sh preconditioner applied to the original matrix \mathcal{K} does not perform very 507well in the heterogeneous case, the size of the coarse space necessary to obtain a condition number 508below the target χ is very large (up to 87 vectors per subdomain). However, using a better local 509preconditioner such as AS or NN can greatly reduce the size of the coarse space, as well as working 510on the Schur matrix \mathcal{S} instead of \mathcal{K} .

5.3. Imposing an *a priori* coarse space size. We showed in the previous section that we 512can effectively control the condition number κ of the method by building the coarse space using 513 two parameters α and β as presented in Theorem 10. However, this can lead to an impractically 514large coarse space and we now consider the context where the size n_v of the local subspace in each 515 subdomain is chosen a priori. Instead of choosing the coarse space by comparing the eigenvalues to a threshold, we thus keep the eigenvectors associated with the n_v smallest eigenvalues. Once the 517 coarse space is computed, we know what threshold would have led us to keep the same number of 518vectors and we can get, a posteriori, a bound on the condition number of the method: if λ_{n_n+1} is 519the lowest eigenvalue corresponding to a vector not in the coarse space, Theorem 10 ensures that 520

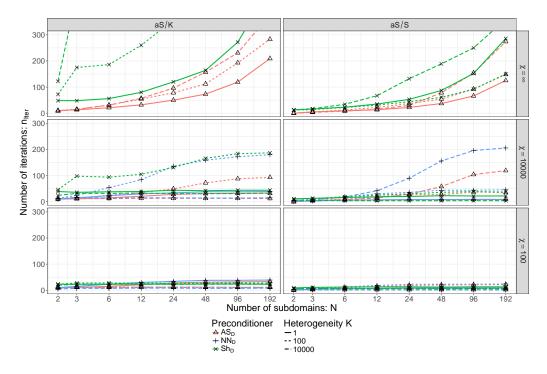


FIG. 2. Number of iterations when imposing an a priori bound χ on the condition number.

521 $\kappa(\mathcal{M}_{Sh,D} \mathcal{A}) \leq N_c(1+1/\lambda_{n_v+1})/\lambda_{n_v+1}$. As in Section 5.2, this bound can be improved for NN and 522 AS preconditioners using Corollary 11 and Theorem 12:

523 • $\kappa(\mathcal{M}_{NN,D} \mathcal{A}) \leq N_c / \lambda_{n_v+1};$

525

- 524 $\kappa(\mathcal{M}_{AS,D} \mathcal{A}) \leq N_c(1+1/\lambda_{n_v+1});$
 - $\kappa(\mathcal{M}_{AS,2} \ \mathcal{A}) \le (N_c + 1) [N_c + 1 + (N_c + 2)/\lambda_{n_v+1}].$

The Schur matrix \mathcal{S} is smaller and better conditioned [5, 27] than the original matrix \mathcal{K} . 526 Furthermore, in a 2-level domain decomposition framework, eliminating the interior unknowns 527significantly improves the convergence by reducing the size of the coarse space needed to take into 528account the physical hetoregeneity in the domain [15]. In accordance with these theoretical results, 529Figure 4 highlights the benefits of operating on \mathcal{S} (Figure 4, right) instead of \mathcal{K} (left): the condition 530number is consistently smaller when applying any aS method on \mathcal{S} instead of \mathcal{K} . Without a coarse 531space $(n_v = 0, \text{ top})$, the results are consistent with Figure 1, top $(\chi = \infty)$: the condition number 532 κ increases with the number of subdomains N. Choosing $n_v = 1$, our coarse space reduces to a classical partition-of-unity coarse space [31] and is sufficient in the homogeneous case (K = 1, plain 534lines); we notice that NN,D/ \mathcal{S} then reduces to classical BDD where the condition number does 535 not depend on N but remains fairly large for large values of K. However, in the heterogeneous 536 cases (K = 100 or 10,000, dashed lines), this simpler coarse space is not enough to get a scalable method: one eigenvector per high-conductivity inclusion is needed in the coarse space to build a 538 robust method [15]. In our case, with 5 high-conductivity layers passing through all the subdomains, 539 $n_v = 5$ eigenvectors are enough to bound the condition number for AS/S and NN/S. Using the 540Sh/S method, since two eigenproblems are solved in each subdomain, 10 vectors are needed to get 541

