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RICAM-Report 2016-20

A UNIFIED FRAMEWORK FOR ADAPTIVE BDDC

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Abstract. In this theoretical study, we explore how to automate the selection of weights and primal constraints in BDDC methods for general SPD problems. In particular, we address the three-dimensional case and non-diagonal weight matrices, such as the deluxe scaling. We provide an overview of existing approaches, show connections between them, and present new theoretical results: A localization of the global BDDC estimate leads to a reliable condition number bound and to a local generalized eigenproblem on each *glob*, i.e., each subdomain face, edge, and possibly vertex. We discuss how the eigenvectors corresponding to the smallest eigenvalues can be turned into generalized primal constraints. These can be either treated as they are, or (which is much simpler to implement) be enforced by (possibly stronger) classical primal constraints. We show that the second option is the better one. Furthermore, we discuss equivalent versions of the face and edge eigenproblem which match with previous works and show an optimality property of the deluxe scaling. Lastly, we give a localized algorithm which guarantees the definiteness of the matrix $\widetilde{S}$ underlying the BDDC preconditioner under mild assumptions on the subdomain matrices.

1. Introduction

The method of *balancing domain decomposition by constraints* (BDDC) (see [18, 33] for closely related methods) is, together with the *dual-primal finite element tearing and interconnecting* (FETI-DP) method [32], among the most advanced non-overlapping domain decomposition methods for partial differential equations. The two methods can be considered as dual to each other, and for symmetric positive definite problems, the corresponding preconditioned operators have identical spectrum (up to values of one and zero) [72, 69, 74, 10].

For a variety of PDEs discretized by the finite element method, a poly-logarithmic bound $C(1+\log(H/h))^2$ of the spectral condition number of the preconditioned system has been established, where H/h is the maximal ratio of subdomain diameter and element size. Covered cases are scalar diffusion problems [78, 59, 71, 55], linear elasticity [58], Stokes flow [68, 44], almost incompressible elasticity [56, 87, 35], Reissner-Mindlin plates [66], as well as positive definite problems in $H(\text{curl})$ [23, 16, 12, 114] and $H(\text{div})$ [84, 85]. The same kind of bound has been obtained for spectral elements [86], boundary elements [88, 89], mortar methods [40, 41], discontinuous Galerkin [27, 14, 16, 28, 99], and isogeometric analysis [5, 7, 60, 63, 6]. Without giving a list of further references,

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we note that BDDC and FETI-DP were successfully applied to many more problems, mostly of a mechanical type. Preconditioners based on Schur complement approximation similar to BDDC were recently proposed by Kraus et al. [61] and Schöberl [98].

The constant C in the bound is usually independent of subdomain diameters and mesh sizes and thus also of the number of subdomains, which is necessary for scalability. Ideally, C is also independent of problem parameters, typically coefficient jumps [59, 92, 35], coefficient ratios [23], or geometry details [55, 12]. As shown in [59, 72, 74], at least for SPD problems, part of the analysis is problem-independent, and the condition number estimate reduces to a single norm estimate of a projection operator (P_D). For a given decomposition into subdomains, this estimate is influenced by two sources: (i) the weights/scalings and (ii) the primal constraints.

(i) Several scalings have been used in the literature. The *multiplicity scaling* is not robust for coefficient jumps. A coefficient-dependent scaling, sometimes called ρ-scaling, based on constant values per vertex/edge/face leads to robustness for coefficient jumps between subdomains. The *stiffness scaling* takes more information into account and may look promising, but can lead to very high condition numbers in the case of irregular meshes [55] or mildly varying coefficients [94, 89]. A trade off "between" the latter two for jumps along interfaces has been proposed in [94, 89], see also [90]. All the scalings above involve diagonal weight matrices. The *deluxe scaling* introduced in [22] (for early experiments see also [21]) breaks with this rule as the weights are dense matrices per subdomain face/edge/vertex. For subdomain faces, it was observed several times, that the deluxe scaling can lead to very good results [23, 84, 7, 16, 66, 50]. Computationally *economic* versions are discussed in [23, 49].

(ii) The selection of good primal constraints is not an easy task either. On the one hand, choosing too few constraints leads to poor performance of the preconditioner [107, Algorithm A]. On the other hand, choosing too many constraints results in a large coarse problem, which leads to a computationally inefficient method. Although large coarse problems can be alleviated using multiple levels [109, 108, 75, 102], it is better to keep the coarse problem size at a necessary minimum. For scalar diffusion and linear elasticity with coefficients that are constant in each subdomain, good selection algorithms are available, see [107] as well as [100] and the references therein. For hard problems with varying coefficients or coefficient jumps along subdomain interfaces, these recipes may happen to work but can also easily lead to poor performance [64, 53, 29, 92] (see [93, 94, 90] for the classical FETI method). This has led to *problem-adapted* algorithms for choosing primal constraints, called *adaptive BDDC/FETI-DP*, which we discuss in the following. Although the adaptive choice means more computational work, this can pay off in highly parallel regimes, where local operations are expected to be comparably cheap [47, 116, 117].

Mandel and Sousedík [73] were the first to investigate, for general diagonal scalings, the influence of primal constraints under quite general assumptions on SPD problems and in an algebraic framework. They came up with a *condition number indicator* which is based on a local estimate per closed face $\overline{F}$, reading

$$\textstyle\sum_{i\in\mathcal{N}_F} |\Xi_{i\overline{F}}(P_D w)_i|^2_{S_i} \le \omega_{\overline{F}} \sum_{i\in\mathcal{N}_F} |w_i|^2_{S_i}\,. \tag{1}$$

Here $\mathcal{N}_F$ is the set of subdomains shared by face F, $\Xi_{i\overline{F}}$ extracts the degrees of freedom on $\overline{F}$, and $|\cdot|_{S_i}$ is the subdomain (semi)norm. The best constant $\omega_{\overline{F}}$ is the maximal eigenvalue of an associated generalized eigenproblem and as such computable. The maximum of all indicators $\omega_{\overline{F}}$ turned out to be quite reliable for some practical applications. The eigenvectors corresponding to the largest eigenvalues can also be used to create new, *adaptive* constraints in order to enhance the condition number. Together with Šístek, this approach was extended to three-dimensional problems [76, 102].

The idea of replacing difficult local estimates by local generalized eigenproblems has been used before, e.g., in smoothed aggregation multigrid [11], balancing Neumann-Neumann methods [9], or spectral AMGe [15]. More recently, this technique has been used in overlapping Schwarz methods [34, 25, 24, 30, 31, 112, 103]. Spillane and Rixen [104] have used it for the classical FETI method, see also [37]. Kraus, Lymbery, and Margenov [61] use a similar idea in the context of the additive Schur complement approximation. Other works on BDDC and FETI-DP will be mentioned below.

There are four limitations of the method in [73, 76, 102]:

(a) The theory considers only diagonal scaling matrices.
(b) In the original works, the local bounds are only *indicators* and were not (yet) proven to be reliable.
(c) To obtain adaptive constraints, the eigenvectors corresponding to $\overline{F}$ have to be *split* into constraints on the corresponding open face F and the edges on its boundary. This can possibly lead to unnecessary constraints. Disregarding the vectors on the face boundary is suggested but not supported theoretically.
(d) It is assumed that the initial set of primal constraints already controls the kernel of the underlying PDE, such as the rigid body modes of elasticity; this is needed to realize the (formal) matrix inverse $\widetilde{S}^{-1}$ in the BDDC preconditioner. It would be good if the local eigenproblems could even detect these kernels and guarantee that $\widetilde{S}$ is definite.

Issue (b) has only been resolved quite recently. In [50], Klawonn, Radtke, and Rheinbach show that for two-dimensional problems, where all vertices are chosen primal, the maximum of all indicators $\omega_{\overline{F}}$ serves as a reliable condition number bound up to a benign factor. In that work, more general scaling matrices are also considered. In a recent preprint, [45], Klawonn, Kühn, and Rheinbach show a reliable condition number bound for general three-dimensional problems, where all vertices are chosen primal, using a diagonal scaling matrix. Up to a benign factor, the bound is the maximum over all the indicators $\omega_{\overline{F}}$ and some additional indicators associated with those subdomain edges that share four or more subdomains. To guarantee the reliability, the obtained face constraints are split into face and edge constraints as described above. The authors also provide some recipes on how the additional work for the edge indicators can be minimized.

In our article, we briefly review the new approach in [45] and show that it can be equally obtained from a *pair-based* localization of the P_D estimate. In the main part of our work, however, we take a different path and provide a similar framework as in [76], but using a *glob-based* localization. Here, a glob is an *open* subdomain face, edge, or possibly vertex. On each glob G, we define an indicator ω_G associated with the local estimate

$$\textstyle\sum_{i\in\mathcal{N}_G} |\Xi_{iG}(P_D w)_i|^2_{S_i} \le \omega_G \sum_{i\in\mathcal{N}_G} |w_i|^2_{S_i}\,. \tag{2}$$

Here, $\mathcal{N}_G$ is the set of subdomains shared by G and Ξ_G extracts the degrees of freedom on G. The best local indicator ω_G can again be obtained by a generalized eigenproblem, and the corresponding eigenvectors associated with the smallest eigenvalues can be used to create adaptive constraints. Solutions are given to all of the above issues:

(a) We allow general scaling matrices that only need to be *block-diagonal* with respect to partitioning into globs.
(b) Up to a benign factor, the maximum over all indicators ω_G serves as a *reliable* computable condition number bound.
(c) The constraints on open faces need not be split and can be used as they are. The eigenvectors obtained on subdomain edges, however, are not in the usual form of primal constraints. We show that we can use them as they are (thereby generalizing the notion of primal constraints), or *convert* them to classical primal constraints, which is more efficient and fully supported theoretically.
(d) The local eigenproblems stay well-defined even if the set of initial primal constraints is empty. Under mild assumptions on the subdomain matrices, we can show that using essentially the eigenvectors corresponding to zero eigenvalues as primal constraints guarantees that the inverse $\widetilde{S}^{-1}$ appearing in the BDDC preconditioner exists.

In the following, we would like to comment on other approaches to this problem. A first group of papers considers two-dimensional problems, where all vertices are a-priori chosen as primal. On subdomain faces (there called edges), generalized eigenvalue problems (and sometimes analytic estimates) are used to adaptively choose additional primal constraints. To review and compare, we need a little more notation: Let F be the subdomain face shared by subdomains i and j, let $S_{kF}^\star$ denote the "Neumann face" matrices ($\widetilde{S}_{FF}^{(k)}$ in the notation of [111, 13]), i.e., the Schur complement of the subdomain matrix eliminating all degrees of freedom (dofs) except those on F, and S_{kF} the "Dirichlet face" matrices ($S_{FF}^{(k)}$ in the notation of [111, 13]), i.e., starting with the subdomain matrix, eliminating all interior dofs, and then selecting the block corresponding to the dofs on face F.

- Klawonn, Radtke, and Rheinbach [49, 46] consider scalar diffusion and compressible elasticity with discontinuous coefficients, discretized by P^1 finite elements. They propose to use three generalized eigenproblems per face,
$$S_{iF}^\star v = \lambda M_{iF} v, \qquad S_{jF}^\star v = \lambda M_{jF} v, \qquad S_{iF}^\star v = \lambda \frac{\widehat{\rho}_i}{\widehat{\rho}_j} S_{jF}^\star v,$$
where $\widehat{\rho}_k$ is the maximal coefficient on subdomain k and M_{kF} a scaled mass matrix. The theory is completed with a discrete Sobolev inequality, $|v|^2_{S_{kF}} \leq C_1 |v|^2_{S_{kF}^\star} + C_2 |v|^2_{M_F}$, and leads to a reliable method for scalar diffusion and linear elasticity with varying coefficients. The authors use a coefficient-dependent scaling similar to the ρ-scaling, based on the values $\widehat{\rho}_k$.
- Chung and Kim [17] have worked out a fully algebraic approach (though limited to two-dimensional problems). They propose to use two eigenproblems per face,
$$(S_{iF} + S_{jF}) v = \lambda (S_{iF}^\star + S_{jF}^\star) v, \qquad S_{iF}^\star v = \lambda S_{jF}^\star v.$$
General scalings are allowed, but the condition number bound depends on the norm of the scaling matrices. For the multiplicity and the deluxe scaling, this norm is bounded by one.

