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A MULTILEVEL SCHWARZ PRECONDITIONER BASED ON A HIERARCHY OF ROBUST COARSE SPACES*

HUSSAM AL DAAS[†], LAURA GRIGORI[†], PIERRE JOLIVET[‡], AND PIERRE-HENRI TOURNIER[§]

Abstract. In this paper we present a multilevel preconditioner based on overlapping Schwarz 5 methods for symmetric positive definite (SPD) matrices. Robust two-level Schwarz preconditioners 6 exist in the literature to guarantee fast convergence of Krylov methods. As long as the dimension of 7 the coarse space is reasonable, that is, exact solvers can be used efficiently, two-level methods scale 8 9 well on parallel architectures. However, the factorization of the coarse space matrix may become costly at scale. An alternative is then to use an iterative method on the second level, combined with 10 11 an algebraic preconditioner, such as a one-level additive Schwarz preconditioner. Nevertheless, the condition number of the resulting preconditioned coarse space matrix may still be large. One of the 12 13difficulties of using more advanced methods, like algebraic multigrid or even two-level overlapping 14Schwarz methods, to solve the coarse problem is that the matrix does not arise from a partial differential equation (PDE) anymore. We introduce in this paper a robust multilevel additive Schwarz 15 preconditioner where at each level the condition number is bounded, ensuring a fast convergence for each nested solver. Furthermore, our construction does not require any additional information than 17 18 for building a two-level method, and may thus be seen as an algebraic extension.

19 **Key words.** domain decomposition, multilevel, elliptic problems, subspace correction

20 AMS subject classifications. 65F08, 65F10, 65N55

12

1. Introduction. We consider the solution of a linear system of equations

22 (1.1)
$$Ax = b$$

23 where $A \in \mathbb{R}^{n \times n}$ is a symmetric positive definite (SPD) matrix, $b \in \mathbb{R}^n$ is the right-

hand side, and $x \in \mathbb{R}^n$ is the vector of unknowns. To enhance convergence, it is common to solve the preconditioned system

26
$$M^{-1}Ax = M^{-1}b$$

Standard domain decomposition preconditioners such as block Jacobi, additive 27 Schwarz, and restricted additive Schwarz methods are widely used [32, 9, 8]. In a 28parallel framework, such preconditioners have the advantage of relatively low com-29 munication costs. However, their role in lowering the condition number of the sys-30 tem typically deteriorates when the number of subdomains increases. Multilevel ap-32 proaches have shown a large impact on enhancing the convergence of Krylov methods 33 [33, 12, 7, 25, 20, 10, 21, 1, 15, 23, 34, 30]. In multigrid and domain decomposition communities, multilevel methods have proven their capacity of scaling up to large 34 numbers of processors and tackling ill-conditioned systems [37, 4, 19]. While some 35 preconditioners are purely algebraic [7, 20, 10, 26, 29, 16, 1], several multilevel meth-36 ods are based on hierarchical meshing in both multigrid and domain decomposition 37 38 communities [35, 9, 25, 15, 23]. Mesh coarsening depends on the geometry of the 39 problem. One has to be careful when choosing a hierarchical structure since it can

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have a significant impact on the iteration count [23, 25]. In [23], the authors propose 40 41 a multilevel Schwarz domain decomposition solver for the elasticity problem. Based on a heuristic approach and following the maximum independent set method [2], they 42 coarsen the fine mesh while preserving the boundary in order to obtain a two-level 43method. This strategy is repeated recursively to build several levels. However, they 44 do not provide a bound on the condition number of the preconditioned matrix of the 45 multilevel method. Multilevel domain decomposition methods are mostly based on 46 non-overlapping approaches [35, 9, 25, 23, 37, 4, 30, 34]. Two-level overlapping domain 47 decomposition methods are well studied and provide robust convergence estimates 48[33, 12, 5]. However, extending such a construction to more than two levels while 49preserving robustness is not straightforward. In [6], the authors propose an algebraic 50 51multilevel additive Schwarz method. Their approach is inspired by algebraic multigrid strategies. One drawback of it is that it is sensitive to the number of subdomains. In [15], the authors suggest applying the two-level Generalized Dryja–Smith–Widlund 53 preconditioner recursively to build a multilevel method. In this case, the condition 54number bound of the two-level approach depends on the width of the overlap, the diameter of discretization elements, and the diameter of the subdomains. They focus 56 on the preconditioner for the three-level case. One drawback of their approach is that the three-level preconditioner requires more iterations than the two-level variant. In 58this paper, the only information from the PDE needed for the construction of the preconditioner consists of the local Neumann matrices at the fine level. These ma-60 trices correspond to the integration of the bilinear form in the weak formulation of 61 62 the studied PDE on the subdomain-decomposed input mesh. No further information is necessary: except on the fine level, our method is algebraic and does not depend 63 on any coarsened mesh or auxiliary discretized operator. For problems not arising 64 from PDE discretization, one needs to supply the local SPSD matrices on the finest 65 level. In [3], a subset of the authors propose a fully algebraic approximation for such 66 matrices. However, their approximation strategy is heuristic and may not be effective 67 68 in some cases.

Our preconditioner is based on a hierarchy of coarse spaces and is defined as following. At the first level, the set of unknowns is partitioned into N_1 subdomains and each subdomain has an associated matrix $A_{1,j} = R_{1,j}AR_{1,j}^{\top}$ obtained by using appropriate restriction and prolongation operators $R_{1,j}$ and $R_{1,j}^{\top}$ respectively, defined in the following section. The preconditioner is formed as an additive Schwarz preconditioner coupled with an additive coarse space correction, defined as,

$$M^{-1} = M_1^{-1} = V_1 A_2^{-1} V_1^{\top} + \sum_{j=1}^{N_1} R_{1,j}^{\top} A_{1,j}^{-1} R_{1,j},$$

where V_1 is a tall-and-skinny matrix spanning a coarse space obtained by solving for 76each subdomain j = 1 to N_1 a generalized eigenvalue problem involving the matrix 77 $A_{1,j}$ and the Neumann matrix associated with subdomain j. The coarse space matrix 78is $A_2 = V_1^{\top} A V_1$. This is equivalent to the GenEO preconditioner, and is described 79in detail in [33] and recalled briefly in section 2. The dimension of the coarse space 80 is proportional to the number of subdomains N_1 . When it increases, factorizing A_2 81 by using a direct method becomes prohibitive, and hence the application of A_2^{-1} to a 82 vector should also be performed through an iterative method. 83

Our multilevel approach defines a hierarchy of coarse spaces V_i and coarse space matrices A_i for i = 2 to any depth L + 1, and defines a preconditioner M_i^{-1} such that the condition number of $M_i^{-1}A_i$ is bounded. The depth L + 1 is chosen such that the

coarse space matrix A_{L+1} can be factorized efficiently by using a direct method. At each level *i*, the graph of the coarse space matrix A_i is partitioned into N_i subdomains, and each subdomain *j* is associated with a local matrix $A_{i,j} = R_{i,j}A_iR_{i,j}^{\top}$ obtained by using appropriate restriction and prolongation operators $R_{i,j}$ and $R_{i,j}^{\top}$, respectively.

91 The preconditioner at level i is defined as,

92
$$M_i^{-1} = V_i A_{i+1}^{-1} V_i^{\top} + \sum_{j=1}^{N_i} R_{i,j}^{\top} A_{i,j}^{-1} R_{i,j},$$

93 where the coarse space matrix is $A_{i+1} = V_i^{\top} A_i V_i$.

One of the main contributions of the paper concerns the construction of the 94 hierarchy of coarse spaces V_i for levels i going from 2 to L, that are built algebraically 95 from the coarse space of the previous level V_{i-1} . This construction is based on the 96 definition of local symmetric positive semi-definite (SPSD) matrices associated with 97 each subdomain j at each level i that we introduce in this paper. These matrices are 98 99 obtained by using the local SPSD matrices of the previous level i-1 and the previous coarse space V_{i-1} . They are then involved, with the local matrices $A_{i,j}$, in concurrent 100 101 generalized eigenvalue problems solved for each subdomain i that allows to compute the local eigenvectors contributing to the coarse space V_i . 102

103 We show in Theorem 5.3, section 5, that the condition number of $M_i^{-1}A_i$ is 104 bounded and depends on the maximum number of subdomains at the first level that 105 share an unknown, the number of distinct colors required to color the graph of A_i so 106 that $\{span\{R_{i,j}^{\top}\}\}_{1 \leq j \leq N_i}$ of the same color are mutually A_i -orthogonal, and a user 107 defined tolerance τ . It is thus independent of the number of subdomains N_i .