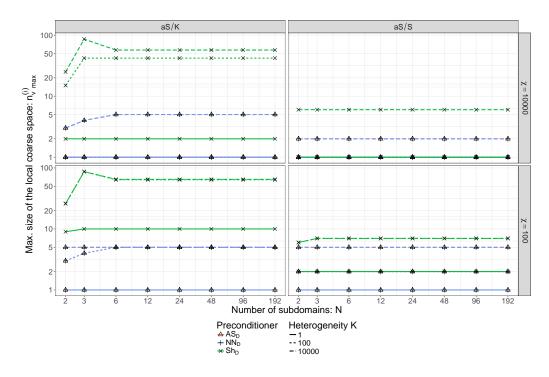


FIG. 3. Maximum size of the local coarse space when imposing an a priori bound χ on the condition number. Note that AS and NN overlap with each other. In most cases, only few vectors per subdomain are enough but the least robust methods can induce a relatively large local coarse space V_i^0 in some cases.

542 a good convergence (bottom right).

543 With a large enough coarse space, the three methods NN,D/S, AS,2/S and AS,D/S perform 544 quite similarly, with a slight advantage for NN. However, when the coarse space is too small ($n_v = 1$ 545 and K = 10,000 for instance), AS,2/S and AS,D/S have a significantly smaller condition number 546 than NN,D/S, and they appear more robust. As a consequence, we will choose for our proposed 547 high performance implementation to focus on the AS,2/S method (Section 5.5).

5485.4. Approximate case: Empirical study of the impact of sparsification. The convergence results for approximate aS methods in sections 2, 3 and 4 apply for both aS/\mathcal{K} and aS/\mathcal{S} 549cases. However, for a matter of conciseness, we now only focus on the latter context for illustrating 550the impact of approximation, as the above experiments showed the numerical benefits of operating on the Schur complement. For that, we approximate the dense matrix \mathcal{S}_i with a sparse matrix $\hat{\mathcal{S}}_i$, by 552dropping some entries in the matrix. This process is called *sparsification*. In a very heterogeneous 553medium $(K \gg 1)$, some entries in S corresponding to couplings between unknown separated by a 554low-conductivity layer, are negligible. We use the symmetry-preserving strategy of dropping s_{ij} if $|s_{ij}| \leq \epsilon(s_{ii} + s_{jj})$, where ϵ is a parameter that controls the sparsity (see, e.g., [6]). 556

The benefits of sparsification are evaluated by assessing the proportion $nnz(LL^T)$ of non-zero elements in the Cholesky factorization $\widehat{S}_i = LL^T$ of the local preconditioner. In Figure 5, we evaluate the impact of sparsification on the robustness of the method. It appears that, up to a certain level, we are still able to find a robust coarse space despite having significantly reduced

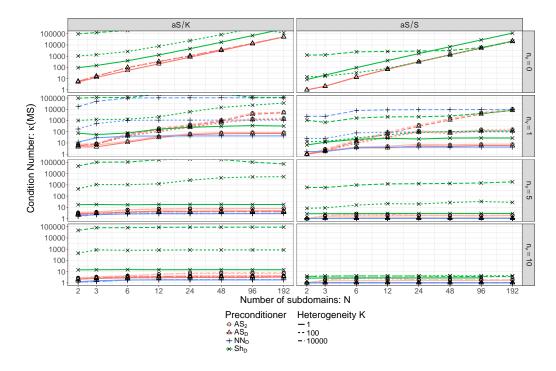


FIG. 4. Condition number when imposing an a priori size n_v for the local coarse space V_i^0 . We are still able to significantly reduce the condition number of the methods. The best convergence results are obtained with the AS, D/S method.

the memory footprint of the preconditioner. For instance, with a sparsity parameter of $\epsilon = 0.001$, although 88.8% of the entries in the factorization of the preconditioner are dropped, our coarse space with $n_v = 5$ vectors per subdomain still significantly improves the convergence.