In both approaches, in contrast to [73, 76], several (simpler) eigenproblems/estimates are combined. Moreover, the influence of the primal constraints on the neighboring vertices (on ∂F) are not included in the local eigenproblems. These two issues raise the question whether the obtained primal constraints are really necessary, or in other words, whether the local bound is efficient; see also [49, 111].

In our approach, we follow Mandel and Sousedík [73] and use a *natural* eigenproblem that directly follows from the localization (2) of the global P_D estimate. This eigenproblem involves unknowns on all subdomains shared by the glob, i.e., for face, about twice as many as for the above eigenproblems. Here, the (good) influence of a-priori chosen primal dofs on *neighboring globs* can (but need not) be included. Disregarding them leads to a much simpler implementation, but including them can reduce the number of primal constraints needed for a desired condition number bound. Besides that, we have collected a number of abstract tools for modifying/simplifying general eigenproblems.

Intermediate steps of our work are documented in the form of slides [21, 91]. In [91], we show that for the *deluxe scaling*, on each subdomain face F shared by subdomains i and j, one can alternatively use the generalized eigenproblem

$$(S^\star_{iF} : S^\star_{jF})v = \lambda(S_{iF} : S_{jF})v \tag{3}$$

where : denotes the *parallel sum of matrices* introduced by Anderson and Duffin [3]. This idea has recently been discussed in a publication by Klawonn, Radtke, and Rheinbach [50] comparing three different methods for the two-dimensional case: the method by Mandel and Sousedík [73], their own approach [49], and our intermediate approach [91] involving the parallel sum, for which they propose a variant for general scalings,

$$(S^\star_{iF} : S^\star_{jF})v = \lambda(D^\top_{jF} S_{iF} D_{jF} + D^\top_{iF} S_{jF} D_{iF})v, \tag{4}$$

where D_{kF} are the face scaling matrices. Sound theory for all three cases is given, but limited to the two-dimensional case. Moreover, *economic* variants are proposed, where S_{iF}, $S^\star_{iF}$, etc. are replaced by matrices where not all subdomain degrees of freedom are eliminated, but only those at a certain distance from the face F. Kim, Chung, and Wang [42, 43] have also compared the method by Chung and Kim [17] with (4). Zampini [116, 115, 117] as well as Calvo and Widlund [111, 13] have experimented with (3) too and give suggestions for the three-dimensional case.

In our current paper, we show a new theoretical link: If one disregards the influence of neighboring globs then the *natural* generalized eigenproblem corresponding to (2) on face $G = F$ shared by subdomains i and j is *equivalent* to (4). In case of the deluxe scaling, (4) is *identical* to (3). Moreover, we show that the deluxe scaling *minimizes* the *matrix trace* of the left-hand side matrix in (4), which is in favor of making the eigenvalues larger. Whereas in [91], we have used the parallel sum as an auxiliary tool, our new minimizing result shows that it is really *encoded* into BDDC.

The three-dimensional case including *subdomain edges* has turned out to be a particularly hard problem. For simplicity, consider an edge E shared by three subdomains i, j, k. Calvo and Widlund [111, 13] suggest to use

$$(S^\star_{iE} : S^\star_{jE} : S^\star_{kE})v = \lambda(T_{iE} + T_{jE} + T_{kE})v, \tag{5}$$

in context of deluxe scaling, where $T_{iE} = S_{iE} : (S_{jE} + S_{kE})$. Kim, Chung, and Wang [42, 43] give a choice for general scalings:

$$(S^\star_{iE} : S^\star_{jE} : S^\star_{kE})v = \lambda(A_{iE} + A_{jE} + A_{kE})v, \tag{6}$$

where $A_{iE} = D^\top_{jE} S_{iE} D_{jE} + D^\top_{kE} S_{iE} D_{kE}$. We provide two alternatives. Firstly, one can use the *natural* edge eigenproblem, optionally simplified by discarding the primal constraints on neighboring globs. We then show how to use the eigenvectors obtained as constraints in the BDDC algorithm. Secondly, we show that with further simplifications, the natural eigenproblem can be *decoupled* into $(n-1)$ independent eigenproblems where n is the number of subdomains shared by the edge. When *recombining* the decoupled problems, one obtains (6) in general, and (5) in case of the deluxe scaling.

Let us note that Stefano Zampini has experimented with

$$(S_{iE}^\star : S_{jE}^\star : S_{kE}^\star)v = \lambda(S_{iE} : S_{jE} : S_{kE})v, \tag{7}$$

which behaves robustly for some $H(\mathrm{curl})$ problems [114], but a theoretical validation is yet missing (and we do not show any).

Apparently, eigenproblems (5) and (6) are simpler than the natural one corresponding to (2), but the primal constraints resulting from (5), (6) may be unnecessary. Vice versa, the natural eigenproblem corresponding to (2) will lead to *efficient* constraints, but is more complicated to be computed. Our decoupled choice is in between.

Note that for all the eigenproblems considered, we show how *initially chosen primal constraints* on the respective glob (G, F, or E) can be built in. Essentially, the eigenproblems has to be projected onto the space where the initial constraints hold.

We hope that our theoretical study will serve as a contribution to better understanding of the proposed methods and the links between them, and to help find a good trade-off between (a) the more efficient, but also more complicated "natural" eigenproblems and (b) simpler eigenproblems that potentially lead to unnecessary constraints but are easier to compute.

The remainder of this paper is organized as follows: In Sect. 2 we discuss the problem setting, the BDDC preconditioner, abstract theory for the condition number, and primal constraints on globs. Sect. 3 provides a localization of the global P_D estimate under mild assumptions on the weight/scaling matrices. Moreover, we localize the condition for $\widetilde{S}$ to be definite. The local estimate is turned into an eigenproblem, which is discussed in detail in Sect. 4. Section 5 is devoted to the choice of the adaptive constraints for both the face and edge eigenproblems. Section 6 discusses the deluxe scaling and its optimality property. In Sect. 7 we combine the local definiteness condition from Sect. 3 and some abstract results from Sect. 4 to show how in practice, and under mild assumptions on the subdomain matrices, the global definiteness of $\widetilde{S}$ can be guaranteed. An appendix contains auxiliary, technical results.

Our paper is meant to be comprehensive and self contained. To get an overview, we recommend to skip the sections marked with an asterisk $(*)$ for the first time. Experienced BDDC readers may initially skip Sect. 2 as well.

Some Notation: X^* denotes the algebraic dual of the finite-dimensional (real) vector space X. We always identify the bi-dual X^{**} with X. If X is a Euclidean space, we even identify X^* with X. For a linear operator $A\colon X \to Y$, the *transpose* $A^\top\colon Y^* \to X^*$ is given by $\langle A^T y^*, x\rangle = \langle y^*, Ax\rangle$, where $\langle\cdot,\cdot\rangle$ are the dual pairings. A linear operator $A\colon X \to X^*$ (with X finite-dimensional) is said to be *symmetric* if $\langle Ax, y\rangle = \langle Ay, x\rangle$ for all x, $y \in X$, *positive semi-definite* if $\langle Ax, x\rangle \geq 0$ for all $x \in X$, and *positive definite* if $\langle Ax, x\rangle > 0$ for all $x \in X \setminus \{0\}$. Symmetric and positive semi-definite (SPSD) operators A, $B\colon X \to X^*$ have the following properties, which we will use frequently:

(i) $\langle Ax, x\rangle = 0 \iff x \in \ker(A)$,
(ii) $\ker(A+B) = \ker(A) \cap \ker(B)$,
(iii) $\mathrm{range}(A+B) = \mathrm{range}(A) + \mathrm{range}(B)$,
(iv) $|v|_A := \langle Av, v\rangle^{1/2}$ is a semi-norm on X.

If $P\colon X \to X$ is a projection ($P^2 = P$), then $X = \ker(P) \oplus \mathrm{range}(P)$, where $\oplus$ denotes the direct sum. Moreover, $(I - P)$ is a projection too, $\ker(I - P) = \mathrm{range}(P)$, and $\mathrm{range}(I - P) = \ker(P)$. Product spaces are denoted by $V_1 \times \cdots \times V_N$ or $\bigotimes_{i=1}^N V_i$.

2. BDDC in an algebraic setting

In this section, we summarize the main components of the BDDC method and fix the relevant notation. For the related FETI-DP method see Appendix B. We give abstract definitions of globs (equivalence classes of degrees of freedom), classical primal constraints, and generalized primal constraints.

2.1. **Problem setting.** We essentially follow the approach and notation in [72]. The problem to be solved is the system of linear equations

$$\text{find } \widehat{u} \in U\colon \quad \underbrace{R^\top S\, R}_{=:\,\widehat{S}}\widehat{u} \;=\; \underbrace{R^\top g}_{=:\,\widehat{g}}, \tag{8}$$

where

$$S = \begin{bmatrix} S_1 & & 0 \\ & \ddots & \\ 0 & & S_N \end{bmatrix}, \qquad g = \begin{bmatrix} g_1 \\ \vdots \\ g_N \end{bmatrix}, \qquad R = \begin{bmatrix} R_1 \\ \vdots \\ R_N \end{bmatrix}, \tag{9}$$

with SPSD matrices S_i. The assembled system matrix $\widehat{S}$ is assumed to be definite, such that (8) has a unique solution. Let W_i be the (real) Euclidean space of *subdomain (interface) degrees of freedom (dofs)* and U the Euclidean space of *global (interface) dofs*, such that

$$\begin{array}{ll} R_i\colon U \to W_i, & \quad R\colon U \to W := W_1 \times \ldots \times W_N, \\ S_i\colon W_i \to W_i, & \quad S\colon W \to W. \end{array} \tag{10}$$

We simply call the indices $i = 1, \ldots, N$ *subdomains.* Each matrix R_i corresponds to a local-to-global mapping $\mathsf{g}_i\colon \{1, \ldots, \dim(W_i)\} \to \{1, \ldots, \dim(U)\}$ and $(R_i)_{\ell k} = 1$ if and only if $k = \mathsf{g}_i(\ell)$ (local dof ℓ on subdomain i corresponds to global dof k), and zero otherwise. We assume that each mapping g_i is injective. Therefore, R_i has row full rank, and we conclude that[1]

$$R_i\, R_i^\top = I, \qquad R_i^\top R_i = \mathrm{diag}(\mu_k^{(i)})_{k=1}^{\dim(U)}, \quad \text{with } \mu_k^{(i)} \in \{0, 1\}. \tag{11}$$

Moreover, $R^\top R = \mathrm{diag}(\mu_k)_{k=1}^{\dim(U)}$ with $\mu_k = \sum_{i=1}^N \mu_k^{(i)}$ being the *multiplicity* of dof k. We assume throughout that $\mu_k \geq 2$ for all k, which implies in particular that R has full column rank and the subspace

$$\widehat{W} := \mathrm{range}(R) \tag{12}$$

is isomorphic to U.

Remark 2.1. Typically, the matrices S_i are constructed from (larger) subdomain finite element stiffness matrices A_i based on a non-overlapping domain decomposition (e.g. using a graph partitioner) by the (formal) static condensation of non-shared dofs. For the corresponding BDDC preconditioner for the non-condensed system see, e.g., [76].