The main contribution of this paper is based on the combination of two previous 108 works on two-level additive Schwarz methods [3, 33]. The coarse space proposed in 109[33] guarantees an upper bound on the condition number that can be prescribed by 110 111 the user. The SPSD splitting in the context of domain decomposition presented in [3] provides an algebraic view for the construction of coarse spaces. The combination 112 113of these two works leads to a robust multilevel additive Schwarz method. Here, robustness refers to the fact that at each level, an upper bound on the condition 114number of the associated matrix can be prescribed by the user a priori. The rest 115of the paper is organized as follows. In the next section, we present the notations 116117 used throughout the paper. In section 2, we present a brief review of the theory of one- and two-level additive Schwarz methods. We extend in section 3 the class of 118SPSD splitting matrices presented in [3] in order to make it suitable for multilevel 119 methods. Afterwards, we define the coarse space at level i based on the extended 120 class of local SPSD splitting matrices associated with this level. Section 4 describes 121 the partitioning of the domain at level i + 1 from the partitioning at level i. In 122Section 5, we explain the computation of the local SPSD matrices associated with each 123 subdomain at level i + 1. We compute them using those associated with subdomains 124at level i. Section 6 presents numerical experiments on highly challenging diffusion 125and linear elasticity problems in two- and three-dimensional problems. We illustrate 126the theoretical robustness and practical usage of our proposed method by performing 127128 strong scalability tests up to 8,192 processes.

129 **Context and notation.** By convention, the finest level, on which (1.1) is de-130 fined, is the first level. A subscript index is used in order to specify which level 131 an entity is defined on. In the case where additional subscripts are used, the first 132 subscript always denotes the level. For the sake of clarity, we omit the subscript corresponding to level 1 when it is clear from context, e.g., matrix A. Furthermore, the subscripts i and j always refer to a specific level i and its subdomain j, respectively. The number of levels is L + 1. Let $A_i \in \mathbb{R}^{n_i \times n_i}$ denote symmetric positive definite matrices, each corresponding to level $i = 1, \ldots, L+1$. We suppose that a direct solver can be used at level L + 1 to compute an exact factorization of A_{L+1} .

Let $B \in \mathbb{R}^{p \times q}$ be a matrix. Let $P \subset [1; p]$ and $Q \subset [1; q]$ be two sets of 138 indices. The concatenation of P and Q is represented by [P,Q]. We note that the 139order of the concatenation is important. B(P, :) is the submatrix of B formed by 140 the rows whose indices belong to P. B(:,Q) is the submatrix of B formed by the 141 columns whose indices belong to Q. B(P,Q) = (B(P,:))(:,Q). The identity matrix 142of size p is denoted I_p . We suppose that the graph of A_i is partitioned into N_i non-143144overlapping subdomains, where $N_i \ll n_i$ and $N_{i+1} \leqslant N_i$ for $i = 1, \ldots, L$. We note that partitioning at level 1 can be performed by using a graph partitioning library such as 145ParMETIS [22] or PT-SCOTCH [11]. Partitioning at greater levels will be described 146later in section 4. In the following, we define for each level $i = 1, \ldots, L$ notations 147for subsets and restriction operators that are associated with the partitioning. Let 148 149 $\Omega_i = [1; n_i]$ be the set of unknowns at level i and let $\Omega_{i,j,I}$ for $j = 1, \ldots, N_i$ be the subset of Ω_i that represents the unknowns in subdomain j. We refer to $\Omega_{i,j,I}$ as the 150*interior unknowns* of subdomain j. Let $\Gamma_{i,j}$ for $j = 1, \ldots, N_i$ be the subset of Ω_i that 151represents the neighbor unknowns of subdomain j, i.e., the unknowns at distance 1 152from subdomain j through the graph of A_i . We refer to $\Gamma_{i,j}$ as the overlapping 153unknowns of subdomain j. We denote $\Omega_{i,j} = [\Omega_{i,j,I}, \Gamma_{i,j}]$, for $j = 1, \ldots, N_i$, the 154155concatenation of interior and overlapping unknowns of subdomain j. We denote $\Delta_{i,j}$, for $j = 1, \ldots, N_i$, the complementary of $\Omega_{i,j}$ in Ω_i , i.e., $\Delta_{i,j} = \Omega_i \setminus \Omega_{i,j}$. In 156Figure 1.1, a triangular mesh is used to discretize a square domain. The set of 157nodes of the mesh is partitioned into 16 disjoint subsets $\Omega_{1,i,I}$, which represent a 158non-overlapping decomposition, for $j = 1, \ldots, 16$ (left). On the left, a matrix A_1 159whose connectivity graph corresponds to the mesh is illustrated. The submatrix 160 161 $A_1(\Omega_{1,j,I},\Omega_{1,j,I})$ is associated with the non-overlapping subdomain j. Each submatrix $A_1(\Omega_{1,j,I},\Omega_{1,j,I})$ is colored with a distinct color. The same color is used to color the 162region that contains the nodes in the non-overlapping subdomain $\Omega_{1,j,I}$. Note that 163if two subdomains j_1, j_2 are neighbors, the submatrix $A_1(\Omega_{1,j_1,I}, \Omega_{1,j_2,I})$ has nonzero 164elements. For $j = 1, ..., N_i$, we denote by $n_{i,j,I}$, $\gamma_{i,j}$ and $n_{i,j}$ the cardinality of $\Omega_{i,j,I}$, 165 $\Gamma_{i,j}$ and $\Omega_{i,j}$ respectively. 166

167 Let $R_{i,j,I} \in \mathbb{R}^{n_{i,j,I} \times n_i}$ be defined as $R_{i,j,I} = I_{n_i}(\Omega_{i,j,I},:)$.

- 168 Let $R_{i,j,\Gamma} \in \mathbb{R}^{\gamma_{i,j} \times n_i}$ be defined as $R_{i,j,\Gamma} = I_{n_i}(\Gamma_{i,j},:)$.
- 169 Let $R_{i,j} \in \mathbb{R}^{n_{i,j} \times n_i}$ be defined as $R_{i,j} = I_{n_i}(\Omega_{i,j},:)$.
- 170 Let $R_{i,j,\Delta} \in \mathbb{R}^{(n_i n_{i,j}) \times n_i}$ be defined as $R_{i,j,\Delta} = I_{n_i}(\Delta_{i,j},:)$.

171 Let $\mathcal{P}_{i,j} = I_{n_i}([\Omega_{i,j,I}, \Gamma_{i,j}, \Delta_{i,j}], :) \in \mathbb{R}^{n_i \times n_i}$, be a permutation matrix associated 172 with the subdomain j, for $j = 1, \ldots, N_i$. The matrix of the overlapping subdomain j, 173 $R_{i,j}A_iR_{i,j}^{\top}$, is denoted $A_{i,j}$. We denote $D_{i,j} \in \mathbb{R}^{n_{i,j} \times n_{i,j}}, j = 1, \ldots, N_i$, any set of 174 non-negative diagonal matrices such that

175
$$I_{n_i} = \sum_{j=1}^{N_i} R_{i,j}^\top D_{i,j} R_{i,j}$$

176 We refer to $\{D_{i,j}\}_{1 \leq j \leq N_i}$ as the algebraic partition of unity. Let $V_i \in \mathbb{R}^{n_i \times n_{i+1}}$ be 177 a tall-and-skinny matrix of full rank. We denote S_i the subspace spanned by the 178 columns of V_i . This subspace will stand for the coarse space associated with level *i*.

179 By convention, we refer to S_i as subdomain 0 at level *i*. Thus, we have $n_{i,0} = n_{i+1}$.



FIG. 1.1. Left: a triangular mesh is used to discretize the unit square. The set of nodes of the mesh is partitioned into 16 disjoint subsets, non-overlapping subdomains, $\Omega_{1,j,I}$ for j = 1, ..., 16. Right: Illustration of the matrix A_1 whose connectivity graph corresponds to the mesh on the left. The diagonal block j of A_1 corresponds to the non-overlapping subdomain $\Omega_{1,j,I}$. Each submatrix $A_1(\Omega_{1,j,I},\Omega_{1,j,I})$ is colored with a distinct color. The same color is used to color the region of the square that contains nodes in $\Omega_{1,j,I}$.

180 The interpolation operator at level i is defined as:

(1.2)
$$\mathscr{R}_{i,2} \colon \prod_{j=0}^{N_i} \mathbb{R}^{n_{i,j}} \to \mathbb{R}^{n_i}$$

181

182

$$(u_j)_{0\leqslant j\leqslant N_i}\mapsto \sum_{j=0}^{N_i} R_{i,j}^\top u_j$$

Finally, we denote $\mathcal{V}_{i,j}$ the set of neighboring subdomains of each subdomain j at level i for $(i, j) \in [\![1; L]\!] \times [\![1; N_i]\!]$.

185
$$\mathcal{V}_{i,j} = \{k \in \llbracket 1; N_i \rrbracket : \Omega_{i,j} \cap \Omega_{i,k} \neq \emptyset\}$$

As previously mentioned, partitioning at level 1 can be performed by graph parti-186tioning libraries such as ParMETIS [22] or PT-SCOTCH [11]. Partitioning at further 187levels will be defined later: the sets $\Omega_{i,j,\Gamma}$, $\Omega_{i,j,\Gamma}$, $\Omega_{i,j}$, and $\Delta_{i,j}$ for i > 1 are defined 188 in subsection 4.2. The coarse spaces S_i as well as the projection and prolongation 189operators V_i^{\top} and V_i are defined in subsection 3.2. We suppose that the connectivity 190 graph between the subdomains on each level is sparse. This assumption is not true in 191 general, however, it is valid in structures based on locally constructed coarse spaces 192193 in domain decomposition as we show in this paper, see [18, Section 4.1 p.81] for the case of two levels. 194

2. Background. In this section, we review briefly several theoretical results related to additive Schwarz preconditioners. We introduce them for the sake of completeness.