These results are very promising as they show we can efficiently apply an approximate scheme to reduce the complexity of two-level aS methods. However, the considered sparsification technique is delicate for ensuring an *a priori* condition number. Approximation through hierarchical matrices [17] might better fit this objective, for bounding ω_{-} and ω_{+} and ensure theorems 10 and 12 apply. This is left for future work (see [1] for preliminary investigations in this direction) and we do not consider approximation techniques in the high performance implementation we propose below.

5.5. Performance of AS_2/S on a modern parallel computer. The excellent numerical 570 properties exhibited above by the AS_2/S method motivated the design of an high-performance code of that variant. For that, we relied on the MaPHyS package and we added a coarse grid correction to the baseline, one-level AS/S variant [3] for the purpose of the present study. MaPHyS 573 574 is a parallel hybrid (direct/iterative) sparse linear solver. Its Setup step relies on third-party sparse direct solvers for efficiently performing the elimination of the interior variables and computing the 575 local Schur complement \mathcal{S}_i . Subdomains are processed concurrently, each subdomain being associ-576 ated with a process. The computation of the one-level preconditioner (still within the Setup step) 577 is then performed with neighbor-to-neighbor communications. The Solve step consists of classical 578preconditioned conjugate gradient iterations. In particular, global synchronizations are only re-579

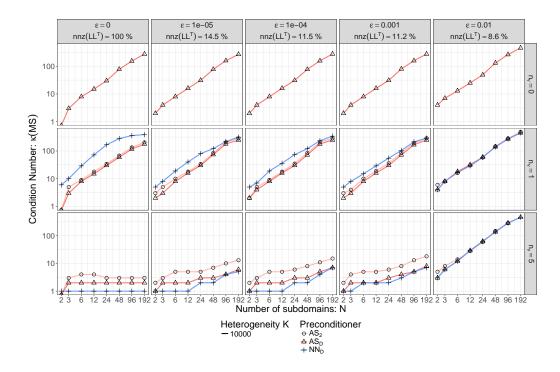


FIG. 5. Up to a certain level, the sparsification does not break the robustness of the method: using a big enough coarse space ($n_v = 5$), it is possible to discard 88.8% of the entries in the factorization of the preconditioner without losing convergence.

quired for computing dot products while the matrix-vector product can be performed concurrently 580 on each subdomain and the application of the (one-level) preconditioner only requires neighbor-to-581 582 neighbor communications. We extended MaPHyS to ensure a coarse grid correction as follows. In the Setup step, the generalized eigenproblems are processed concurrently on each subdomain; the 583matrix associated with the resulting coarse space is then assembled and factorized using a third-584party parallel sparse direct solver. In the Solve step, a coarse solve is added in the application of the 585 preconditioner at each iteration. Due to the nature of the coarse space, these operations add global 586communications and synchronizations in the algorithm and particular care must be taken in their 587 implementation in order to achieve good scalability and parallel efficiency. Several parallelization 588 strategies for the coarse correction are currently investigated and will be discussed in a future work. 589In the current experiment, the coarse matrix \mathcal{A}_0 is assembled and factorized redundantly on disjoint 590sub-communicators (obtained by splitting the global one) in order to reduce the number of global 591communications during the solve step. 592

We now present a weak scalability study conducted on test cases similar to the ones introduced in Section 5.1, but with larger subdomains. Each subdomain is indeed a cube discretized on $31 \times 31 \times 31$ mesh with 29,791 unknowns. There are now 6 alternating conductivity layers (K = 10,000), and we consider a scenario with an imposed coarse space size (as in Section 5.3) using 3 vectors per subdomain. No approximation is performed. The same stopping criterion as above is used. The experiments have been conducted on the Occigen machine at CINES. Each node is composed of two Haswell (E5-2690V3) 12-core processors running at 2.6 GHz. A subdomain is associated with a process, binded on a CPU core. MaPHyS was compiled with Intel 17.0 and Intel
MPI 2017.0.098. All dense operations are performed with the Intel Math Kernel Library (MKL)
2017 (including the Lapack dsygvx routine for solving the eigenproblems, that allows one to only
compute a targeted subset of eigenpairs). Sparse factorizations are performed with the MUMPS
5.0.2 sparse direct solver [4] together with the ParMetis 4.0.3 partitioner [21].