[1] Note that $R^\top$ in (8) actually maps W^* to U^* and assembles local contributions to the global residual (i.e., a *functional*), whereas $R_i^\top$ in (11) plays a different role as it extends a *function* in W_i to U by putting all dofs zero that are not shared by subdomain i.

Remark 2.2. The assumption that each dof is at least shared by two subdomains is purely to simplify our presentation. All our results can be generalized to the case $\mu_k \geq 1$, which is, e.g., convenient for BETI [65]. Moreover, we could allow that R_i is rank-deficient and assume that $R_i^\top R_i = I$ is diagonal with ones and zeros. Then, however, some formulas would need adaptations. Such "phantom dofs" appear in the TFETI method [26]. See also [89] for both cases.

2.2. **The BDDC preconditioner.** There are two main ingredients for the BDDC preconditioner. The first one is the *averaging operator*

$$E_D \colon W \to U, \qquad E_D w \;:= \sum_{i=1}^N R_i^\top D_i w_i\,, \tag{13}$$

where $D_i \colon W_i \to W_i$ are *weight matrices* fulfilling

Condition 2.3 (partition of unity)**.** $\sum_{i=1}^N R_i^\top D_i R_i = I$ *(or equivalently* $E_D R = I$*).*

Note that the matrices D_i themselves need not be SPSD.

Proposition 2.4. *Under Condition 2.3 (partition of unity),* $\operatorname{range}(E_D) = U$ *and* $R E_D \colon W \to W$ *is a projection onto* $\widehat{W}$*.*

Proof. We have $U \supset \operatorname{range}(E_D) \supset \operatorname{range}(E_D R) = U$ and $(RE_D)^2 = RE_D RE_D = RE_D$. Finally, $\operatorname{range}(RE_D) = R(\operatorname{range}(E_D)) = \operatorname{range}(R) = \widehat{W}$. □

The simplest weights are given by the *multiplicity scaling*, $D_i = \operatorname{diag}(1/\mu_{\mathsf{g}_i(\ell)})_{\ell=1}^{\dim(W_i)}$, where $\mathsf{g}_i(\ell)$ is the global dof corresponding to the local dof ℓ on subdomain i. In some papers ([72, p. 180], [69, 76]), the weight matrices D_i are assumed to be diagonal with positive entries. In the current paper, we allow more general weights (see Condition 3.4 below). A special choice, the *deluxe scaling*, is discussed in Sect. 6.

The second ingredient is an *intermediate subspace* $\widetilde{W}$ that fulfills:

Condition 2.5. $\widehat{W} \subset \widetilde{W} \subset W$.

Condition 2.6. *S is definite on $\widetilde{W}$ (*$\ker(S) \cap \widetilde{W} = \{0\}$*).*

The construction of $\widetilde{W}$ is further described in Sect. 2.5.2 below. Condition 2.6 is needed for both the practical application of the BDDC preconditioner and its analysis, and it will be further discussed in Sect. 3.1 as well as in Sect. 7. Let

$$\tilde{I} \colon \widetilde{W} \to W. \tag{14}$$

denote the natural embedding operator and define the restricted operator

$$\widetilde{S} := \tilde{I}^\top S \tilde{I} \colon \widetilde{W} \to \widetilde{W}^*. \tag{15}$$

Due to Condition 2.6, $\widetilde{S}$ is definite and thus has a well-defined inverse. The BDDC preconditioner for problem (8) is defined by

$$M_{\text{BDDC}}^{-1} \;:=\; E_D\,(\tilde{I}\,\widetilde{S}^{-1}\,\tilde{I}^\top) E_D^\top \colon U \to U. \tag{16}$$

If we *explicitly* choose a basis for $\widetilde{W}$, then $\tilde{I}$ and $\tilde{S}$ have matrix representations and $\widetilde{S}^{-1}$ can be constructed via a block Cholesky factorization (see e.g. [69, 58]). Depending on the structure of the space $\widetilde{W}$, this can cause a loss of sparsity, which leads to inefficient local solvers when using, e.g., nested dissection. The original BDDC method [19] is based on *primal dofs* (explained in Sect. 2.5), and provides an efficient algorithm

(Appendix C) to realize $(\tilde{I}\,\widetilde{S}^{-1}\,\tilde{I}^\top)$ using a change of basis only *implicitly* and preserving sparsity. A more general construction of the space $\widetilde{W}$ (cf. [76]) has certain importance to our work as well and will be investigated in Sect. 2.6, Sect. 5.4, and Appendix C.3.

2.3. **Abstract Analysis.** Theorem 2.8 below has been shown several times in the literature (see, e.g., [72, 74]). For its statement we need the projection operator

$$P_D := I - R\,E_D \colon W \to W. \tag{17}$$

The following properties can be derived from Proposition 2.4.

Proposition 2.7. *Under Condition 2.3 and Condition 2.5,*

(i) $P_D^2 = P_D$,
(ii) $P_D w = 0 \iff w \in \mathrm{range}(R) = \widehat{W}$,
(iii) $P_D w \in \widetilde{W} \iff w \in \widetilde{W}$, *in particular* $P_D(\widetilde{W}) \subset \widetilde{W}$, $\mathrm{range}(P_D) \cap \widetilde{W} = P_D(\widetilde{W})$.

Theorem 2.8 ([72, Theorem 5])**.** *Let assumptions from Sect. 2.1 hold and let Condition 2.3 (partition of unity), Condition 2.5 ($\widehat{W} \subset \widetilde{W} \subset W$), and Condition 2.6 ($S$ definite on $\widetilde{W}$) be fulfilled. Then*

$$\lambda_{\min}(M_{\mathrm{BDDC}}^{-1}\widehat{S}) \;\geq\; 1.$$

Moreover, the three estimates

$$|RE_D w|_S^2 \;\leq\; \omega\,|w|_S^2 \qquad \forall w \in \widetilde{W}, \tag{18}$$

$$|P_D w|_S^2 \;\leq\; \omega\,|w|_S^2 \qquad \forall w \in \widetilde{W}, \tag{19}$$

$$\lambda_{\max}(M_{\mathrm{BDDC}}^{-1}\widehat{S}) \;\leq\; \omega \tag{20}$$

are equivalent. Summarizing, (19) *implies* $\kappa(M_{\mathrm{BDDC}}^{-1}\widehat{S}) \leq \omega$.

A proof based on the fictitious space lemma is provided in Appendix A, see also [61].

Remark 2.9. In general, the definiteness of $\widetilde{S}$ *does not* follow from (18) or (19). Consider one global dof ($U = \mathbb{R}$) shared by two subdomains with $S_1 = D_1 = 1$, $S_2 = D_2 = 0$ and $\widetilde{W} = W = \mathbb{R}^2$. Then $\widetilde{S}$ is singular but $|P_D w|_S^2 = 0$ and $|RE_D w|_S^2 = |w|_S^2$.

Remark 2.10. For a fixed problem matrix S and weight matrices D_i, consider two BDDC preconditioners based on spaces $\widetilde{W}^{(1)} \subset \widetilde{W}^{(2)}$ (typically meaning that $\widetilde{W}^{(1)}$ has more primal constraints than $\widetilde{W}^{(2)}$) and let $\lambda_{\max}^{(1)}$, $\lambda_{\max}^{(2)}$ denote the corresponding maximal eigenvalues. Then $\lambda_{\max}^{(1)} \leq \lambda_{\max}^{(2)}$. Since in practice, $\lambda_{\min}$ is close or even equal to one [10, 69, 74, 73], we can expect the smaller space (with the larger set of primal constraints) to lead to a smaller condition number.

2.4. **Globs.** In BDDC and FETI-DP the intermediate space $\widetilde{W}$ is described using *primal dofs*, or *coarse dofs*. In this particular paper, we restrict ourselves to primal dofs that are associated with *globs*[2].

Definition 2.11 (globs)**.** For each global dof $k \in \{1, \dots, \dim(U)\}$, we define the set

$$\mathcal{N}_k := \bigl\{ i = 1, \dots, N : \mu_k^{(i)} = 1 \bigr\}$$

[2]Note that many different definitions of globs are used in the literature: sometimes globs are geometrical sets [79, 89], sometimes the set of globs excludes vertices [73].

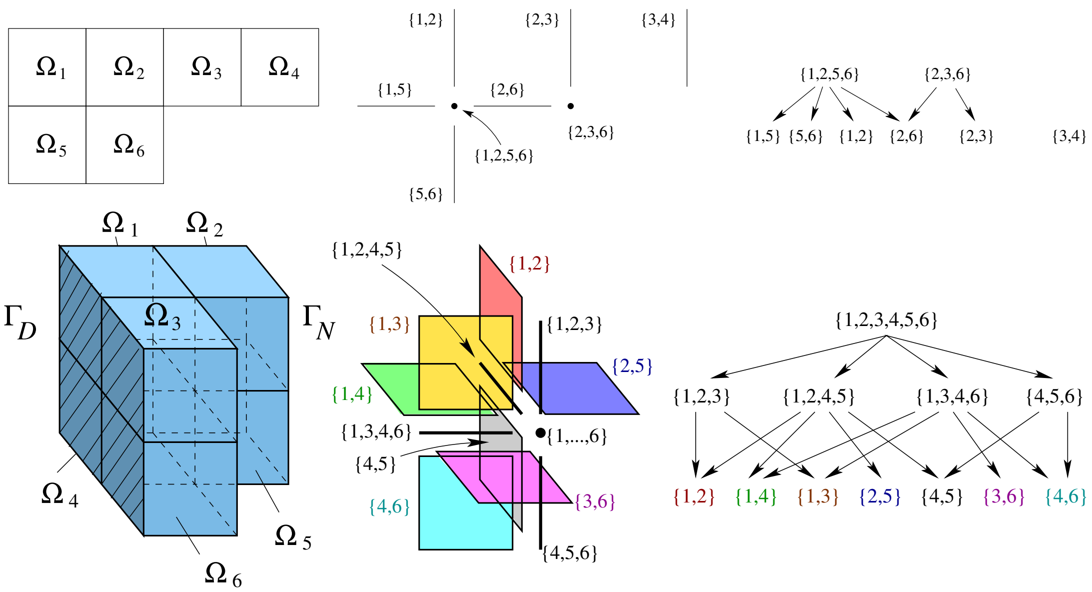

FIGURE 1. Two examples of subdomain decompositions and globs. *Top:* 2D example, *bottom:* 3D example, *left:* subdomain decomposition, *middle:* visualization of globs with $\mathcal{N}_G$ displayed, *right:* parent graph; arrow points from parent to "child".

of sharing subdomains. The set $\{1, \ldots, \dim(U)\}$ of global dofs is partitioned into equivalence classes, called *globs*, w.r.t. the equivalence relation $k \sim k' \iff \mathcal{N}_k = \mathcal{N}_{k'}$. We denote by $\mathcal{G}$ the set of all globs and by $\mathcal{N}_G$ the set of subdomains shared by glob G. Finally, we define the set

$$\mathcal{G}_i := \{G \in \mathcal{G} : i \in \mathcal{N}_G\}$$

of globs for subdomain i. If $|\mathcal{N}_G| = 2$, we call G a *face*, and we denote the set of all faces (of subdomain i) by $\mathcal{F}$ ($\mathcal{F}_i$, respectively).