198 LEMMA 2.1 (fictitious subspace lemma). Let $A \in \mathbb{R}^{n_A \times n_A}, B \in \mathbb{R}^{n_B \times n_B}$ be two

symmetric positive definite matrices. Let \mathscr{R} be an operator defined as 199

$$\mathscr{R}: \mathbb{R}^{n_B} \to \mathbb{R}^{n_A}$$

 $v \mapsto \mathscr{R}v$. 201

and let \mathscr{R}^{\top} be its transpose. Suppose that the following conditions hold: 202

1. The operator \mathscr{R} is surjective. 203

2. There exists $c_u > 0$ such that 204

205
$$(\mathscr{R}v)^{\top} A(\mathscr{R}v) \leqslant c_u v^{\top} B v, \quad \forall v \in \mathbb{R}^{n_B}.$$

3. There exists $c_l > 0$ such that for all $v_{n_A} \in \mathbb{R}^{n_A}, \exists v_{n_B} \in \mathbb{R}^{n_B} | v_{n_A} = \mathscr{R} v_{n_B}$ 206207and

$$c_l v_{n_B}^{\top} B v_{n_B} \leqslant \left(\mathscr{R} v_{n_B} \right)^{\top} A \left(\mathscr{R} v_{n_B} \right) = v_{n_A}^{\top} A v_{n_A}$$

Then, the spectrum of the operator $\mathscr{R}B^{-1}\mathscr{R}^{\top}A$ is contained in the segment $[c_l, c_{\mu}]$. 209

Proof. We refer the reader to [12, Lemma 7.4 p.164] or [28, 27, 13] for a detailed 210 proof. 211

212LEMMA 2.2. The operator $\mathcal{R}_{i,2}$ as defined in (1.2) is surjective.

Proof. The proof follows from the definition of $\mathcal{R}_{i,2}$ (1.2). 213

LEMMA 2.3. Let $k_{i,c}$ for i = 1, ..., L be the minimum number of distinct colors 214 so that $\{span\{R_{i,j}^{\top}\}\}_{1 \leq j \leq N_i}$ of the same color are mutually A_i -orthogonal. Then, we 215have 216217

218
$$\left(\mathscr{R}_{i,2}u_{\mathcal{B}_{i}}\right)^{\top}A_{i}\left(\mathscr{R}_{i,2}u_{\mathcal{B}_{i}}\right)$$

$$\leqslant (k_{i,c}$$
 -

220 221

 $+1)\sum_{i=0}^{N_i} u_j^{\top} \left(R_{i,j} A_i R_{i,j}^{\top} \right) u_j, \quad \forall u_{\mathcal{B}_i} = \left(u_j \right)_{0 \leq j \leq N_i} \in \prod_{j=0}^N \mathbb{R}^{n_{i,j}}.$ 219

We note that at level *i*, the number $k_{i,c}$ is smaller than the maximum number of 2.2.2 neighbors over the set of subdomains $[1; N_i]$ 223

Proof. We refer the reader to [9, Theorem 12 p.93] for a detailed proof.

224
$$k_{i,c} \leqslant \max_{1 \leqslant j \leqslant N_i} \# \mathcal{V}_{i,j}$$

Due to the sparse structure of the connectivity graph between the subdomains at 225level *i*, the maximum number of neighbors over the set of subdomains $[1; N_i]$ is 226227independent of the number of subdomains N_i . Then, so is $k_{i,c}$.

LEMMA 2.4. Let $u_{A_i} \in \mathbb{R}^{n_{A_i}}$ and $u_{\mathcal{B}_i} = \{u_j\}_{0 \leq j \leq N_i} \in \prod_{j=0}^{N_i} \mathbb{R}^{n_{i,j}}$ such that $u_{A_i} = \mathscr{R}_{i,2}u_{\mathcal{B}_i}$. The additive Schwarz operator without any other restriction on the coarse 228 229 230 space S_i verifies the following inequality

231
$$\sum_{j=0}^{N_i} u_j^\top \left(R_{i,j} A_i R_{i,j}^\top \right) u_j \leqslant 2u_{A_i}^\top A_i u_{A_i} + (2k_{i,c}+1) \sum_{j=1}^{N_i} u_j^\top R_{i,j} A_i R_{i,j}^\top u_j,$$

where $k_{i,c}$ is defined in Lemma 2.3. 232

Proof. We refer the reader to [12, Lemma 7.12, p. 175] to view the proof in 233 234detail. Π

LEMMA 2.5. Let $A, B \in \mathbb{R}^{m \times m}$ be two symmetric positive semi-definite matrices. 235Let ker(A), range(A) denote the null space and the range of A respectively. Let P_0 236 be an orthogonal projection on range(A). Let τ be a positive real number. Consider 237the generalized eigenvalue problem, 238

$$P_0 B P_0 u_k = \lambda_k A u_k,$$

$$(u_k, \lambda_k) \in range(A) \times \mathbb{R}$$

Let P_{τ} be an orthogonal projection on the subspace 241

242
$$Z = ker(A) \oplus span\{u_k | \lambda_k > \tau\},$$

then, the following inequality holds: 243

244 (2.1)
$$(u - P_{\tau}u)^{\top} B(u - P_{\tau}u) \leqslant \tau u^{\top} A u, \quad \forall u \in \mathbb{R}^{m}.$$

Proof. We refer the reader to [3, Lemma 2.4] and [12, Lemma 7.7] for a detailed 245246proof.

2.1. GenEO coarse space. In [33, 12] the authors present the GenEO coarse 247 space which relies on defining appropriate symmetric positive semi-definite (SPSD) 248matrices $\tilde{A}_j \in \mathbb{R}^{n \times n}$ for $j = 1, \dots, N$. These are the unassembled Neumann matrices, 249corresponding to the integration on each subdomain of the operator defined in the 250variational form of the PDE. These matrices are local, i.e., $R_{j,\Delta} \hat{A}_j = 0$. Furthermore, 251252they verify the relations

$$u^{\top} A_{j} u \leqslant u^{\top} A u, \quad \forall u \in \mathbb{R}^{n},$$
$$u^{\top} \sum_{i=1}^{N} \tilde{A}_{j} u \leqslant k_{\text{GenEO}} u^{\top} A u, \quad \forall u \in \mathbb{R}^{n},$$

253254

239

$$u^{\top} \sum_{j=1}^{N} \tilde{A}_{j} u \leqslant k_{\text{GenEO}} u^{\top} A u, \quad \forall u \in \mathbb{R}^{n},$$

where $k_{\text{GenEO}} \leq N$ is the maximum number of subdomains that share an unknown. 255

2.2. Local SPSD splitting of an SPD matrix. In [3], the authors present 256the local SPSD splitting of an SPD matrix. Given the permutation matrix \mathcal{P}_j , a local 257SPSD splitting matrix \tilde{A}_j of A associated with subdomain j is defined as 258

259 (2.2)
$$\mathcal{P}_{j}\tilde{A}_{j}\mathcal{P}_{j}^{\top} = \begin{pmatrix} R_{j,I}AR_{j,I}^{\top} & R_{j,I}AR_{j,\Gamma}^{\top} \\ R_{j,\Gamma}AR_{j,I}^{\top} & \tilde{A}_{\Gamma}^{j} \\ & & 0 \end{pmatrix}$$

where $\tilde{A}_{\Gamma}^{j} \in \mathbb{R}^{\gamma_{j} \times \gamma_{j}}$ satisfies the two following conditions: For all $u \in \mathbb{R}^{\gamma_{j}}$, 260

261 •
$$u^{\top} \left(R_{j,\Gamma} A R_{j,I}^{\top} \right) \left(R_{j,I} A R_{j,I}^{\top} \right)^{-1} \left(R_{j,I} A R_{j,\Gamma}^{\top} \right) u \leqslant u^{\top} \tilde{A}_{\gamma}^{j} u$$

$$262 \qquad \bullet \ u^{\top} A_{\Gamma}^{\top} u \leqslant u^{\top} \left(\left(R_{j,\Gamma} A R_{j,\Gamma}^{\top} \right) - \left(R_{j,\Gamma} A R_{j,\Delta}^{\top} \right) \left(R_{j,\Delta} A R_{j,\Delta}^{\top} \right)^{-1} \left(R_{j,\Delta} A R_{j,\Gamma}^{\top} \right) \right) u.$$

The authors prove that the matrices A_i defined in such a way verify the following 263relations: 264

$$265 \quad (2.3) \qquad \qquad R_{j,\Delta} \tilde{A}_j = 0,$$

266 (2.4)
$$u^{\top} \tilde{A}_j u \le u^{\top} A u, \quad \forall u \in \mathbb{R}^n$$

267 (2.5)
$$u^{\top} \sum_{j=1}^{N} \tilde{A}_{j} u \leqslant k u^{\top} A u, \quad \forall u \in \mathbb{R}^{n},$$

\

where k is a number that depends on the local SPSD splitting matrices and can be at most equal to the number of subdomains $k \leq N$. The authors also show that the local matrices defined in GenEO [33, 12] can be seen as a local SPSD splitting.