Table 1 compares the behavior of our extension of MaPHyS relying on the proposed coarse grid 605 correction described above (AS_2/S) with the baseline, one-level version of MaPHyS [3] (AS/S). 606 The number of subdomains N, which is equal to the number of MPI processes and CPU cores used 607 608 for the respective computation, the total number of unknowns $n = (30N+1) \times 31 \times 31$ and the size of the coarse space n_0 are provided in the table along with the maximum (among all subdomains) 609 time in seconds needed to perform the Setup step, the Solve step or both steps (Total) and the 610 number of PCG iterations performed during the *Solve* step, for both the AS/S method (left) and 611 the AS.2/S method (right). The Setup step includes the time spent in the factorization of the 612 local matrices and the computation of the local Schur complement matrix using a sequential sparse 613 614 direct solver, the assembly and factorization of the local Schur complement, the solution of the generalized eigenproblems, the construction and the factorization of the coarse matrix. The Solve 615step corresponds to the PCG iterations and the final computation of the interior unknowns. We 616 observe that the addition of the coarse correction increases the *Setup* time and the individual cost 617 of each iteration (up to a factor 2), mainly due to the induced global communications. On the 618 other hand, the number of iterations of AS_2/S remains stable, leading to a drastically overall 619 reduced Solve time compared to the baseline AS/S method (up to a factor 37 when the 44,283,841) 620 unknowns are distributed among 1,536 subdomains). As a consequence, in a scenario consisting of 621 solving a linear system with a single right-hand side, the coarse grid usage reduces the total time 622 623 to solution (Setup + Solve) when the number of subdomains (and CPU cores) is equal to or higher 624 than 384. In another common application scenario where multiple (say, p), successive, right-hand sides must be solved, the total time to solution (Setup + p Solve) may then essentially be governed 625 by the Solve step if p is large. In that latter case, the benefits of the coarse grid may then thus be 626 tremendous on large scale computers. 627

TABLE 1

A weak scalability study was performed using the MaPHyS parallel solver. The Setup, Solve and Total times are the max among all subdomains, in seconds (s). Each subdomain is associated with one MPI process binded on one CPU core. N is the number of subdomains, n is the size of K and n_0 is the size of the coarse space. Without coarse correction, the Setup time remains stable, whereas the Solve time grows linearly with the number of domains. The coarse correction adds to the Setup time but keeps the number of iterations constant, thus improving the scalability. Without coarse correction, no convergence was achieved on 3,072 domains.

				AS/\mathcal{S}				AS,2/S		
N	n	n_0	Setup	Solve	Total	# iter	Setup	Solve	Total	# iter
24	692k	72	3,64	$0,\!47$	4,12	33	6,13	$0,\!30$	$6,\!44$	15
48	1.4M	144	$3,\!67$	$0,\!87$	$4,\!54$	62	6,52	$0,\!30$	$6,\!83$	15
96	$2.8 \mathrm{M}$	288	3,79	$1,\!62$	$5,\!41$	119	6,52	$0,\!31$	$6,\!84$	15
192	$5.6 \mathrm{M}$	576	3,75	$3,\!17$	6,92	233	6,59	$0,\!33$	$6,\!92$	15
384	11.1M	1.1k	$3,\!87$	5,02	8,90	371	6,61	$0,\!32$	$6,\!93$	14
768	$22.1 \mathrm{M}$	2.3k	3,78	8,30	12,1	609	6,61	$0,\!33$	$6,\!95$	14
1536	44.3M	4.6k	$4,\!13$	15,1	19,2	1,077	6,96	$0,\!40$	$7,\!38$	14
3072	88.6M	9.2k	-	-	-	-	7,24	$0,\!42$	7,70	14