Definition 2.12 (glob relationships)**.** A glob G_1 is called an *ancestor* of G_2 if $\mathcal{N}_{G_1} \supsetneq \mathcal{N}_{G_2}$ and G_1 is called a *parent* of G_2 if G_1 is an ancestor of G_2 and there is no other glob G_3 with $\mathcal{N}_{G_1} \supsetneq \mathcal{N}_{G_3} \supsetneq \mathcal{N}_{G_2}$. Certainly, a glob can have several parents. If a glob has no parents, we call it a *base glob*. Two globs $G_1 \neq G_2$ are called *neighbors* if $|\mathcal{N}_{G_1} \cap \mathcal{N}_{G_2}| \geq 2$, i.e., if they share at least two common subdomains.

Figure 1 illustrates these definitions (assuming a relatively fine mesh and a finite element space with node-based dofs, such that sets of nodes look like geometrical sets).

Remark 2.13. For general partitions of 3D finite element meshes, e.g., obtained from a graph partitioner, it can be hard to classify globs geometrically, in particular to distinguish between vertices and edges. For some rules/heuristics see [51, Sect. 2], [58, Sect. 3], [23, Sect. 5]. For our purposes, such a classification is not needed. The above definition also resembles the *fat* faces/edges/vertices for isogeometric analysis [5]. Moreover, the setting is not only limited to two- and three-dimensional problems. Lastly, note that our theory holds for any alternative definition of globs that *refines* Definition 2.11 in the sense that each glob of Definition 2.11 is a union of the refined globs. For instance, one may want to split a glob if it is not connected geometrically; see also [58, 89, 116, 117].

symbol	explanation	reference
$\mathcal{F}$ ($\mathcal{F}_i$)	set of faces (associated with subdomain i)	Def. 2.11
$\mathcal{G}$ ($\mathcal{G}_i$)	set of globs (associated with subdomain i)	Def. 2.11
$\mathcal{G}^*$ ($\mathcal{G}_i^*$)	subset of $\mathcal{G}$ ($\mathcal{G}_i$), not totally primal	Def. 2.20
$\mathcal{N}_G$	set of subdomain indices associated with glob G	Def. 2.11
D_{iG}	glob scaling matrix $U_G \to U_G$	Ass. 3.4
R_{iG}	restriction matrix $W_i \to U_G$	Def. 2.14
$\widehat{R}_G$	restriction matrix $U \to U_G$	(21)
$Q_G^\top$	evaluation of primal dofs	Def. 2.15
Ξ_G (Ξ_{iG})	filter matrix $W \to W$ ($W_i \to W_i$)	(23)
$\widehat{\Xi}_G$	filter matrix $U \to U$	(23)

TABLE 1. Notation concerning globs.

Definition 2.14. Let U_G denote the space of dofs on G (with a fixed numbering). For any $i \in \mathcal{N}_G$, let $R_{iG} \colon W_i \to U_G$ be the (zero-one) restriction matrix (of full rank) extracting these dofs, such that $R_{iG} R_{iG}^\top = I$.

Since U_G has a fixed dof numbering, we can conclude that there exists a matrix $\widehat{R}_G \colon U \to U_G$ such that

$$R_{iG} R_i = \widehat{R}_G \quad \forall i \in \mathcal{N}_G\,, \qquad \widehat{R}_G \widehat{R}_G^\top = I \quad \forall G \in \mathcal{G}. \tag{21}$$

Since the globs are disjoint to each other,

$$R_{iG_1} R_{iG_2}^\top = \begin{cases} I & \text{if } G_1 = G_2 \in \mathcal{G}_i \\ 0 & \text{otherwise.} \end{cases} \tag{22}$$

We define the cut-off/filter matrices

$$\Xi_{iG} := R_{iG}^\top R_{iG}\,, \qquad \Xi_G := \operatorname{diag}(\Xi_{iG})_{i=1}^N\,, \qquad \widehat{\Xi}_G := \widehat{R}_G^\top \widehat{R}_G\,, \tag{23}$$

which are diagonal matrices with entry one if the corresponding dof is on G and zero otherwise.[3] From the previous definitions and properties we conclude that

$$\Xi_{iG} R_i = R_i \widehat{\Xi}_G\,, \qquad \Xi_G R = R \widehat{\Xi}_G\,, \qquad \Xi_G^2 = \Xi_G\,, \qquad \widehat{\Xi}_G^2 = \widehat{\Xi}_G\,. \tag{24}$$

By construction, we have the following partitions of unity on W_i and U,

$$\sum_{G \in \mathcal{G}_i} \Xi_{iG} = I, \qquad \sum_{G \in \mathcal{G}} \widehat{\Xi}_G = I, \tag{25}$$

as well as the following characterization of the "continuous" space (cf. [72])

$$\widehat{W} \;:=\; \operatorname{range}(R) \;=\; \{ w \in W \colon \forall G \in \mathcal{G}\ \forall i, j \in \mathcal{N}_G \colon R_{iG} w_i - R_{jG} w_j = 0 \}. \tag{26}$$

2.5. **Primal dofs and the space $\widetilde{W}$.** Various definitions of primal dofs have been used for FETI-DP [32, 67, 59, 58, 89, 107] and BDDC [19, 72, 73] in the literature. Here, we require that a primal dof must be associated with a glob and is nothing but a linear combination of regular dofs within that glob. In Sect. 2.5.3 below, we discuss a more general definition of primal dofs and the space $\widetilde{W}$ based on *closed* globs, which we, however, do not use in the main part of our theory.

[3] Our expression $\Xi_{iG} w_i$ corresponds to $I^h(\theta_G w_i)$ in the terminology of [107].

2.5.1. *Classical primal dofs.* The following definition is more common in BDDC methods, which is why we term it "classical"; see Sect. 2.5.3 for a more general definition.

Definition 2.15. *Classical primal dofs* on the open glob G are described by a matrix

$$Q_G^\top \colon U_G \to U_{\Pi G} := \mathbb{R}^{n_{\Pi G}},$$

where $n_{\Pi G} \geq 0$ is the number of primal dofs associated with glob G. The subspace of U_G where the primal dofs vanish is

$$U_{G\Delta} := \{y \in U_G \colon Q_G^\top y = 0\}. \tag{27}$$

We set

$$W_{\Pi i} := \bigotimes_{G \in \mathcal{G}_i} U_{\Pi G}\,, \quad W_\Pi := \bigotimes_{i=1}^N W_{\Pi i}\,, \quad \text{and} \quad U_\Pi := \bigotimes_{G \in \mathcal{G}} U_{\Pi G} \simeq \mathbb{R}^{n_\Pi},$$

with $n_\Pi = \sum_{G \in \mathcal{G}} n_{\Pi G}$ the total number of primal dofs. Analogously to Sect. 2.1, we can find zero-one matrices

$$R_{\Pi i} \colon U_\Pi \to W_{\Pi i}\,, \quad R_\Pi \colon U_\Pi \to W_\Pi\,, \quad \text{and} \quad R_{\Pi i G} \colon W_{\Pi i} \to U_{\Pi G}\,, \tag{28}$$

and a matrix $\widehat{R}_{\Pi G} : U_\Pi \to U_{\Pi G}$ such that $R_{\Pi i G} R_{\Pi i} = \widehat{R}_{\Pi G}$ independent of $i \in \mathcal{N}_G$. Let

$$C_i \colon W_i \to W_{\Pi i}\,, \qquad C_i := \sum_{G \in \mathcal{G}_i} R_{\Pi i G}^\top Q_G^\top R_{iG}\,.$$

be the matrix evaluating all primal dofs associated with subdomain i and define the *dual subspaces* [72, 107]

$$W_{i\Delta} := \ker(C_i) = \{w_i \in W_i \colon \forall G \in \mathcal{G}_i \colon Q_G^\top R_{iG} w_i = 0\}, \qquad W_\Delta := \bigotimes_{i=1}^N W_{i\Delta}. \tag{29}$$

Remark 2.16. The operators/spaces R_Π, U_Π, W_Π correspond to R_c, U_c, X, respectively, from [73, Sec. 2.3]). The operator Q_P from [72, 73] reads (in our notation) $Q_P^\top = \sum_{G \in \mathcal{G}} \widehat{R}_{\Pi G}^\top Q_G^\top \widehat{R}_G \colon U \to U_\Pi$. So Definition 2.15 is equivalent to saying that $Q_P^\top$ is *block-diagonal* with respect to the partitions of (primal) dofs into globs.

The next condition states that the primal dofs on G are linearly independent. This can always be achieved by (modified) Gram-Schmidt orthonormalization or, more generally, by a QR factorization [36, Sect. 5.2].

Condition 2.17 (linearly independent primal dofs)**.** *For each glob $G \in \mathcal{G}$, the columns of the matrix Q_G are linearly independent.*

The following condition is needed later on:

Condition 2.18 (C_i surjective)**.** $\ker(C_i^\top) = \{0\}$ *for all* $i = 1, \ldots, N$*.*

Proposition 2.19. *Let $\{Q_G^\top\}_{G \in \mathcal{G}}$ be primal dofs in the sense of Definition 2.15. Then Condition 2.17 $\iff$ Condition 2.18.*

Proof. Recall that $C_i^\top = \sum_{G \in \mathcal{G}_i} R_{iG}^\top Q_G R_{\Pi i G}$, i.e., $C_i^\top$ is block-diagonal with respect to the partition of W_i into globs and to the partition of $W_{\Pi i}$ into $\{U_{\Pi G}\}_{G \in \mathcal{G}_i}$. Hence $C_i^\top$ is injective if and only if all the matrices $\{Q_G\}_{G \in \mathcal{G}_i}$ are injective. □

Some special primal dofs control *all* dofs on a glob (in applications, these are typically subdomain vertices):

Definition 2.20 (totally primal glob)**.** We call a glob G *totally primal* if $Q_G^\top$ is injective (typically the identity). The set of globs (for subdomain i) which are *not* totally primal is denoted by $\mathcal{G}^*$ ($\mathcal{G}_i^*$ respectively).

2.5.2. *The space* $\widetilde{W}$. Following [19, 72, 69, 73], we define the "partially continuous space" $\widetilde{W}$ based on primal dofs.

Definition 2.21. For given primal dofs $\{Q_G^\top\}_{G\in\mathcal{G}}$ in the sense of Definition 2.15, we set

$$\widetilde{W} := \{w \in W\colon \forall G \in \mathcal{G}\ \forall i, j \in \mathcal{N}_G\colon Q_G^\top (R_{iG}w_i - R_{jG}w_j) = 0\}. \tag{30}$$

Obviously, the space above fulfills Condition 2.5, i.e., $\widehat{W} \subset \widetilde{W} \subset W$. The following characterization can be shown using the properties of the restriction matrices $R_{\Pi\ldots}$, cf. [72], [73, Sect. 2.3].

Proposition 2.22. *If the primal dofs are linearly independent (Condition 2.17) then*

$$\widetilde{W} = \{w \in W\colon \exists u_\Pi \in U_\Pi\ \forall i = 1, \ldots, N\colon C_i w_i = R_{\Pi i} u_\Pi\}. \tag{31}$$

The side conditions in (30) are called *primal constraints*, and they fulfill two jobs: First, we need enough constraints such that Condition 2.6 holds ($\widetilde{S}$ is invertible). Second, additional constraints may be needed to get a good constant in the bound (19) (recall Remark 2.10: the smaller the space $\widetilde{W}$, the (potentially) smaller the constant ω). In particular this is important for 3D problems or parameter-dependent problems. The first job is treated in Sect. 3.1 and in Sect. 7. The rest of the paper is mainly devoted to the second job. Here, one has to take into account that, although a smaller space leads to a better condition number, the amount of coupling within $\widetilde{W}$ should be kept at a minimum, otherwise the algorithm is not efficient. For example, if $\widetilde{W} = \widehat{W}$, then $\widetilde{S}$ (which should actually be cheaper to invert) is the same as the original problem matrix.

Before proceeding, we provide two basic results on the space $\widetilde{W}$. The first one clarifies its dimension.