In [3], the authors highlight that the key idea to construct a coarse space relies on the ability to identify the so-called local SPSD splitting matrices. They present a class of algebraically constructed coarse spaces based on the local SPSD splitting matrices. Moreover, this class can be extended to a larger variety of local SPSD matrices. This extension has the advantage of allowing to construct efficient coarse spaces for a multilevel structure in a practical way. This is discussed in the following section.

3. Extension of the class of coarse spaces. In this section we extend the class of coarse spaces presented in [3]. To do so, we present a class of matrices, that is larger than the class of local SPSD splitting matrices. This will be our main building block in the construction of efficient coarse spaces. Furthermore, this extension can lead to a straightforward construction of hierarchical coarse spaces in a multilevel Schwarz preconditioner setting.

3.1. Extension of the class of local SPSD splitting matrices. Regarding the two-level additive Schwarz method, the authors of [3] introduced the local SPSD splitting related to a subdomain as defined in (2.2). As it can be seen from the theory presented in that paper, it is not necessary to have the exact matrices $R_{j,I}AR_{j,I}^{\top}$, $R_{j,I}AR_{j,\Gamma}^{\top}$, and $R_{j,\Gamma}AR_{j,I}^{\top}$ in the definition of the local SPSD splitting in order to build an efficient coarse space. Indeed, the one and only necessary condition is to define for each subdomain j an SPSD matrix \tilde{A}_{j} for $j = 1, \ldots, N$ such that:

$$R_{j,\Delta}\tilde{A}_{j} = 0,$$

$$u^{\top} \sum_{j=1}^{N} \tilde{A}_{j}u \leqslant ku^{\top}Au, \forall u \in \mathbb{R}^{n},$$

$$u^{\top} \sum_{j=1}^{N} \tilde{A}_{j}u \leqslant ku^{\top}Au, \forall u \in \mathbb{R}^{n},$$

where k is a number that depends on the local SPSD matrices \tilde{A}_j for j = 1, ..., N. The first condition means that \tilde{A}_j has the local SPSD structure associated with subdomain j, i.e., it has the following form:

297
$$\mathcal{P}_{j}\tilde{A}_{j}\mathcal{P}_{j}^{\top} = \begin{pmatrix} \tilde{A}_{I,\Gamma}^{j} & 0\\ 0 & 0 \end{pmatrix},$$

where $\tilde{A}_{I,\Gamma}^{j} \in \mathbb{R}^{n_j \times n_j}$. The second condition is associated with the stable decomposition property [36, 12]. Note that with regard to the local SPSD matrices, the authors in [33] only use these two conditions. That is to say, with matrices that verify conditions (3.1) the construction of the coarse space is straightforward through the theory presented in either [33] or [3]. To this end, we define in the following the local SPSD (LSPSD) matrix associated with subdomain j as well as the associated local filtering subspace that contributes to the coarse space.

DEFINITION 3.1 (local SPSD matrices). An SPSD matrix $\tilde{A}_{i,j} \in \mathbb{R}^{n_i \times n_i}$ is called local SPSD (LSPSD) with respect to subdomain j if

307 •
$$R_{i,j,\Delta}\tilde{A}_{i,j} = 0,$$

308 • $u^{\top}\sum_{j=1}^{N_i}\tilde{A}_{i,j}u \leqslant k_i u^{\top}A_i u,$

309 where $k_i > 0$.

We note that the local SPSD splitting matrices form a subset of the local SPSD matrices.

312 3.2. Multilevel coarse spaces. This section summarizes the steps to be per-313 formed in order to construct the coarse space at level *i* once we have the LSPSD 314 matrices associated with each subdomain at that level.

DEFINITION 3.2 (coarse space based on LSPSD matrices). Let $\tilde{A}_{i,j} \in \mathbb{R}^{n_i \times n_i}$ for $j = 1, \ldots, N_i$ be LSPSD matrices. Let $D_{i,j} \in \mathbb{R}^{n_{i,j}}$ for $j = 1, \ldots, N_i$ be the partition of unity. Let $\tau_i > 0$ be a given number. For a subdomain $j \in [1; N_i]$, let

318
$$G_{i,j} = D_{i,j} \left(R_{i,j} A_i R_{i,j}^{\dagger} \right) D_{i,j}.$$

119 Let $\tilde{P}_{i,j}$ be the projection on range $(R_{i,j}\tilde{A}_jR_{i,j}^{\top})$ parallel to $ker(R_{i,j}\tilde{A}_jR_{i,j}^{\top})$. Let $K_{i,j} = ker(R_{i,j}\tilde{A}_{i,j}R_{i,j}^{\top})$. Consider the generalized eigenvalue problem:

$$\tilde{P}_{i,j}G_{i,j}\tilde{P}_{i,j}u_{i,j,k} = \lambda_{i,j,k}R_{i,j}\tilde{A}_{i,j}R_{i,j}^{\top}u_{i,j,k}$$

 $(u_{i,j,k},\lambda_{i,j,k}) \in range(R_{i,j}\tilde{A}_{i,j}R_{i,j}^{\top}) \times \mathbb{R}.$

323 Set

324 (3.3)
$$Z_{i,j} = K_{i,j} \oplus span\{u_{i,j,k} | \lambda_{i,j,k} > \tau_i\}$$

Then, the coarse space associated with LSPSD matrices $A_{i,j}$ for $j = 1, ..., N_i$ at level i is defined as:

327 (3.4)
$$\mathcal{S}_i = \bigoplus_{j=1}^{N_i} R_{i,j}^\top D_{i,j} Z_{i,j}$$

Following notations from section 1, the columns of V_i span the coarse space S_i . The matrix A_{i+1} is defined as:

330 (3.5)
$$A_{i+1} = V_i^{\top} A_i V_i.$$

The local SPSD splitting matrices at level 1 will play an important role in the construction of the LSPSD matrices at subsequent levels. In the following, we present an efficient approach for computing LSPSD matrices for levels greater than 1.

4. Partitioning for levels strictly greater than 1. In this section, we explain how to obtain the partitioning sets $\Omega_{i,j,I}$ for $(i,j) \in [\![2;L]\!] \times [\![1;N_i]\!]$. Once the sets $\Omega_{i,j,I}$ for $j = 1, \ldots, N_i$ are defined at level *i*, the following elements are readily available: sets $\Gamma_{i,j}, \Delta_{i,j}$, and $\Omega_{i,j}$; restriction operators $R_{i,j,I}, R_{i,j,\Gamma}, R_{i,j,\Delta}$, and $R_{i,j}$; permutation matrices $\mathcal{P}_{i,j}$ for $j = 1, \ldots, N_i$. The partition of unity is constructed in an algebraic way. The *m*th diagonal element of $D_{i,j}$ is 1 if $m \leq n_{i,j,I}$ and 0 otherwise.

4.1. Superdomains as unions of several subdomains. In this section, we 340introduce the notion of a *superdomain*. It refers to the union of several neighboring 341subdomains. Let $\mathcal{G}_{i,1}, \ldots, \mathcal{G}_{i,N_{i+1}}$ be disjoint subsets of $[\![1; N_i]\!]$, where $\bigcup_{j=1}^{N_{i+1}} \mathcal{G}_{i,j} = [\![1; N_i]\!]$. We call the union of the subdomains $\{k \in [\![1; N_i]\!] : k \in \mathcal{G}_{i,j}\}$ superdomain j, 342 343 344 for $j = 1, \ldots, N_{i+1}$. Figure 4.1 gives an example of how to set superdomains. Though this definition of superdomains may look somehow related to the fine mesh, it is in 345346 practice done at the algebraic level, as explained later on. Note that the indices of columns and rows of A_{i+1} are associated with the vectors contributed by the subdo-347 mains at level i in order to build the coarse space S_i , see Figure 4.2. Hence, defining 348 subdomains on the structure of A_{i+1} is natural once we have the subsets $\mathcal{G}_{i,i}$, for 349 $j = 1, \ldots, N_{i+1}.$ 350

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FIG. 4.1. Left: 16 subdomains at level 1. Right: 4 superdomains at level 1. $\mathcal{G}_{1,j} = \llbracket 4(j-1) + 1; 4(j-1) + 4 \rrbracket$.



FIG. 4.2. Illustration of the correspondence of indices between the columns of V_i (left) and the rows and columns of A_{i+1} (right). Having no overlap in V_i is possible through a non-overlapping partition of unity.