6. Conclusion. In this paper, we have proposed a new class of aS preconditioners, so-called 628 approximate aS preconditioners. These preconditioners are fully algebraic in the sense that they 629 do not require any other information apart from SPSD subdomain matrices. This class is wide as 630 it consists of all aS preconditioners, provided that their coarse space results from the assembly of 631 local components that contain the kernel of some local operators (Definition 1). In particular, it 632 generalizes the class of approximate NN preconditioners introduced in [25] (named generalized NN 633 in the original paper). We exhibited a bound on the condition number of all approximate deflated aS 634 preconditioners (Theorem 2). This bound depends on generalized Rayleigh quotients and generalizes 635 636 the result from [25] beyond the class of approximate NN methods. Applying a GenEO procedure on two well chosen generalized eigenproblems, we proposed to explicitly compute the coarse space 637 while bounding these Rayleigh quotients leading to a bound on the condition number (hence on the 638 number of iterations of PCG) independent of the number of subdomains. We also showed that a 639 640 similar bound can be obtained when the coarse space is applied additively for the subclass of newly introduced approximate AS methods. 641

642 The results presented in this paper can be readily derived to retrieve the bounds previously obtained via generalized eigenproblems in the particular cases of AS/ \mathcal{K} [11, 33], NN/ \mathcal{S} [34] and 643 optimized Robin (SORAS) [18]. It also generalizes these results when used with approximate local 644 solvers. Furthermore, they allowed us to define a coarse space for the AS method applied on the 645Schur complement (AS/S) [6], leading to an extremely robust substructuring method, for which 646 the coarse space can be applied either with deflation or additively, and with the freedom of relying 647 on an approximate local Schur complement. Numerical experiments illustrated these statements. 648 In particular, they motivated an high-performance design of a coarse grid correction for AS/ \mathcal{S} . We 649 implemented it within the MaPHyS package. Parallel experiments showed the significant benefits 650 651 that the resulting AS_{2}/S solver could bring.

A challenge opened by the present study is to determine an explicit procedure to perform the approximation while achieving a given *a priori* bound on the condition number. We also plan to study the effects of the method on the spectrum and on the empirical convergence of non symmetric test cases.

7. Acknowledgments. The authors would like to thank Nicole Spillane for proofreading 656 an early draft of this manuscript. Experiments presented in sections 5.2 to 5.4 were carried 657 out using the PLAFRIM experimental testbed, being developed under the Inria PlaFRIM de-658 velopment action with support from Bordeaux INP, LABRI and IMB and other entities: Conseil 659 Régional d'Aquitaine, Université de Bordeaux and CNRS (and ANR in accordance to the pro-660 gramme d'investissements d'Avenir). Experiments presented in Section 5.5 were performed on the 661 GENCI Occigen cluster at CINES by Matthieu Kuhn and Gilles Marait. We would also like to 662 thank the anonymous referees whose constructive comments enabled us to significantly improve 663 the manuscript. Finally, this work was partially supported by the French research agency ANR in 664 665 the framework of the DEDALES project (ANR-14-CE23-0005), in particular the PhD thesis of the 666 third author (in the alphabetical order) was funded by this project.

667 **References.**

- E. AGULLO, E. DARVE, L. GIRAUD, AND Y. HARNESS, Low-Rank Factorizations in Data Sparse Hierarchical Algorithms for Preconditioning Symmetric Positive Definite Matrices, SIAM Journal on Matrix Analysis and Applications, 39 (2018), pp. 1701–1725, https://hal.
 inria.fr/hal-01940053.
- 672 [2] E. AGULLO, L. GIRAUD, A. GUERMOUCHE, AND J. ROMAN, Parallel hierarchical hy-