Proposition 2.23. *If the primal dofs are linearly independent (Condition 2.17), then* $\dim(\widetilde{W}) = n_\Pi + \sum_{i=1}^N \dim(W_{i\Delta})$.

The second result allows us to write $\widetilde{W}$ as a direct sum of a *continuous* and a *discontinuous* space, see also [72, Sect. 5], [107, Sect. 6.4].

Proposition 2.24. *If the primal dofs are linearly independent (Condition 2.17), then*

$$\widetilde{W} = \widehat{W}_\Pi \oplus W_\Delta\,,$$

where $\widehat{W}_\Pi = \mathrm{range}(\widehat{\Phi}) \subset \widehat{W}$ *is given by the full-rank matrix*

$$\widehat{\Phi}\colon U_\Pi \to \widehat{W}, \quad \widehat{\Phi} := RQ_P = R \sum_{G\in\mathcal{G}} \widehat{R}_G^\top Q_G \widehat{R}_{\Pi G}\,.$$

Moreover, $\widehat{\Phi}_i = C_i^\top R_{\Pi i} = (\sum_{G\in\mathcal{G}_i} R_{iG}^\top Q_G R_{\Pi i G}) R_{\Pi i}$, *so the basis has local support.*

Remark 2.25. If the primal dofs are orthogonal, i.e., for all $G \in \mathcal{G}$: $Q_G^\top Q_G = I$, then $C_i \widehat{\Phi}_i = I$. Otherwise, one can redefine $\widehat{\Phi}$ to fulfill the latter property, cf. [72, Lemma 9].

2.5.3. *Primal dofs on closed globs**. In some references and implementations, primal dofs are defined on the *closure of globs*, cf. [107, 48, 76].

Definition 2.26. The *closure* $\overline{G}$ of glob G is given by G and all its ancestors, i.e.,

$$\overline{G} := \bigcup \{G' \in \mathcal{G}_{\overline{G}}\}, \quad \text{where} \quad \mathcal{G}_{\overline{G}} := \{G' \in \mathcal{G}\colon \mathcal{N}_{G'} \supseteq \mathcal{N}_G\}.$$

Let $U_{\overline{G}}$ denote the space of dofs on $\overline{G}$ (with a fixed numbering). Analogously to the above, we can find zero-one matrices $R_{i\overline{G}}\colon W_i \to U_{\overline{G}}$ and $\widehat{R}_{\overline{G}}\colon U \to U_{\overline{G}}$ extracting these dofs such that $R_{i\overline{G}} R_i = \widehat{R}_{\overline{G}}$ independent of $i \in \mathcal{N}_G$.

Definition 2.27. *Primal dofs* on the *closed glob* $\overline{G}$ are described by a matrix

$$Q_{\overline{G}}^\top\colon U_{\overline{G}} \to U_{\Pi G} := \mathbb{R}^{n_{\Pi G}}.$$

The analogous definitions of $C_i\colon W_i \to W_{\Pi i}$ and $Q_P^\top\colon U \to U_\Pi$ are

$$C_i = \sum_{G \in \mathcal{G}_i} R_{\Pi i G}^\top Q_{\overline{G}}^\top R_{i\overline{G}}, \qquad Q_P^\top = \sum_{G \in \mathcal{G}} R_{\Pi G}^\top Q_{\overline{G}}^\top \widehat{R}_{\overline{G}}$$

and the space $\widetilde{W}$ can now be defined as in (31).

Recall that for the classical primal dofs (on "open" globs), the proof of Proposition 2.19 is very simple. For the closed case, an analogue is not presently known. Yet, the following is easily verified:

Proposition 2.28. *Let $R_{G\overline{G}} := \widehat{R}_G \widehat{R}_{\overline{G}}^\top$ denote the restriction matrix from the dofs on $\overline{G}$ to the (fewer) dofs on the open glob G. If for each $G \in \mathcal{G}$, the matrix $R_{G\overline{G}} Q_{\overline{G}}$ has full column rank, then also $Q_{\overline{G}}$ has full column rank (analogous to Condition 2.17).*

If $R_{G\overline{G}} Q_{\overline{G}}$ has linearly *dependent* columns, we can *split* each primal dof on the closed glob $\overline{G}$ into primal dofs on all the *open* globs $G' \in \mathcal{G}_{\overline{G}}$, orthonormalize them together with the existing ones, and finally obtain linearly independent primal dofs on *open* globs (Condition 2.17). However, to our best knowledge, no algorithm exists to date which gets Condition 2.17 to hold by modifying $Q_{\overline{G}}$ *without increasing* the overall number of primal dofs. See also [76, p. 1819]. This is one of the reasons why we use Definition 2.15.

2.6. **Generalized primal constraints***. Mandel, Sousedík, and Šístek [76] use a more general definition of the space $\widetilde{W}$, which is of central importance to our own work:

$$\widetilde{W} \;=\; \{w \in W\colon Lw = 0\}, \tag{32}$$

where $L\colon W \to X := \mathbb{R}^M$ is a matrix with M linearly independent rows. One easily shows that $\widehat{W} \subset \widetilde{W} \subset W$ (Condition 2.5) if and only if $LR = 0$, or equivalently,

$$Lw \;=\; 0 \qquad \forall w \in \widehat{W}. \tag{33}$$

Apparently, Definition 2.21 (based on the classical primal dofs) is a special case of (32) but not vice versa. For the general form (32), the application $y = \tilde{I}\widetilde{S}^{-1}\tilde{I}^\top \psi$ for $\psi \in W$ is equivalent to solving the global saddle point problem

$$\begin{bmatrix} S & L^\top \\ L & 0 \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix} = \begin{bmatrix} \psi \\ 0 \end{bmatrix}. \tag{34}$$

For the special case of L discussed below, a more viable option is given in Appendix C.

Remark 2.29. Actually, for any space $\widetilde{W}$ with $\widehat{W} \subset \widetilde{W} \subset W$ (Condition 2.5), there is a matrix L such that (32)–(33) holds. In a FETI-DP framework (see Appendix B), (33) implies that $L = \bar{L}B$ for some $\bar{L}$, and so, such constraints can be implemented by *deflation* [54, 38, 49, 42, 43]. The balancing Neumann-Neumann method [70] can be interpreted as a BDDC method with (32), however the constraints L are global, cf. [89, p. 110].

In [76], Mandel et al. require that each constraint (each row of L) is *local to a glob*, i.e., for each glob $G \in \mathcal{G}$, there exist matrices $L_{jG} \colon U_G \to X_G$, $j \in \mathcal{N}_G$ such that

$$Lw = \sum_{G \in \mathcal{G}} R_{XG}^\top \sum_{j \in \mathcal{N}_G} L_{jG} R_{jG} w_j \,, \tag{35}$$

where X is isomorphic to $\bigotimes_{G \in \mathcal{G}} X_G$ and $R_{XG} \colon X \to X_G$ is the zero-one matrix extracting the "G" component. If L is of form (35) then

(i) L has linearly independent rows if and only if for all $G \in \mathcal{G}$ the block row matrix $[\cdots | L_{jG} | \cdots]_{j \in \mathcal{N}_G}$ has linearly independent rows.

(ii) $Lw = 0$ holds if and only if

$$\sum_{j \in \mathcal{N}_G} L_{jG} R_{jG} w_j \;=\; 0 \qquad \forall G \in \mathcal{G}, \tag{36}$$

(iii) $Lw = 0$ for all $w \in \widehat{W}$ (Condition (33)) if and only if

$$\sum_{j \in \mathcal{N}_G} L_{jG} = 0 \qquad \forall G \in \mathcal{G}. \tag{37}$$

The above form of constraints is important to our study, because our localized bounds (implying the central bound (19) of the P_D operator) hold (and are sharp) if constraints of form (35), (37) are imposed (in addition to previously fixed primal constraints). In particular, they pop out of local generalized eigenproblems associated with globs that share more than two subdomains and that involve more than just a few dofs such as subdomain edges.

Mandel, Sousedík, and Šístek provide an algorithm for the efficient solution of the global saddle point problem (34) based the multifrontal massively parallel sparse direct solver MUMPS [1]. In Appendix C.3, we give an extension of the algorithm proposed in [19] which realizes $\tilde{I}\,\widetilde{S}^{-1}\tilde{I}^\top$ by solving local saddle point problems and one global (coarse) SPD problem. Under the perspective of the extended algorithm, BDDC with generalized (but still glob-based) primal constraints becomes amenable for multiple levels [109, 52, 75, 102] which is a rather attractive option if one thinks of problems with high contrast coefficients [93, 94, 92, 16, 49] and/or a detailed underlying geometry [73, 20, 23]. Nevertheless, as we will show in Sect. 5.4 below, it is much more favorable to use potentially stronger classical primal constraints and the conventional algorithm from Appendix C.1–C.2 (which is naturally amenable to multiple levels). Although our result holds for the general case, we will describe it later in Sect. 5, when needed.

3. Localization

In this section, we provide a local condition implying the global definiteness of $\widetilde{S}$ (Sect. 3.1, Condition 2.6). After introducing our mild assumptions on the weight/scaling matrices D_i and showing some technical results in Sect. 3.2, we provide local estimates implying the global estimate (19) of the P_D-operator in Sect. 3.3. We also review a similar approach by Klawonn, Kühn, and Rheinbach [45] (Sect. 3.4). Throughout this section, we assume a space $\widetilde{W}$ based on classical primal dofs (Def. 2.15 and Def. 2.21).

3.1. A local, glob-based condition for the definiteness of $\widetilde{S}$.

The problem of how to guarantee definiteness of $\widetilde{S}$ already arose in the original FETI-DP method [32]. Suitable choices of primal constraints are known for scalar diffusion and linear elasticity problems ([67, 107]). For the general SPD case, however, an all-purpose recipe is yet

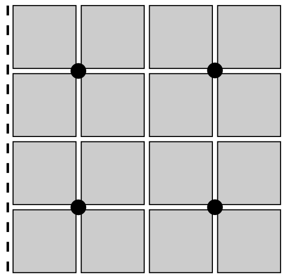

FIGURE 2. Example where (38) is not sufficient to guarantee that $\widetilde{S}$ is definite; 2D Laplace problem with Dirichlet boundary conditions on the dashed line. Bullet indicates primal constraint on subdomain vertex.

missing (to our best knowledge). As one can see easily, the definiteness of S on $\widetilde{W}$ (Condition 2.6) implies the necessary local condition

$$S_i \text{ is definite on } W_{i\Delta} \qquad \forall i = 1, \ldots, N, \tag{38}$$

which is, however, not sufficient (see Fig. 2 for a counterexample).

Condition 3.1 below is local and sufficient (Lemma 3.2), although not necessary. In Sect. 7, we provide an algorithm that computes a set of primal constraints such Condition 3.1 can be guaranteed under mild assumptions on the problem. For each glob $G \in \mathcal{G}$, we define the (Euclidean) space

$$W_{\mathcal{N}_G} := \{w = [w_i]_{i \in \mathcal{N}_G} \colon w_i \in W_i\},$$

where $[w_i]_{i \in \mathcal{N}_G}$ simply designates a block vector. We denote by $w_{\mathcal{N}_G} \in W_{\mathcal{N}_G}$ the restriction of $w \in W$ to the subdomains in $\mathcal{N}_G$ and define the subspace

$$\begin{aligned} \widetilde{W}_{\mathcal{N}_G} &:= \{w \in W_{\mathcal{N}_G} \colon \exists z \in \widetilde{W} \colon w_i = z_i \ \forall i \in \mathcal{N}_G\} \\ &= \{w \in W_{\mathcal{N}_G} \colon \forall i \neq j \in \mathcal{N}_G \ \forall G', \{i,j\} \subset \mathcal{N}_{G'} \colon Q_{G'}^\top (R_{iG'} w_i - R_{jG'} w_j) = 0\}, \end{aligned} \tag{39}$$

i.e., the space of functions living "around" G, where (previously fixed) primal constraints are enforced on all the *neighboring* globs of G, cf. Def. 2.12. See Fig. 3 for a two-dimensional example where G is a vertex. If G is a typical edge in a three-dimensional problem, then in addition to the previously fixed edge constraints, also previously fixed face and vertex constraints are enforced.