4.2. Heritage from superdomains. Let $e_{i,j}$ be the set of indices of the vectors that span $R_{i,j}^{\top}D_{i,j}Z_{i,j}$ in the matrix V_i for some $(i,j) \in [\![1;L-1]\!] \times [\![1;N_i]\!]$, see Figure 4.2. We define $\Omega_{i+1,j,I} = \bigcup_{k \in \mathcal{G}_{i,j}} e_{i,k}$, for $j = 1, \ldots, N_{i+1}$. We denote $\Omega_{i+1,j,\Gamma}$ the subset of $[\![1;n_{i+1}]\!] \setminus \Omega_{i+1,j,I}$ whose elements are at distance 1 from $\Omega_{i+1,j,I}$ through the graph of A_{i+1} . We note that

356
$$\Omega_{i+1,j,\Gamma} \subset \bigcup_{p \in \mathcal{G}_{i,j}} \bigcup_{k \in \mathcal{V}_{i,p}} e_{i,k},$$

where $\mathcal{V}_{i,j}$ represents the set of subdomains that are neighbors of subdomain j at level i for $j = 1, ..., N_i$. The overlapping subdomain j is defined by the set $\Omega_{i+1,j} =$ $[\Omega_{i+1,j,I}, \Omega_{i+1,j,\Gamma}]$. The rest of the sets, restriction, and prolongation operators can be defined as given in section 1.

5. LSPSD matrices for levels strictly greater than 1. In [33, 12, 3], differ-361 362ent methods are suggested to obtain local SPSD splitting matrices at level 1. These matrices are used to construct efficient two-level additive Schwarz preconditioners. 363 Here in this section, we do not discuss the construction of these matrices at level 1. We 364 suppose that we have the local SPSD matrices $A_{1,j} \in \mathbb{R}^{n_1 \times n_1}$ for $j = 1, \ldots, N_1$. We 365 focus on computing LSPSD matrices $\tilde{A}_{i,j} \in \mathbb{R}^{n_i \times n_i}$ for $(i,j) \in [\![2;L]\!] \times [\![1;N_i]\!]$. We also 366 suppose that the coarse space S_1 is available, i.e., the matrices V_1 and $A_2 = V_1^{\top} A_1 V_1$ 367 are known explicitly. 368

PROPOSITION 5.1. Let *i* be a fixed level index, and let $A_{i,j}$ be an LSPSD of A_i , 369 (see Definition 3.1), associated with subdomain j, for $j = 1, \ldots, N_i$. Let $\mathcal{G}_{i,1}, \ldots, \mathcal{G}_{i,N_{i+1}}$ 370 be a set of superdomains at level i associated with the partitioning at level i + 1, see 371 subsection 4.1. Let V_i^{\top} be the restriction matrix to the coarse space at level i. Then, 372 the matrix $A_{i+1,j}$ which is defined as: 373

$$\tilde{A}_{i+1,j} = \sum_{k \in \mathcal{G}_{i,j}} V_i^\top \tilde{A}_{i,k} V_i,$$

satisfies the conditions in Definition 3.1. That is, $\tilde{A}_{i+1,j}$ is LSPSD of A_{i+1} with 375 respect to subdomain j for $j = 1, \ldots, N_{i+1}$. 376

Proof. To prove that $\tilde{A}_{i+1,j}$ is LSPSD of A_{i+1} with respect to subdomain j, we 377 have to prove the following 378

379

• $R_{i+1,j,\Delta}\tilde{A}_{i+1,j} = 0$ • $u^{\top} \sum_{j=1}^{N_{i+1}} \tilde{A}_{i+1,j} u \leq k_{i+1} u^{\top} A_{i+1} u$ for all $u \in \mathbb{R}^{n_{i+1}}$. 380

First, note that $R_{i,k}\tilde{A}_{i,j} = 0$ for all non-neighboring subdomains k of subdomain j. 381 This yields $Z_{i,k}^{\top} D_{i,k} R_{i,k} \tilde{A}_{i,j} = 0$ for these subdomains k. 382

Now, let $m \in [[1; n_{i+1}]] \setminus \Omega_{i+1,j}$. We will show that the *m*th row of $\tilde{A}_{i+1,j}$ is zero. 383 Following the partitioning of subdomains at level i + 1, there exists a subdomain Ω_{p_0} 384 such that the *m*th column of V_i is part of $R_{i,p_0}^{\top} D_{i,p_0} Z_{i,p_0}$. We denote this column vector by v_m . Furthermore, the subdomain p_0 is not a neighbor of any subdomain 385 386 that is a part of the superdomain $\mathcal{G}_{i,j}$. Hence, $v_m^{\top} \tilde{A}_{i,k} = 0$ for $k \in \mathcal{G}_{i,j}$. The *m*th row 387 of $\tilde{A}_{i+1,j}$ is given as $v_m^{\top} \sum_{k \in \mathcal{G}_{i,j}} \tilde{A}_{i,k} V_i$. Then, $v_m^{\top} \sum_{k \in \mathcal{G}_{i,j}} \tilde{A}_{i,k} = 0$, and the *m*th row 388 of $A_{i+1,j}$ is zero. 389

390 To prove the second condition, we have

391
392
$$u^{\top} \sum_{j=1}^{N_{i+1}} \tilde{A}_{i+1,j} u = u^{\top} \sum_{j=1}^{N_{i+1}} \sum_{k \in \mathcal{G}_{i,j}} V_i^{\top} \tilde{A}_{i,k} V_i u.$$

Since $\{\mathcal{G}_{i,j}\}_{1 \le j \le N_{i+1}}$ form a disjoint partitioning of $[1; N_i]$, we can write 393

394
$$u^{\top} \sum_{j=1}^{N_{i+1}} \tilde{A}_{i+1,j} u = u^{\top} \sum_{k=1}^{N_i} V_i^{\top} \tilde{A}_{i,k} V_i u,$$

$$= u^{\top} V_i^{\top} \sum_{k=1}^{N_i} \tilde{A}_{i,k} V_i u.$$

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397 $A_{i,k}$ is an LSPSD matrix of A_i for $k = 1, \ldots, N_i$. Hence, we have

398
$$u^{\top} \sum_{i=1}^{N_{i+1}} \tilde{A}_{i+1,j} u \leqslant k_i u^{\top} V_i^{\top} A_i V_i u,$$

$$\leqslant k_i u^\top A_{i+1} u.$$

401 We finish the proof by setting $k_{i+1} = k_i$.

Figure 5.1 gives an illustration of the LSPSD construction provided by Proposi-402tion 5.1. Figure 5.1 (top left) represents the matrix A_1 . The graph of A_1 is partitioned 403 404 into 16 subdomains. Each subdomain is represented by a different color. Figure 5.1 (top right) represents the matrix V_1 whose column vectors form a basis of the coarse 405space S_1 . Colors of columns of V_1 correspond to those of subdomains in A_1 . Figure 5.1 406 (bottom left) represents the matrix $A_2 = V_1^{\top} A_1 V_1$. Note that column and row indices 407of A_2 are associated with column indices of V_1 . Four subdomains are used at level 2. 408 The partitioning at level 2 is related to the superdomain $\mathcal{G}_{1,j} = \llbracket 4(j-1)+1; 4(j-1)+4 \rrbracket$ 409for j = 1, ..., 4. Figure 5.1 (bottom right) represents an LSPSD matrix of A_2 with 410 respect to subdomain 1 at level 2. 411

Theorem 5.2 shows that the third condition of the fictitious subspace lemma Lemma 2.1 holds at level i for i = 1, ..., L.

414 THEOREM 5.2. Let $A_{i,j}$ be an LSPSD of A_i associated with subdomain j, for $(i,j) \in [\![1;L]\!] \times [\![1;N_i]\!]$. Let $\tau_i > 0$, $Z_{i,j}$ be the subspace associated with $\tilde{A}_{i,j}$, and $P_{i,j}$ be the projection on $Z_{i,j}$ as defined in Lemma 2.5. Let $u_i \in \mathbb{R}^{n_i}$ and let $u_{i,j} =$ $(D_{i,j} (I_{n_{i,j}} - P_{i,j}) R_{i,j}u_i)$ for $(i,j) \in [\![1;L]\!] \times [\![1;N_i]\!]$. Let $u_{i,0}$ be defined as,

418
$$u_{i,0} = \left(V_i^{\top} V_i\right)^{-1} V_i^{\top} \left(\sum_{j=1}^{N_i} R_{i,j}^{\top} D_{i,j} P_{i,j} R_{i,j} u_i\right).$$

419 Let $m_i = (2 + (2k_{i,c} + 1)k_i\tau_i)^{-1}$. Then,

420
$$u_i = \sum_{i=0}^{N_i} R_{i,j}^{\top} u_{i,j},$$

421 and

422 (5.1)
$$m_i \sum_{j=0}^{N_i} u_{i,j}^{\top} R_{i,j} A_i R_{i,j}^{\top} u_{i,j} \leqslant u_i^{\top} A_i u_i.$$

423 *Proof.* We have

424
$$\sum_{j=0}^{N_i} R_{i,j}^{\top} u_{i,j} = V_i \left(V_i^{\top} V_i \right)^{-1} V_i^{\top} \left(\sum_{j=1}^{N_i} R_{i,j}^{\top} D_{i,j} P_{i,j} R_{i,j} u_i \right) + \sum_{j=1}^{N_i} R_{i,j}^{\top} u_{i,j}$$

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FIG. 5.1. Illustration of the LSPSD construction provided by Proposition 5.1. Top left: the matrix A_1 , top right: V_1 , bottom left: the matrix $A_2 = V_1^{\top} A_1 V_1$, bottom right: $\tilde{A}_{2,1} = \sum_{j \in \mathcal{G}_{1,1}} V_1^{\top} \tilde{A}_{1,j} V_1$, where $\mathcal{G}_{1,1} = 1, \ldots, 4$