- brid linear solvers for emerging computing platforms, Comptes Rendus Mécanique, 339
 (2011), pp. 96–103, https://doi.org/10.1016/j.crme.2010.11.005, http://www.sciencedirect.
 com/science/article/pii/S1631072110002068 (accessed 2018-03-08).
- 010
- [3] E. AGULLO, L. GIRAUD, S. NAKOV, AND J. ROMAN, *Hierarchical hybrid sparse linear solver* for multicore platforms, report, INRIA Bordeaux, Oct. 2016, https://hal.inria.fr/hal-01379227/
 document (accessed 2018-03-26).
- [4] P. R. AMESTOY, I. S. DUFF, J.-Y. L'EXCELLENT, AND J. KOSTER, A fully asynchronous multifrontal solver using distributed dynamic scheduling, SIAM Journal on Matrix Analysis and Applications, 23 (2001), pp. 15–41.
- [5] S. C. BRENNER, The condition number of the Schur complement in domain decomposition,
 Numerische Mathematik, 83 (1999), pp. 187–203.
- [6] L. M. CARVALHO, L. GIRAUD, AND G. MEURANT, Local preconditioners for two-level non overlapping domain decomposition methods, Numerical linear algebra with applications, 8
 (2001), pp. 207–227.
- [7] B. COCKBURN, J. GOPALAKRISHNAN, AND R. LAZAROV, Unified hybridization of discontinuous Galerkin, mixed, and continuous Galerkin methods for second order elliptic problems, SIAM Journal on Numerical Analysis, 47 (2009), pp. 1319–1365.
- [8] Y.-H. DE ROECK AND P. LE TALLEC, Analysis and test of a local domain decomposition
 preconditioner, in Fourth International Symposium on Domain Decomposition Methods for
 Partial Differential Equations, vol. 4, 1991.
- [9] C. R. DOHRMANN, A preconditioner for substructuring based on constrained energy minimiza tion, SIAM Journal on Scientific Computing, 25 (2003), pp. 246–258.
- [10] V. DOLEAN, P. JOLIVET, AND F. NATAF, An Introduction to Domain Decomposition Methods:
 Algorithms, Theory, and Parallel Implementation, vol. 144, SIAM, 2015.
- [11] Y. EFENDIEV, J. GALVIS, R. LAZAROV, AND J. WILLEMS, Robust domain decomposition
 preconditioners for abstract symmetric positive definite bilinear forms, ESAIM: Mathematical
 Modelling and Numerical Analysis, 46 (2012), pp. 1175–1199, http://www.esaim-m2an.org/
 articles/m2an/abs/2012/05/m2an110073/m2an110073.html (accessed 2017-06-08).
- [12] C. FARHAT, M. LESOINNE, P. LETALLEC, K. PIERSON, AND D. RIXEN, FETI-DP: A dual-primal unified FETI method—part I: A faster alternative to the two-level FETI method, International journal for numerical methods in engineering, 50 (2001), pp. 1523–1544.
- [13] C. FARHAT AND F.-X. ROUX, A method of finite element tearing and interconnecting and its parallel solution algorithm, International Journal for Numerical Methods in Engineering, 32 (1991), pp. 1205–1227.
- [14] V. FRAYSSÉ AND L. GIRAUD, A set of conjugate gradient routines for real and complex arith metics, CERFACS Technical Report TR/PA/00/47, (2000).
- [15] J. GALVIS AND Y. EFENDIEV, Domain Decomposition Preconditioners for Multiscale Flows in High-Contrast Media, Multiscale Modeling & Simulation, 8 (2010), pp. 1461–1483, https://doi. org/10.1137/090751190, http://epubs.siam.org/doi/abs/10.1137/090751190 (accessed 2016-09-15).
- [16] M. J. GANDER, *Optimized schwarz methods*, SIAM Journal on Numerical Analysis, 44 (2006),
 pp. 699–731.
- 715 [17] L. GRASEDYCK AND W. HACKBUSCH, Construction and Arithmetics of H-Matrices, Comput-
- ing, 70 (2003), pp. 295–334, https://doi.org/10.1007/s00607-003-0019-1, https://link.springer.
 com/article/10.1007/s00607-003-0019-1 (accessed 2018-03-26).
- 718 [18] R. HAFERSSAS, P. JOLIVET, AND F. NATAF, An Additive Schwarz Method Type Theory for