Condition 3.1 (local kernel condition)**.** *For each glob $G \in \mathcal{G}^*$ (i.e. not totally primal), assume that*

$$\forall w \in \widetilde{W}_{\mathcal{N}_G} \colon \quad \big(\forall i \in \mathcal{N}_G \colon S_i\, w_i = 0\big) \implies (\forall i,j \in \mathcal{N}_G \colon R_{iG} w_i = R_{jG} w_j).$$

Lemma 3.2. *Condition 3.1 $\implies$ Condition 2.6 (S is definite on $\widetilde{W}$).*

Proof. Let Condition 3.1 hold and let $w \in \ker(S) \cap \widetilde{W}$ be arbitrary but fixed. Then $S_i w_i = 0$ for all $i = 1, \ldots, N$. Due to Condition 3.1 for all not totally primal globs G,

$$\forall i,j \in \mathcal{N}_G \colon R_{iG} w_i = R_{jG} w_j\,.$$

On the remaining totally primal globs, we get the same condition from Def. 2.21 and Def. 2.20. So, *all* dofs are continuous across *all* globs, and with (26), $w \in \widehat{W}$. Since $\ker(S) \cap \widehat{W} = \{0\}$ (cf. Sect. 2.1), $w = 0$. Summarizing, $\ker(S) \cap \widetilde{W} = \{0\}$. □

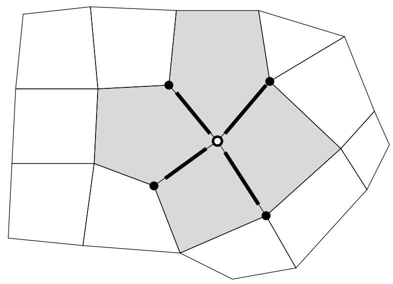

FIGURE 3. Sketch of a vertex G (marked with $\circ$) and the neighboring globs where constraints enforced in the associated space $\widetilde{W}_{\mathcal{N}_G}$ (marked with thick lines and black dots).

Remark 3.3. Condition 3.1 is similar to but substantially different from [73, Assumption 8]. The latter reads as follows. For all *faces* $F \in \mathcal{F}$,

$$\forall w \in \widetilde{W}_{\mathcal{N}_F}: \quad (S_i w_i = 0,\ S_j w_j = 0) \implies (R_{i\overline{F}} w_i = R_{j\overline{F}} w_j), \tag{40}$$

where $\{i, j\} = \mathcal{N}_F$ and $\overline{F}$ is the closed face (Def. 2.26). Under the additional assumption that for each glob $G \in \mathcal{G} \setminus \mathcal{F}$, one can connect each pair $\{i, j\} \subset \mathcal{N}_G$ via a path through faces (which is fulfilled for usual domain decompositions), one can show that Condition 2.6 holds. Neither Condition 3.1 nor (40) are necessary for Condition 2.6 to hold.

3.2. **Assumption on the weight matrices.** In our subsequent theory, we need the following, mild assumption on the scaling matrices D_i:

Assumption 3.4 (D_i block diagonal)**.** *Each scaling matrix D_i is block diagonal with respect to the glob partition, i.e., there exist matrices $D_{iG}\colon U_G \to U_G$, $G \in \mathcal{G}_i$ such that*

$$D_i \;=\; \sum_{G \in \mathcal{G}_i} R_{iG}^\top D_{iG} R_{iG}\,.$$

The condition below is a glob-wise partition of unity and the proposition thereafter is easily verified.

Condition 3.5 (glob-wise partition of unity)**.** *For each glob $G \in \mathcal{G}$, there holds $\sum_{j \in \mathcal{N}_G} D_{jG} = I$.*

Proposition 3.6. *Let Assumption 3.4 hold. Then for all $G \in \mathcal{G}$ and $i \in \mathcal{N}_G$,*

$$\Xi_{iG} D_i \;=\; D_i \Xi_{iG}\,, \qquad \Xi_G D = D \Xi_G \tag{41}$$

(where $D = \operatorname{diag}(D_i)_{i=1}^N$) and

$$E_D w \;=\; \sum_{G \in \mathcal{G}} \widehat{R}_G^\top \sum_{i \in \mathcal{N}_G} D_{iG} R_{iG} w_i\,. \tag{42}$$

Moreover, Condition 2.3 (partition of unity) is equivalent to Condition 3.5.

Proof. Firstly, we show (41) and (42):

$$\Xi_{iG} D_i \overset{\text{Ass. 3.4}}{=} \sum_{G \in \mathcal{G}_i} \underbrace{\Xi_{iG} R_{iG}^\top}_{= R_{iG}^\top} D_{iG} \underbrace{R_{iG}}_{= R_{iG}\Xi_{iG}} \overset{\text{Ass. 3.4}}{=} D_i \Xi_{iG}$$

$$E_D w \;=\; \sum_{i=1}^N R_i^\top D_i w_i \overset{\text{Ass. 3.4}}{=} \sum_{i=1}^N \sum_{G \in \mathcal{G}_i} \underbrace{R_i^\top R_{iG}^\top}_{= \widehat{R}_G^\top} D_{iG} R_{iG} w_i \;=\; \sum_{G \in \mathcal{G}} \widehat{R}_G^\top \sum_{i \in \mathcal{N}_G} D_{iG} R_{iG} w_i \,.$$

Secondly, (42) implies $E_D R = \sum_{G' \in \mathcal{G}} \widehat{R}_{G'}^\top \sum_{i \in \mathcal{N}_{G'}} D_{iG'} \widehat{R}_{G'}$.

If Condition 2.3 holds, the left-hand side evaluates to I and we obtain Condition 3.5 by multiplying from the left by $\widehat{R}_G$ and from the right by $\widehat{R}_G^\top$ (for an arbitrary $G \in \mathcal{G}$ and using (21)). Conversely, if Condition 3.5 holds, the right-hand side evaluates to I due to (25), so Condition 2.3 is fulfilled. ☐

The following two results will be helpful for Section 3.3.

Lemma 3.7. *Let Assumption 3.4 (D_i block diagonal) and Condition 3.5 (glob-wise partition of unity) hold. Then*

(i)

$$\widehat{\Xi}_G E_D = E_D \Xi_G \,, \qquad (R E_D \Xi_G)^2 = R E_D \Xi_G \,,$$
$$\Xi_G P_D = P_D \Xi_G \,, \qquad (P_D \Xi_G)^2 = P_D \Xi_G \,.$$

(ii)

$$\Xi_{iG} (P_D w)_i \;=\; R_{iG}^\top \sum_{j \in \mathcal{N}_G \setminus \{i\}} D_{jG} (R_{iG} w_i - R_{jG} w_j).$$

In particular,

$$\Xi_G P_D w = 0 \quad \Longleftrightarrow \quad \big(\forall i, j \in \mathcal{N}_G : R_{iG} w_i = R_{jG} w_j\big).$$

(iii) *If G is totally primal ($G \notin \mathcal{G}^*$, cf. Sect. 2.5.1) then*

$$\Xi_G P_D w = 0 \qquad \forall w \in \widetilde{W}.$$

Proof. (i) By definition, $E_D = R^\top D$ with $D = \operatorname{diag}(D_i)_{i=1}^N$. From (24), (41) we get

$$\widehat{\Xi}_G E_D = \widehat{\Xi}_G R^\top D = R^\top \Xi_G D = R^\top D \Xi_G = E_D \Xi_G \,.$$

The other assertions follow immediately from (24), the fact that $(R E_D)^2 = R E_D$ (Proposition 3.6 and Proposition 2.4) and the definition of P_D.

(ii) From the definitions of E_D and P_D we get

$$R_{iG} (P_D w)_i \;=\; R_{iG} w_i - \widehat{R}_G E_D w \qquad \forall i \in \mathcal{N}_G \,. \tag{43}$$

Applying $\widehat{R}_G$ to formula (42), we find that

$$\widehat{R}_G E_D w \overset{(42)}{=} \sum_{G' \in \mathcal{G}} \widehat{R}_G \widehat{R}_{G'}^\top \sum_{j \in \mathcal{N}_{G'}} D_{jG'} R_{jG'} w_j \overset{(22)}{=} \sum_{j \in \mathcal{N}_G} D_{jG} R_{jG} w_j \,.$$

Substituting the latter result into (43) yields

$$R_{iG}^\top R_{iG} (P_D w)_i \;=\; R_{iG}^\top \Big(R_{iG} w_i - \sum_{j \in \mathcal{N}_G} D_{jG} R_{jG} w_j \Big).$$

The definition of Ξ_{iG} and Condition 3.5 yield the desired formula.
(iii) If $G \notin \mathcal{G}^*$ and $w \in \widetilde{W}$ then, $Q_G^\top(R_{iG}w_i - R_{jG}w_j) = 0$ for all i, $j \in \mathcal{N}_G$, cf. Def 2.21. Since $Q_G^\top$ is non-singular, $R_{iG}w_i = R_{jG}w_j$ and Lemma 3.7(ii) implies that $\Xi_G P_D w = 0$. □

3.3. **A glob-based localization of the P_D estimate (19).** Recall the formula in Lemma 3.7(ii). We define

$$(44)\qquad P_{D,G}\colon W_{\mathcal{N}_G} \to W_{\mathcal{N}_G}\colon \quad (P_{D,G}w)_i := R_{iG}^\top \sum_{j\in\mathcal{N}_G\setminus\{i\}} D_{jG}(R_{iG}w_i - R_{jG}w_j).$$

Lemma 3.8. *Let Assumption 3.4 (D_i block diagonal) and Condition 3.5 (glob-wise partition of unity) hold. Then*

(i) $\Xi_{iG}(P_D w)_i = (P_{D,G}w_{\mathcal{N}_G})_i \qquad \forall w \in W,$

(ii) $P_{D,G}^2 = P_{D,G}.$

(iii) $\ker(P_{D,G}) = \{w \in W_{\mathcal{N}_G}\colon \forall i,j \in \mathcal{N}_G\colon R_{iG}w_i = R_{jG}w_j\}.$

(iv) $P_{D,G}w \in \widetilde{W}_{\mathcal{N}_G} \iff w \in \widetilde{W}_{\mathcal{N}_G}$,
in particular, $P_{D,G}(\widetilde{W}_{\mathcal{N}_G}) \subset \widetilde{W}_{\mathcal{N}_G}$ *and* $\mathrm{range}(P_{D,G}) \cap \widetilde{W}_{\mathcal{N}_G} = P_{D,G}(\widetilde{W}_{\mathcal{N}_G})$,

(v) *there exists a projection operator* $\widetilde{P}_{D,G}\colon \widetilde{W}_{\mathcal{N}_G} \to \widetilde{W}_{\mathcal{N}_G}$ *such that* $P_{D,G}\widetilde{I}_{\mathcal{N}_G} = \widetilde{I}_{\mathcal{N}_G}\widetilde{P}_{D,G}$, *where* $\widetilde{I}_{\mathcal{N}_G}\colon \widetilde{W}_{\mathcal{N}_G} \to W_{\mathcal{N}_G}$ *is the natural embedding.*

Proof. Part (i) follows from Lemma 3.7(ii) and the definition of $P_{D,G}$, and Part (ii) from Lemma 3.7(i). Part (iii) can be derived using Lemma 3.7(ii). Part (iv): For $y \in W_{\mathcal{N}_G}$ and $w = P_{D,G}y$ one easily shows that

$$Q_G^\top R_{iG}w_i \;=\; Q_G^\top R_{iG}(\Xi_{iG}y_i - R_{iG}^\top \overline{y}_G), \quad \text{where } \overline{y}_G = \sum_{j\in\mathcal{N}_G} D_{iG}R_{jG}w_j\,,$$

$$Q_G^\top(R_{iG}w_i - R_{jG}w_j) \;=\; Q_G^\top(R_{iG}y_i - R_{jG}y_j).$$

Finally, Part (v) follows from Parts (ii) and (iii). □

Remark 3.9. If $\widetilde{W}$ does not originate from primal dofs on open globs (Definition 2.15), then Parts (iii) and (v) do not necessarily hold.