Since for all $y \in S_i$, $V_i \left(V_i^\top V_i \right)^{-1} V_i^\top y = y$, we have 426

427
$$\sum_{j=0}^{N_{i}} R_{i,j}^{\top} u_{i,j} = \sum_{j=1}^{N_{i}} R_{i,j}^{\top} D_{i,j} P_{i,j} R_{i,j} u_{i} + \sum_{j=1}^{N_{i}} R_{i,j}^{\top} \left(D_{i,j} \left(I_{n_{i,j}} - P_{i,j} \right) R_{i,j} u_{i} \right)$$
428
$$= \sum_{j=1}^{N_{i}} R_{i,j}^{\top} D_{i,j} R_{i,j} u_{i},$$

To prove the inequality (5.1), we start with the inequality from Lemma 2.4. We 431432have

433 (5.2)
$$\sum_{j=0}^{N_i} u_{i,j}^{\top} R_{i,j} A_i R_{i,j}^{\top} u_{i,j} \leqslant 2u_i^{\top} A_i u_i + (2k_{i,c}+1) \sum_{j=1}^{N_i} u_{i,j}^{\top} R_{i,j} A_i R_{i,j}^{\top} u_{i,j},$$

435where we chose $u_{\mathcal{B}_i}$ in Lemma 2.4 to be $(u_{i,j})_{j=0,\ldots,N_i}$ and $u_{A_i} = u_i$. In Definition 3.2,

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436 we defined $Z_{i,j}$, such that for all $w \in \mathbb{R}^{n_{i,j}}$ we have

$$\overset{437}{_{438}} \qquad \left(\left(I_{n_{i,j}} - P_{i,j} \right) w \right)^{\top} \left(D_{i,j} R_{i,j} A_i R_{i,j}^{\top} D_{i,j} \right) \left(\left(I_{n_{i,j}} - P_{i,j} \right) w \right) \leqslant \tau_i w^{\top} \left(R_{i,j} \tilde{A}_{i,j} R_{i,j}^{\top} \right) w$$

439 Hence, in the special case $w = R_{i,j}u_i$, we can write

14

441
$$((I_{n_{i,j}} - P_{i,j})R_{i,j}u_i)^{\top} (D_{i,j}R_{i,j}A_iR_{i,j}^{\top}D_{i,j}) ((I_{n_{i,j}} - P_{i,j})R_{i,j}u_i)$$

442
443 $\leq \tau_i (R_{i,j}u_i)^{\top} (R_{i,j}\tilde{A}_{i,j}R_{i,j}^{\top}) (R_{i,j}u_i).$

444 Equivalently,

445
$$u_{i,j}^{\top} R_{i,j} A_i R_{i,j}^{\top} u_{i,j} \leqslant \tau_i (R_{i,j} u_i)^{\top} R_{i,j} \tilde{A}_{i,j} R_{i,j}^{\top} (R_{i,j} u_i).$$

447 Plugging this inequality in (5.2) gives

448
$$\sum_{j=0}^{N_i} u_{i,j}^{\top} R_{i,j} A_i R_{i,j}^{\top} u_{i,j} \leqslant 2u_i^{\top} A_i u_i + (2k_{i,c}+1) \tau_i \sum_{j=1}^{N_i} (R_{i,j} u_i)^{\top} R_{i,j} \tilde{A}_{i,j} R_{i,j}^{\top} (R_{i,j} u_i).$$

450 Since $\tilde{A}_{i,j}$ is local, we have

451
$$(R_{i,j}u_i)^{\top}R_{i,j}\tilde{A}_{i,j}R_{i,j}^{\top}(R_{i,j}u_i) = u_i^{\top}\tilde{A}_{i,j}u_i, \text{ for } j = 1, \dots, N_i.$$

452 By using the fact that $\hat{A}_{i,j}$ is LSPSD of A_i for $j = 1, \ldots, N_i$, we obtain the following:

453
454
$$\sum_{j=0}^{N_i} u_{i,j}^{\top} R_{i,j} A_i R_{i,j}^{\top} u_{i,j} \leqslant 2u_i^{\top} A_i u_i + (2k_{i,c}+1) k_i \tau_i u_i^{\top} A_i u_i.$$

455 Multiplying both sides with m_i ends the proof, i.e.,

$$m_i \sum_{j=0}^{N_i} u_{i,j}^{\top} R_{i,j} A_i R_{i,j}^{\top} u_{i,j} \leqslant u_i^{\top} A_i u_i. \qquad \square$$

In [3], the authors presented the minimal subspace that replaces $Z_{i,j}$ (defined in (3.3) 458and used in Theorem 5.2) that is required to prove Theorem 5.2. The main difference 459with respect to the subspace that we define in (3.3) is that it is not necessary to include 460the entire kernel of the LSPSD matrix, $K_{i,j}$, in $Z_{i,j}$, see Definition 3.2. Nevertheless, 461in this work, we include the entire kernel of the LSPSD matrix in the definition of 462 $Z_{i,j}$. This allows us to ensure that the kernels of Neumann matrices are transferred 463 across the levels, see Theorem 5.4. And in addition, this corresponds to the definition 464used in GenEO [12, Lemma 7.7] and to its implementation in the HPDDM library 465[19]466

467 Theorem 5.3 provides an upper bound on the condition number of the precondi-468 tioned matrix $M_i^{-1}A_i$ for i = 1, ..., L.

469 THEOREM 5.3. Let M_i be the additive Schwarz preconditioner at level *i* combined 470 with the coarse space correction induced by S_i defined in (3.4). The following inequality 471 holds,

472
$$\kappa \left(M_i^{-1} A_i \right) \leqslant (k_{i,c} + 1) \left(2 + (2k_{i,c} + 1)k_i \tau_i \right).$$

473 *Proof.* Lemma 2.2, Lemma 2.3, and Theorem 5.2 prove that the multilevel precon-474 ditioner verifies the conditions in Lemma 2.1 at each level *i*. Hence, the spectrum of the

475 preconditioned matrix $M_i^{-1}A_i$ is contained in the interval $\left[\left(2 + \left(2k_{i,c} + 1\right)k_i\tau_i\right)^{-1}, k_{i,c} + 1\right)k_i\tau_i\right]$

476 1]. Equivalently, the condition number of the preconditioned matrix at level *i* verifies

477 the following inequality

478

504

505

$$\kappa \left(M_i^{-1} A_i \right) \leqslant (k_{i,c} + 1) \left(2 + (2k_{i,c} + 1)k_i \tau_i \right).$$

Proposition 5.1 shows that the constant k_i associated with the LSPSD matrices at level *i* is independent of the number of levels and bounded by the number of subdomains at level 1. Indeed,

 $\ldots, L.$

$$k_1 \ge k_i \text{ for } i = 2,.$$

Furthermore, in the case where the LSPSD matrices at the first level are the Neumann matrices, k_i is bounded by the maximum number of subdomains at level 1 that share an unknown.

The constant $k_{i,c}$ for i = 1, ..., L is the minimum number of distinct colors so that $\{span\{R_{i,j}^{\top}\}\}_{1 \leq j \leq N_i}$ of the same color are mutually A_i -orthogonal. Both constants k_i and $k_{i,c}$ are independent of the number of subdomains for each level i.

The constant τ_i can be chosen such that the condition number of the preconditioned system at level *i* is upper bounded by a prescribed value. Hence, this allows to have a robust convergence of the preconditioned Krylov solver at each level.

492Algorithm 5.1 presents the construction of the multilevel additive Schwarz method by using GenEO. The algorithm iterates over the levels. At each level, three main 493operations are performed. First, the construction of the LSPSD matrices. At level 1, 494 the LSPSD matrices are the Neumann matrices, otherwise, Proposition 5.1 is used 495to compute them. Once the LSPSD matrix is available, the generalized eigenvalue 496497 problem in (3.2) has to be solved concurrently. Given the prescribed upper bound on the condition number, $Z_{i,j}$ can be set. Finally, the coarse space is available and the 498coarse matrix is assembled. 499

500 The following Theorem 5.4, describes how the kernel of Neumann matrices are 501 transferred across the levels.

THEOREM 5.4. Suppose that $\tilde{A}_{1,j}$ is the Neumann matrix associated with the subdomain $\Omega_{1,j}$ for $j \in [\![1; N_1]\!]$. For $(i, j) \in [\![2; L]\!] \times [\![1; N_i]\!]$, let

- $\tilde{A}_{i,j}$ be the LSPSD matrices associated with $A_{i,j}$ defined in Proposition 5.1,
 - $\mathcal{G}_{i-1,j}$ be the corresponding superdomains,
- 506 $\mathcal{G}_{i-1,j}^1$ be the union of subdomains at level 1 which contribute hierarchically 507 to obtain $\mathcal{G}_{i-1,j}$,
- 508 $\tilde{A}_{\mathcal{G}_{i-1,j}}$ be the Neumann matrix associated with $\mathcal{G}_{i-1,j}^1$ (seeing $\mathcal{G}_{i-1,j}^1$ as a subdomain),
- 510 $A_{\mathcal{G}_{i-1,j}}$ be the restriction of A to the subdomain $\mathcal{G}_{i-1,j}^1$.