- Lions's Algorithm and a Symmetrized Optimized Restricted Additive Schwarz Method, SIAM
 Journal on Scientific Computing, 39 (2017), pp. A1345–A1365.
- [19] P. HÉNON, P. RAMET, AND J. ROMAN, PASTIX: A high-performance parallel direct solver for sparse symmetric positive definite systems, Parallel Computing, 28 (2002), pp. 301–321.
- [20] P. JOLIVET, F. HECHT, F. NATAF, AND C. PRUD'HOMME, Scalable Domain Decomposition Preconditioners for Heterogeneous Elliptic Problems, in Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis, SC '13, New York, NY, USA, 2013, ACM, pp. 80:1–80:11, https://doi.org/10.1145/2503210.2503212, http://doi.acm.org/10.1145/2503210.2503212 (accessed 2018-03-26).
- [21] G. KARYPIS AND V. KUMAR, MeTis: Unstructured Graph Partitioning and Sparse Matrix
 Ordering System, Version 4.0, 2009, http://www.cs.umn.edu/~metis.
- [22] A. KLAWONN, M. KUHN, AND O. RHEINBACH, Adaptive coarse spaces for FETI-DP in three
 dimensions, SIAM Journal on Scientific Computing, 38 (2016), pp. A2880–A2911.
- [23] A. KLAWONN, M. KÜHN, AND O. RHEINBACH, Adaptive FETI-DP and BDDC methods with
 a generalized transformation of basis for heterogeneous problems, Electronic Transactions on
 Numerical Analysis, 49 (2018), pp. 1–27.
- [24] A. KLAWONN, P. RADTKE, AND O. RHEINBACH, A comparison of adaptive coarse spaces for
 iterative substructuring in two dimensions, Electron. Trans. Numer. Anal, 45 (2016), pp. 75–
 106.
- [25] P. LE TALLEC AND M. VIDRASCU, Generalized Neumann-Neumann preconditioners for iterative substructuring, in Domain Decomposition Methods in Sciences and Engineering, 1998.
- [26] J. MANDEL, Balancing domain decomposition, International Journal for Numerical Methods
 in Biomedical Engineering, 9 (1993), pp. 233–241.
- [27] L. MANSFIELD, On the Conjugate Gradient Solution of the Schur Complement System Obtained from Domain Decomposition, SIAM Journal on Numerical Analysis, 27 (1990), pp. 1612– 1620, https://doi.org/10.1137/0727094, http://epubs.siam.org/doi/abs/10.1137/0727094 (accessed 2015-07-16).
- [28] T. P. A. MATHEW, Domain Decomposition Methods for the Numerical Solution of Partial Differential Equations, vol. 61, Springer Science & Business Media, 2008.
- [29] F. NATAF, H. XIANG, V. DOLEAN, AND N. SPILLANE, A Coarse Space Construction Based on Local Dirichlet-to-Neumann Maps, SIAM Journal on Scientific Computing, 33 (2011), pp. 1623– 1642, https://doi.org/10.1137/100796376, http://epubs.siam.org/doi/abs/10.1137/100796376
 (accessed 2014-11-18).
- [30] A. QUARTERONI AND A. VALLI, Domain Decomposition Methods for Partial Differential Equa tions, Oxford University Press, 1999.
- [31] M. SARKIS, Partition of unity coarse spaces: Enhanced versions, discontinuous coefficients and applications to elasticity, Domain decomposition methods in science and engineering, (2003), pp. 149–158.
- [32] N. SPILLANE, Méthodes de Décomposition de Domaine Robustes Pour Les Problèmes
 Symétriques Définis Positifs, PhD Thesis, Paris 6, 2014.
- [33] N. SPILLANE, V. DOLEAN, P. HAURET, F. NATAF, C. PECHSTEIN, AND R. SCHE-ICHL, Abstract robust coarse spaces for systems of PDEs via generalized eigenproblems in the overlaps, Numerische Mathematik, 126 (2014), pp. 741–770, https://doi.org/ 10.1007/s00211-013-0576-y, https://link.springer.com/article/10.1007/s00211-013-0576-y (accessed 2018-03-26).
- [34] N. SPILLANE AND D. J. RIXEN, Automatic spectral coarse spaces for robust finite element tear-

- ing and interconnecting and balanced domain decomposition algorithms, International Journal
- for Numerical Methods in Engineering, 95 (2013), pp. 953–990, https://doi.org/10.1002/nme.
- 767 4534, https://onlinelibrary.wiley.com/doi/abs/10.1002/nme.4534.
- [35] A. TOSELLI AND O. WIDLUND, Domain Decomposition Methods-Algorithms and Theory,
 vol. 34, Springer Science & Business Media, 2006.