As the next theorem shows, the global bound (19) can be established from local bounds associated with individual globs:

Local glob estimate:

$$(45)\qquad \sum_{i\in\mathcal{N}_G} |(P_{D,G}w)_i|_{S_i}^2 \;\le\; \omega_G \sum_{i\in\mathcal{N}_G} |w_i|_{S_i}^2 \qquad \forall w \in \widetilde{W}_{\mathcal{N}_G}.$$

Theorem 3.10. *Let Assumption 3.4 (D_i block diagonal) and Condition 3.5 (glob-wise partition of unity) be fulfilled and let $\widetilde{W}$ be defined by classical primal dofs (Def. 2.21). For each glob $G \in \mathcal{G}^*$ (that is not totally primal), assume that the local estimate* (45) *holds with some constant $\omega_G < \infty$. Then the global P_D-estimate* (19) *holds with*

$$\omega = \Big(\max_{i=1,\ldots,N} |\mathcal{G}_i^*|^2\Big)\big(\max_{G\in\mathcal{G}^*}\omega_G\big),$$

where $|\mathcal{G}_i^*|$ denotes the cardinality of the set $\mathcal{G}_i^*$. In particular, if, in addition, $\widetilde{S}$ is definite (Condition 2.6), then Theorem 2.8 implies $\kappa_{BDDC} \le \omega$.

Proof. Firstly, we use (25), Lemma 3.7(iii) and Lemma 3.8(i) to obtain

$$(P_D w)_i \;=\; \sum_{G \in \mathcal{G}_i} \Xi_{iG} (P_D w)_i \;=\; \sum_{G \in \mathcal{G}_i^*} \Xi_{iG} (P_D w)_i \;=\; \sum_{G \in \mathcal{G}_i^*} (P_{D,G} w_{\mathcal{N}_G})_i \,.$$

Secondly, the Cauchy-Bunyakovsky-Schwarz inequality and the local bounds (45) imply

$$\begin{aligned}
\sum_{i=1}^N |(P_D w)_i|_{S_i}^2 \;&\leq\; \sum_{i=1}^N |\mathcal{G}_i^*| \sum_{G \in \mathcal{G}_i^*} |(P_{D,G} w_{\mathcal{N}_G})_i|_{S_i}^2 \\
&\leq\; \big(\max_{i=1,\ldots,N} |\mathcal{G}_i^*| \big) \sum_{G \in \mathcal{G}^*} \sum_{j \in \mathcal{N}_G} |(P_{D,G} w)_j|_{S_j}^2 \\
&\leq\; \big(\max_{i=1,\ldots,N} |\mathcal{G}_i^*| \big) \sum_{G \in \mathcal{G}^*} \sum_{j \in \mathcal{N}_G} \omega_G \, |w_i|_{S_i}^2 \\
&\leq\; \big(\max_{i=1,\ldots,N} |\mathcal{G}_i^*| \big) \sum_{i=1}^N \sum_{G \in \mathcal{G}_i^*} \omega_G \, |w_i|_{S_i}^2 \,.
\end{aligned}$$

Finally, $\sum_{G \in \mathcal{G}_i^*} \omega_G \leq (\max_{i=1,\ldots,n} |\mathcal{G}_i^*|)(\max_{G \in \mathcal{G}^*} \omega_G)$. □

The arguments in the proof above are not new and are used in all the known theoretical condition number bounds of FETI, FETI-DP and BDDC for specific PDEs and discretizations, see, e.g., [7, 22, 57, 59, 77, 78, 107]. The more recent works [16, 49] make implicitly use of Thm. 3.10, and a similar result for the two-dimensional case can be found in [50, Thm. 5.1].

Remark 3.11. If Assumption 3.4 did not hold, i.e, if the matrices D_i were not block-diagonal w.r.t. the globs, we would need an estimate of the form

$$\sum_{i \in \mathcal{N}_G} |\Xi_{iG} (P_D w)_i|_{S_i}^2 \;\leq\; \omega_G \sum_{j \in \mathcal{N}_G^+} |w_j|_{S_j}^2 \qquad \forall w \in \widetilde{W},$$

where $\mathcal{N}_G^+$ are the subdomains of $\mathcal{N}_G$ and all their next neighbors.

Remark 3.12. Certainly, if the local glob estimate (45) holds on a *larger* space than $\widetilde{W}_{\mathcal{N}_G}$, we get a similar result (possibly with a pessimistic bound ω_G). A possible choice for such a space is

$$\widetilde{W}_{\mathcal{N}_G}^G \;:=\; \{ w = [w_i]_{i \in \mathcal{N}_G} : \forall i \neq j \in \mathcal{N}_G : Q_G^\top R_{iG}^\top w_i = Q_G^\top R_{jG}^\top w_j \}, \tag{46}$$

i.e., the space of functions living "around" G, where only the primal constraints associated with G are enforced. We shall make use of this later in Sect. 4.2, Strategy 4.

Remark 3.13. Whereas the local estimate (45) is *glob*-based, other localizations used in the literature are *subdomain*-based. For example, translating the suggestion by Kraus et al. [61, Sect. 5] to our framework leads to the estimate

$$|(P_D w)_i|_{S_i}^2 \;\leq\; \omega_i \sum_{j \in \mathcal{N}_i} |w_j|_{S_j}^2 \qquad \forall w \in \widetilde{W}_{\mathcal{N}_i} \,,$$

where $\mathcal{N}_i$ are the neighboring subdomains of i and $\widetilde{W}_{\mathcal{N}_i}$ is the restriction of $\widetilde{W}$ to these. Another option, probably related to the work by Spillane and Rixen [104], is

$$\sum_{j \in \mathcal{N}_i} |(P_D w)_j|_{S_j}^2 \;\leq\; \omega_i \, |w_i|_{S_i}^2$$

for all $w \in W$ that vanish in all but the i-th subdomain.

3.4. **A review of a pair-based localization***. The local estimate (45) was first proposed in [73] (see also [101, 76, 102]), there, however, in slightly different form on every *closed* face F

$$\big(|\Xi_{i,\overline{F}}(P_D w)_i|^2_{S_i} + |\Xi_{j,\overline{F}}(P_D w)_j|^2_{S_j}\big) \;\le\; \omega_{\overline{F}}\big(|w_i|^2_{S_i} + |w_j|^2_{S_j}\big) \qquad \forall w \in \widetilde{W}, \tag{47}$$

where $\mathcal{N}_F = \{i,j\}$ and $\Xi_{i,\overline{F}} := \sum_{G\subset\overline{F}} \Xi_{i,G}$ is the filter matrix corresponding to $\overline{F}$. Under Assumption 3.4 (D_i block diagonal) and Condition 3.5 (glob-wise partition of unity), the estimate can be expressed using a space $\widetilde{W}_{\overline{F}}$ and an operator $P_{D,\overline{F}}$ defined analogously to $\widetilde{W}_G$ and $P_{D,G}$, respectively. In [73, 76], the local bounds are used to define the *condition number indicator*

$$\widetilde{\omega} := \max_{F\in\mathcal{F}} \omega_{\overline{F}}\,. \tag{48}$$

If every glob G is either totally primal or $|\mathcal{N}_G| = 2$ (typical for two-dimensional problems), then it does not matter whether one uses the open or closed face, and (19) holds with $\omega = \widetilde{\omega}$, so $\widetilde{\omega}$ is indeed a reliable bound for the condition number; see also [50, Thm. 5.1].

For the three-dimensional case, the reliablity of (48) was open for quite a long time. In their recent preprint [45], Klawonn, Kühn, and Rheinbach show that in general, (48) is reliable, if (i) all vertices are totally primal and (ii) one includes some estimates associated with those subdomain edges that share more than three subdomains. In the following, we present this latest theory under a slightly different perspective.

If Assumption 3.4 (glob-wise partition of unity) holds then

$$(P_D w)_i \;=\; \sum_{j\in\mathcal{N}_i} \sum_{\substack{G\in\mathcal{G}^*\\ \{i,j\}\subset\mathcal{N}_G}} R_{iG}^\top D_{jG}(R_{iG}w_i - R_{jG}w_j), \tag{49}$$

where $\mathcal{N}_i := \bigcup_{G\in\mathcal{G}_i} \mathcal{N}_G$ is the set of neighboring subdomains of subdomain i. This formula motivates a *neighbor-based* viewpoint and the following definition.

Definition 3.14 (generalized facet)**.** For each pair $\{i,j\}$, $i \neq j$, we define the *generalized facet*

$$\Gamma_{ij} := \bigcup_{G\in\mathcal{G}^*\colon \{i,j\}\subset\mathcal{N}_G} G,$$

i.e., the set of dofs shared by subdomains i and j, excluding totally primal dofs. Note that $\Gamma_{ji} = \Gamma_{ij}$. The set of non-trivial generalized facets is given by

$$\Upsilon^* := \{\Gamma_{ij}\colon i,j = 1,\ldots,N,\ i\neq j,\ \Gamma_{ij}\neq\emptyset\}.$$

Remark 3.15. Most of these generalized facets are *closed faces*. Assume that every vertex is chosen totally primal, then in two dimensions, all generalized facets are actually closed faces. In three dimensions, if we have a regular subdomain edge E shared by four or more subdomains, then for each pair $i \neq j$ with $\{i,j\} \in \mathcal{N}_E$ where no face F exists such that $\{i,j\} \in \mathcal{N}_F$ we get a generalized facet Γ_{ij}. According to [95, 45], for decompositions generated from a graph partitioner, most of the subdomain edges share only three subdomains.

We fix an ordering of the dofs for each set Γ_{ij} and denote by $R_{i\Gamma_{ij}}\colon W_i \to U_{\Gamma_{ij}}$ the corresponding zero-one restriction matrix. For each sub-glob $G \subset \Gamma_{ij}$, we denote by $R_{G\Gamma_{ij}}\colon U_{\Gamma_{ij}} \to U_G$ the zero-one restriction matrix such that $R_{iG} = R_{G\Gamma_{ij}} R_{i\Gamma_{ij}}$.

Moreover, for each *pair* (i, j) with $\Gamma_{ij} \in \Upsilon^*$, we denote by W_{ij}, $\widetilde{W}_{ij}$ the restriction of W, $\widetilde{W}$, respectively, to the two components i, j. The restriction of a vector $w \in \widetilde{W}$ or W is denoted by w_{ij}. With this notation, we deduce from (49) that

$$
\begin{aligned}
(P_D w)_i &= \sum_{j\colon \Gamma_{ij}\in\Upsilon^*} R_{i\Gamma_{ij}}^\top \underbrace{\Big(\sum_{G\subset\Gamma_{ij}} R_{G\Gamma_{ij}}^\top D_{jG} R_{G\Gamma_{ij}} \Big)}_{=:\ D_{j\Gamma_{ij}}} (R_{i\Gamma_{ij}} w_i - R_{j\Gamma_{ij}} w_j) \\
&= \sum_{j\colon \Gamma_{ij}\in\Upsilon^*} \underbrace{R_{i\Gamma_{ij}}^\top D_{j\Gamma_{ij}} (R_{i\Gamma_{ij}} w_i - R_{j\Gamma_{ij}} w_j)}_{=:\ (P_{D,\Gamma_{ij}} w_{ij})_i},
\end{aligned} \tag{50}
$$

where $P_{D,\Gamma_{ij}} \colon W_{ij} \to W_{ij}$. The following result was first shown in [45, Lemma 6.1] with essentially the same constant.