511 Then, the kernel of $\tilde{A}_{\mathcal{G}_{i-1,j}}$ is included in the kernel of $\left(\prod_{l=1}^{i-1} V_l\right) \tilde{A}_{i,j} \left(\prod_{l=1}^{i-1} V_l\right)^{\top}$.

Proof. First, note that for any LSPSD matrix computed as in Proposition 5.1, we have

$$\left(\prod_{l=1}^{i-1} V_l\right) \tilde{A}_{i,j} \left(\prod_{l=1}^{i-1} V_l\right)^{\top} = \left(\prod_{l=1}^{i-1} V_l\right) \left(\prod_{l=1}^{i-1} V_l\right)^{\top} \sum_{k \in \mathcal{G}_{i,j}^1} \tilde{A}_{1,k} \left(\prod_{l=1}^{i-1} V_l\right) \left(\prod_{l=1}^{i-1} V_l\right)^{\top}.$$

Algorithm 5.1 Multilevel GenEO

Require: $A_1 = A \in \mathbb{R}^{n \times n}$ SPD, L + 1 number of levels, N_i number of subdomains at each level, $\mathcal{G}_{i,j}$ sets of superdomains

Ensure: preconditioner at each level *i*, M_i^{-1} with bounded condition number of $M_i^{-1}A_i$

1: for i = 1, ..., L do

2: for each subdomain $j = 1, \ldots, N_i$ do

3: $A_{i,j} = R_{i,j}A_i R_{i,j}^{\top}$ (local matrix associated with subdomain j)

4: if i = 1 then

5: local SPSD $A_{i,j}$ is Neumann matrix of subdomain j

6: **else**

7: compute local SPSD matrix as

$$\tilde{A}_{i,j} = \sum_{k \in \mathcal{G}_{i,j}} V_{i-1}^{\top} \tilde{A}_{i-1,k} V_{i-1}$$

8: end if 9: solve the generalized eigenvalue problem (3.2), set $Z_{i,j}$ as in (3.3) 10: end for 11: $S_i = \bigoplus_{j=1}^{N_i} D_{i,j} R_{i,j}^\top Z_{i,j}, V_i$ basis of S_i 12: coarse matrix $A_{i+1} = V_i^\top A_i V_i, A_{i+1} \in \mathbb{R}^{n_{i+1} \times n_{i+1}}$ 13: end for 14: $M_i^{-1} = V_i A_{i+1}^{-1} V_i^\top + \sum_{j=1}^{N_i} R_{i,j}^\top A_{i,j}^{-1} R_{i,j}$

Moreover, due to the fact that $\hat{A}_{\mathcal{G}_{i-1,j}}$ and $\hat{A}_{1,k}$ are Neumann matrices, we have

$$u^{\top} \tilde{A}_{\mathcal{G}_{i-1,j}} u \leqslant u^{\top} \sum_{k \in \mathcal{G}_{i,j}^1} \tilde{A}_{1,k} u \leqslant k_1 u^{\top} \tilde{A}_{\mathcal{G}_{i-1,j}} u.$$

On one hand, the kernels of $\tilde{A}_{1,k}$ for $k \in \mathcal{G}_{i,j}^1$ are included, by construction, in the image of V_1 , see Definition 3.2. So is their intersection which is the kernel of $\sum_{k \in \mathcal{G}_{i,j}^1} \tilde{A}_{1,k}$. On the other hand, the previous two-sided inequality implies that the kernels of $\tilde{A}_{\mathcal{G}_{i-1,j}}$ and $\sum_{k \in \mathcal{G}_{i,j}^1} \tilde{A}_{1,k}$ are identical. Hence, the kernel of $\tilde{A}_{\mathcal{G}_{i-1,j}}$ is included in the image of QQ^{\top} , where $Q = \left(\prod_{l=1}^{i-1} V_l\right)$.

Theorem 5.4 proves that the kernel of the Neumann matrix of a union of subdomains at level 1 that hierarchically contribute to form a subdomain at level i is conserved by the construction of the hierarchical coarse spaces. For example in the case of linear elasticity, it is essential to include the rigid body motions in the coarse space in order to have a fast convergence. As these are included in the kernel of the Neumann matrix of the subdomain, the hierarchical coarse space includes them, consequently.

6. Numerical experiments. In this section, the developed theory is validated numerically with FreeFEM [14] for finite element discretizations and HPDDM [19] for domain decomposition methods. We present numerical experiments on two highly challenging problems illustrating the efficiency and practical usage of the proposed method. For both problems, we use $N_1 = 2,048$ MPI processes (equal to the number of subdomains at level 1), and the domain partitioning is performed using ParMETIS [22], with no control on the alignments of subdomain interfaces. We compare the two-level GenEO preconditioner and its multilevel extension by varying N_2 between 4 and 256. For the two-level method, N_2 corresponds to the number of MPI processes that solve the coarse problem in a distributed fashion using MKL CPARDISO [17]. For the multilevel method, N_3 is set to 1, i.e., a three-level method is used. The goal of these numerical experiments is to show that when one switches from a two-level method with an exact coarse solver, to our proposed multilevel method, the number of outer iterations is not impacted. Thus, three levels are sufficient. As an outer solver, since all levels but the coarsest are solved approximately, the flexible GMRES [31] is used. It is stopped when relative unpreconditioned residuals are lower than

537 [31] is used. It is stopped when relative unpreconditioned residuals are lower than 538 10⁻⁶. Subdomain matrices $\{A_{i,j}\}_{1 \leq i \leq 2, 1 \leq j \leq N_i}$ are factorized concurrently using MKL PARDISO, and eigenvalue problems are solved using ARPACK [24]. In both, two-540and three-level GenEO, we factorize the local matrices $A_{1,j}$ for $j \in [1; N_1]$ and solve 541the generalized eigenvalue problems concurrently at the first level. For this reason, we do not take into account the time needed for these two steps which are performed 543 544without any communication between MPI processes. We compare the time needed to assemble and factorize A_2 in the two-level approach against the time needed to 545assemble A_2 and local SPSD matrices $\tilde{A}_{2,j}$ for $j \in [1; N_2]$, solve the generalized 546eigenvalue problems concurrently on the second level, assemble, and factorize the 547 matrix A_3 in the three-level approach. We also compare the time spent in the outer 548Krylov solver during the solution phase. Readers interested by a comparison of the 549efficiency of GenEO and multigrid methods such as GAMG [1] are referred to [18]. FreeFEM scripts used to produce the following results are available at the following 551 URL: https://github.com/prj-/aldaas2019multi¹.

553 **6.1. Diffusion test cases.** The scalar diffusion equation with highly heteroge-554 neous coefficient κ is solved in $[0,1]^d$ (d = 2 or 3). The strong formulation of the 555 equation is:

$$\begin{aligned}
-\nabla \cdot (\kappa \nabla u) &= 1 & \text{in } \Omega, \\
556 & u &= 0 & \text{on } \Gamma_D, \\
557 & \frac{\partial u}{\partial n} &= 0 & \text{on } \Gamma_N.
\end{aligned}$$

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558The exterior normal vector to the boundary of Ω is denoted n. Γ_D is the subset 559of the boundary of Ω corresponding to x = 0 in 2D and 3D. Γ_N is defined as the complementary of Γ_D with respect to the boundary of Ω . We discretize the equation 560 using \mathbb{P}_2 and \mathbb{P}_4 finite elements in the 3D and 2D test cases, respectively. The number 561of unknowns is 441×10^6 and 784×10^6 , with approximately 28 and 24 nonzero 562elements per row in the 3D and 2D cases, respectively. The heterogeneity is due 563 to the jumps in the diffusion coefficient κ , see Figure 6.1, which is modeled using 564a combination of jumps and channels, cf. the file coefficients.idp from https: 565//github.com/prj-/aldaas2019multi. 566

The results in two dimensions are reported in Table 6.1. The number of outer iterations for both two- and three-level GenEO is 32. The size of the level 2 operator is $n_2 = 25 \times 2,048 = 51,200$. In all numerical results, the number of eigenvectors per subdomain, here 25, is fixed. This is because ARPACK cannot a priori compute all eigenpairs below a certain threshold, and an upper bound has to be provided instead.

¹note to reviewers: the repository is now public



FIG. 6.1. Variation of the coefficient κ used for the diffusion test case

HPDDM is capable of filtering the eigenpairs for which eigenvalues are above the userspecified GenEO threshold from Lemma 2.5. However, this means that the coarse 573operator may be unevenly distributed. With a fixed number of eigenvectors per sub-574domain, it is possible to use highly optimized uniform MPI routines and block matrix 575576 formats. Hence, for performance reasons, all eigenvectors computed by ARPACK are 577 kept when building coarse operators. It is striking that the multilevel method does not deteriorate the numerical performance of the outer solver. For the two-level method, 578the first column corresponds to the time needed to assemble the Galerkin operator A_2 from (3.5) (assuming V_1 has already been computed by ARPACK), and to factorize it 580 using N_2 MPI processes. For the three-level method, the first column corresponds to 581the time needed to assemble level 2 local subdomain matrices $\{A_{2,j}\}_{1 \leq j \leq N_2}$, level 2 582 local SPSD matrices, solve the generalized eigenvalue problem (3.2) concurrently, as-583 semble the Galerkin operator A_3 and factorize it on a single process. The size of 584the level 3 operator is $n_3 = 20 \times N_2$. For both two- and three-level methods, the 585 second column is the time spent in the outer Krylov solver once the preconditioner 586has been set up. In the last column of the three-level method, the number of inner 587 iterations for solving systems involving A_2 , which is not inverted exactly anymore, 588 is reported. For all tables, this column is an average over all successive outer itera-589tions. Another important numerical property of our method is that, thanks to fully 590 591 controlled bounds at each level, the number of inner iterations is low, independently of the number of superdomains N_2 . Because this problem is not large enough, it is still tractable by a two-level method, for which HPDDM was highly optimized for. 593 Thus, there is no performance gain to be expected at this scale. However, one can 594notice that the construction of the coarse operator(s) scales nicely with N_2 for the 596 three-level method, whereas the performance of the direct solver MKL CPARDISO quickly stagnates because of the finer and finer parallel workload granularity. 597

The results in three dimensions are reported in Table 6.2. The number of outer iterations for both the two- and three-level GenEO is 19. The observations made in two dimensions still hold, and the dimensions of A_2 and A_3 are the same. Once again, it is important to note that the number of outer iterations is the same for both methods.

	two-level GenEO			three-level GenEO			
N_2	CS	solve	$\%$ of nnz A_2	CS	solve	inner it.	% of nnz A_3
4	2.4	11.9	0.19	6.5	27.4	14	56.0
16	1.8	11.3		3.6	15.4	15	19.0
64	1.9	12.1		3.0	16.7	14	5.5
256	2.4	18.4		2.8	13.9	13	1.4

TABLE 6.1 Diffusion 2D test case, comparison between two- and three-level GenEO. The percentage of nonzero entries in A_1 is 0.3%.

	two-level GenEO			three-level GenEO			
N_2	CS	solve	$\%$ of nnz A_2	CS	solve	inner it.	$\%$ of nnz A_3
4	7.0	20.9	0.36	16.9	43.6	17	62.0
16	5.0	19.8		7.7	26.7	17	28.0
64	5.1	20.1		5.8	32.7	15	8.9
256	5.2	24.1		5.3	22.6	14	2.6

TABLE 6.2 Diffusion 3D test case, comparison between two- and three-level GenEO. The percentage of nonzero entries in A_1 is 0.5%.

603 **6.2. Linear elasticity test cases.** The system of linear elasticity with highly 604 heterogeneous elastic moduli is solved in 2D and 3D. The strong formulation of the 605 equation is given as:

606 (6.1)
$$\operatorname{div} \sigma(u) + f = 0 \quad \text{in } \Omega,$$
$$u = 0 \quad \text{on } \Gamma_D,$$

 $\sigma(u) \cdot n = 0 \quad \text{on } \Gamma_N.$

The physical domain Ω is a beam of dimensions $[0, 10] \times [0, 1]$, extruded for $z \in [0, 1]$ in 3D. The Cauchy stress tensor $\sigma(\cdot)$ is given by Hooke's law: it can be expressed in terms of Young's modulus E and Poisson's ratio ν .

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$$\sigma_{ij}(u) = \begin{cases} 2\mu\varepsilon_{ij}(u) & i \neq j\\ 2\mu\varepsilon_{ii}(u) + \lambda \operatorname{div}(u) & i = j \end{cases}$$

612 where

613
$$\varepsilon_{ij}(u) = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_i} + \frac{\partial u_j}{\partial x_j} \right), \mu = \frac{E}{2(1+\nu)}, \text{ and } \lambda = \frac{E\nu}{1-2\nu}.$$

The exterior normal vector to the boundary of Ω is denoted *n*. Γ_D is the subset 614 of the boundary of Ω corresponding to x = 0 in 2D and 3D. Γ_N is defined as the 615complementary of Γ_D with respect to the boundary of Ω . We discretize (6.1) using 616 the following vectorial finite elements: $(\mathbb{P}_2, \mathbb{P}_2, \mathbb{P}_2)$ in 3D and $(\mathbb{P}_3, \mathbb{P}_3)$ in 2D. The 617 number of unknowns is 146×10^6 and 847×10^6 , with approximately 82 and 34 618 nonzero elements per row in the 3D and 2D cases, respectively. The heterogeneity is 619 due to the jumps in E and ν . We consider discontinuous piecewise constant values 620 for E and ν : $(E_1, \nu_1) = (2 \times 10^{11}, 0.25), (E_2, \nu_2) = (10^7, 0.45)$, see Figure 6.2. 621

Results in two (resp. three) dimensions are reported in Table 6.3 (resp. Table 6.4). The number of outer iterations are 73 and 45 respectively. For these test cases, we



FIG. 6.2. Variation of the structure coefficients used for the elasticity test case

	two-level GenEO			three-level GenEO				
N_2	CS	solve	$\%$ of nnz A_2	CS	solve	inner it.	$\%$ of nnz A_3	
4	4.8	52.7	0.18	22.5	179.3	31	43.0	
16	3.9	50.3		9.3	124.9	57	17.0	
64	4.0	53.1		7.2	71.5	34	4.9	
256	4.8	63.2		6.8	71.2	44	1.4	

TABLE 6.3 Elasticity 2D test case, comparison between two- and three-level GenEO. The percentage of nonzero entries in A_1 is 0.4%.

slightly relaxed the criterion for selecting eigenvectors in coarse spaces, which explains 624 why the iteration counts increase. However, the same observations as for the diffusion 625test cases still hold. The dimension of the level 2 matrix is $n_2 = 50 \times 2,048 = 1.02 \cdot 10^5$, 626 while for the level 3 matrix it is $n_3 = 20 \times N_2$. This means that 50 (resp. 20) 627 eigenvectors are kept per level 1 (resp. level 2) subdomains. We observe that the 628 number of iterations of the inner solver increases slowly when increasing the number 629 of subdomains from 4 to 256 in the 2D case and remains almost constant in the 3D 630 case. In terms of runtime, the two-level GenEO is faster than three-level GenEO for 631 these matrices of medium dimensions. 632

To show the potential of our method at larger scales, a three-dimensional linear 633 elasticity problem of size 593×10^6 is now solved on $N_1 = 16,384$ processes and 634 $N_2 = 256$ superdomains. With the two-level method, A_2 is assembled and factorized 635 in 40.8 seconds. With the three-level method, this step now takes 35.1 seconds, see 636 637 Table 6.5. There is a two iterations difference in the iteration count. Not taking into account the preconditioner setup, the problem is solved in 222.5 seconds in the 638 639 two-level case and 90.1 seconds in the multilevel case. In this test case the cost of applying the two-level preconditioner on a given vector is approximately twice the cost 640 of applying the multilevel variant. At this regime, it is clear that there are important 641 gains for the solution phase. At even greater scales, gains for the setup phase are 642643 also expected. Moreover, another interesting fact to note regarding computation time is that the generalized eigenvalue problems solved concurrently at the first level to 644obtain V_1 actually represents a significant part of the total time of 377.6 seconds (resp. 645 244.8 seconds) with the two- (resp. three-)level method: 78.2 seconds. This cost can 646be reduced by taking a larger number of (smaller) subdomains, with the drawback of 647 increasing the size of V_1 and thus A_2 . This drawback represents a clear bottleneck 648 for the two-level method but is alleviated by using the three-level method, making it 649 a good candidate for problems at greater scales. 650

7. Conclusion. In this paper, we reviewed general properties of overlapping Schwarz preconditioners and presented a framework for its multilevel extension. We

	two-level GenEO			three-level GenEO			
N_2	CS	solve	$\%$ of nnz A_2	CS	solve	inner it.	% of nnz A_3
4	28.5	46.9	0.38	78.9	296.7	23	43.0
16	17.3	35.4		24.5	124.5	23	19.0
64	15.0	33.2		15.4	62.2	21	7.9
256	13.6	40.7		10.6	50.7	23	2.5

TABLE 6.4 Elasticity 3D test case, comparison between two- and three-level GenEO. The percentage of nonzero entries in A_1 is 3.3%.

	two-lev	vel GenEO	three-level GenEO				
N_2	CS	solve	CS	solve	inner it.		
256	40.8	222.5	35.1	90.1	11		
TABLE 6.5							

Elasticity 3D test case, comparison between two- and three-level GenEO

generalized the local SPSD splitting presented in [3] to cover a larger set of matrices 653 654 leading to more flexibility for building robust coarse spaces. Based on local SPSD matrices on the first level, we presented how to compute local SPSD matrices for 655 coarser levels. The multilevel solver based on hierarchical local SPSD matrices is 656 robust and guarantees a bound on the condition number of the preconditioned matrix 657 at each level depending on predefined values. Numerical experiments illustrate the 658 theory and prove the efficiency of the method on challenging problems of large size 659 arising from heterogeneous linear elasticity and diffusion problems with jumps in the 660 661 coefficients of multiple orders of magnitude.

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