Lemma 3.16. *Let Assumption 3.4 (glob-wise partition of unity) be fulfilled. If for every* $\Gamma_{ij} \in \Upsilon^*$, *the inequality*

$$
|(P_{D,\Gamma_{ij}} w_{ij})_i|_{S_i}^2 + |(P_{D,\Gamma_{ij}} w_{ij})_j|_{S_j}^2 \;\le\; \omega_{ij}\Big(|w_i|_{S_i}^2 + |w_j|_{S_j}^2 \Big) \qquad \forall w_{ij} \in \widetilde{W}_{ij}
$$

holds, then

$$
|P_D w|_S^2 \;\le\; \omega\, |w|_S^2 \qquad \forall w \in \widetilde{W},
$$

with $\omega = \big(\max_{i=1,\ldots,N} n_i^2\big)\,\big(\max_{\Gamma_{ij}\in\Upsilon^*} \omega_{ij}\big)$, *where* $n_i := |\{j\colon \Gamma_{ij} \in \Upsilon^*\}|$.

Proof. The Cauchy-Bunyakovsky-Schwarz inequality implies

$$
\begin{aligned}
\sum_{i=1}^N |(P_D w)_i|_{S_i}^2 &\le \sum_{i=1}^N n_i \sum_{j\colon \Gamma_{ij}\in\Upsilon^*} |(P_{D,\Gamma_{ij}} w_{ij})_i|_{S_i}^2 \\
&\le \big(\max_{i=1,\ldots,N} n_i\big) \sum_{\Gamma_{ij}\in\Upsilon^*} \Big(|(P_{D,\Gamma_{ij}} w_{ij})_i|_{S_i}^2 + |(P_{D,\Gamma_{ij}} w_{ij})_j|_{S_j}^2 \Big).
\end{aligned}
$$

Employing the local estimate and using Cauchy-Bunyakovsky-Schwarz another time yields

$$
\begin{aligned}
\sum_{i=1}^N |(P_D w)_i|_{S_i}^2 &\le \big(\max_{i=1,\ldots,N} n_i\big) \sum_{\Gamma_{ij}\in\Upsilon^*} \omega_{ij} \Big(|w_i|_{S_i}^2 + |w_j|_{S_i}^2 \Big) \\
&= \big(\max_{i=1,\ldots,N} n_i\big) \sum_{i=1}^N \sum_{j\colon \Gamma_{ij}\in\Upsilon^*} \omega_{ij} |w_i|_{S_i}^2 \\
&\le \big(\max_{i=1,\ldots,N} n_i^2\big) \big(\max_{\Gamma_{ij}\in\Upsilon^*} \omega_{ij}\big) \sum_{i=1}^N |w_i|_{S_i}^2 .
\end{aligned}
$$

□

Unlike the glob-based operator $P_{D,G}$, the pair-based operator $P_{D,\Gamma_{ij}}$ *fails* to be a projection. For this reason and the fact that adaptive constraints on the generalized facets Γ_{ij} would have to be specially treated (e.g., split) in order to ensure that the constraints associated with each subdomain are linearly independent, we do not pursue the pair-based localization further. Note, however, that parts (not all) of our theory could be transferred to the pair-based localization.

4. The glob eigenproblem for general scalings

The local glob estimate (45) is directly related to a generalized eigenproblem $A = \lambda B$, where A, B correspond to the right- and left-hand side of the estimate, respectively, and the best constant is the inverse of the minimal eigenvalue. We show this relation in detail (Sect. 4.1), allowing both A, B to be singular (in this, our presentation differs from [74, 76]). Next, we show how to reduce generalized eigenproblems by using Schur complements and how to modify them, obtaining the same or related estimates. In Sect. 4.2, we discuss the eigenproblem associated with estimate (45) and provide some strategies on how it could be computed in practice.

4.1. **Technical tools for generalized eigenproblems***. The following definition and lemma are common knowledge, but stated and proved for the sake of completeness; see also [36, Sect. 7.7.1], [76, Lem. 2], [103, Def. 2.10, Lem. 2.11], and [30, 49] for similar results.

Definition 4.1. Let V be a finite-dimensional (real) Hilbert space and A, $B\colon V \to V^*$ linear operators. We call (λ, y) a (real) *generalized eigenpair* of (A, B) if either

(a) $\lambda \in \mathbb{R}$ and $y \in V \setminus \{0\}$ fulfill $Ay = \lambda By$, or
(b) $\lambda = \infty$ and $y \in \ker(B) \setminus \{0\}$.

We will not need complex eigenvalues in the sequel. In this text, we say that λ is a *genuine eigenvalue* of (A, B) if there is an associated eigenvector in $V \setminus (\ker(A) \cap \ker(B))$.

Apparently, λ is a generalized eigenvalue of (A, B) if and only if $1/\lambda$ is a generalized eigenvalue of (B, A), where $1/0 := \infty$ and $1/\infty := 0$. The eigenspaces corresponding to $\lambda = 0$ and $\lambda = \infty$ are $\ker(A)$ and $\ker(B)$, respectively. If $\ker(A) \cap \ker(B)$ is non-trivial then every (λ, y) with $\lambda \in \mathbb{R} \cup \{\infty\}$ and $y \in \ker(A) \cap \ker(B)$ is a generalized eigenpair. If an eigenvalue λ has only eigenvectors in $\ker(A) \cap \ker(B)$, we call it *ambiguous* in the sequel. If B is non-singular then the generalized eigenvalues of (A, B) are the same as the regular eigenvalues of $B^{-1}A$, and if B is SPD as those of $B^{-1/2}AB^{-1/2}$, where $B^{1/2}$ is the SPD matrix square root. The next lemma treats the general SPSD case, and its proof is given on p. 25.

Lemma 4.2. *Let V be a finite-dimensional (real) Hilbert space and A, $B\colon V \to V^*$ linear operators that are SPSD. Then there exist at least $n = \dim(V) - \dim(\ker(B))$ genuine generalized eigenvalues*

$$0 \le \lambda_1 \le \lambda_2 \le \ldots \le \lambda_n < \infty$$

and a basis $\{y_k\}_{k=1}^{\dim(V)}$ of V such that $(\lambda_k, y_k)_{k=1}^n$ and $(\infty, y_k)_{k=n+1}^{\dim(V)}$ are generalized eigenpairs of (A, B) and

$$\langle By_k, y_\ell\rangle = \delta_{k\ell}, \qquad \langle Ay_k, y_\ell\rangle = \lambda_k \delta_{k\ell} \qquad\qquad \forall k, \ell = 1, \ldots, n,$$

and $\ker(B) = span\{y_k\}_{k=n+1}^{\dim(V)}$. Furthermore, for any $k \in \{0, \ldots, n-1\}$ with $\lambda_{k+1} > 0$,

$$\langle Bz, z\rangle \;\le\; \frac{1}{\lambda_{k+1}} \langle Az, z\rangle \qquad \forall z \in V,\ \langle By_\ell, z\rangle = 0,\ \ell = 1, \ldots, k.$$

The constant in this bound cannot be improved.

The next result is interesting in itself, cf. [103, Lem. 2.11].

Corollary 4.3. *Let $k \in \{0, \ldots, n-1\}$ with $\lambda_{k+1} > 0$ as in the previous lemma and let $\Pi_k \colon V \to V$ be the projection defined by $\Pi_k v := \sum_{\ell=1}^k \langle Bv, y_\ell \rangle y_\ell$. Then*

$$|\Pi_k v|_A \le |v|_A\,, \quad |(I-\Pi_k)v|_A \le |v|_A\,, \quad |\Pi_k v|_B \le |v|_B\,, \quad |(I-\Pi_k)v|_B \le |v|_B\,.$$

Moreover,

$$|(I-\Pi_k)v|_B^2 \;\le\; \frac{1}{\lambda_{k+1}} |(I-\Pi_k)v|_A^2 \;\le\; \frac{1}{\lambda_{k+1}} |v|_A^2 \qquad \forall v \in V.$$

Proof. All the estimates can be easily verified by using that any $v \in V$ can be written by $v = \sum_{\ell=1}^{\dim(V)} \beta_\ell y_\ell$ and by using the results of Lemma 4.2. □

For the proof of Lemma 4.2, we need an auxiliary result.

Principle 4.4 ("Schur principle": reduction of infinite eigenvalues by Schur complement)**.** *Let V be a finite-dimensional (real) Hilbert space and A, $B \colon V \to V^*$ two linear and self-adjoint operators. Let $V_2 \subset \ker(B)$ be a subspace and V_1 some complementary space such that $V = V_1 \oplus V_2$ (direct sum, not necessarily orthogonal). In that situation, we may identify V with $V_1 \times V_2$ and write*

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \qquad B = \begin{bmatrix} B_{11} & 0 \\ 0 & 0 \end{bmatrix}.$$

Assume that $\ker(A_{22}) \subset \ker(A_{12})$ (cf. Lemma D.3) and let $S_1 := A_{11} - A_{12}A_{22}^\dagger A_{21}$ be a generalized Schur complement (cf. Appendix D). Then the following holds:

(i) *(λ, y) is a generalized eigenpair of (A, B) if and only if either $\lambda = \infty$ and $y \in \ker(B)$, or*

$$y = \begin{bmatrix} y_1 \\ -A_{22}^\dagger A_{21} y_1 + v_2^K \end{bmatrix}, \quad \textit{for some } v_2^K \in \ker(A_{22})$$

and (λ, y_1) is a generalized eigenpair of (S_1, B_{11}).

(ii) *Assume that A, B are positive semi-definite and let $y_1, \ldots, y_m \in V_1$ be fixed. Then*

$$\langle Bz, z\rangle \le \gamma \langle Az, z\rangle \qquad \forall z \in V \colon \langle B \begin{bmatrix} y_\ell \\ 0 \end{bmatrix}, z\rangle = 0,\ \ell = 1, \ldots, m$$

if and only if

$$\langle B_{11} z_1, z_1\rangle \le \gamma \langle S_1 z_1, z_1 \rangle \qquad \forall z_1 \in V_1 \colon \langle B_{11} y_\ell, z_1\rangle = 0,\ \ell = 1, \ldots, m.$$

Proof of the "Schur" Principle 4.4. Part (i): Let (λ, y) be a generalized eigenpair of (A, B) and assume that $y \notin \ker(B)$. Consequently $\lambda \neq \infty$ and

$$\begin{aligned} A_{11} y_1 + A_{12} y_2 &= \lambda B_{11} y_1\,, \\ A_{21} y_1 + A_{22} y_2 &= 0. \end{aligned}$$

The second line holds if and only if $y_2 = -A_{22}^\dagger y_1 + v_2^K$ for some $v_2^K \in \ker(A_{22})$. Substituting y_2 into the first line yields

$$A_{11} y_1 - A_{12}(A_{22}^\dagger A_{21} y_1 + v_2^K) \;=\; \lambda B_{11} y_1\,.$$

Due to our assumption $v_2^K \in \ker(A_{12})$ and so $S_1 y_1 = \lambda B_{11}$. Conversely, assume that (λ, y_1) is a generalized eigenpair of (S_1, B_{11}). If $\lambda = \infty$ then $y_1 \in \ker(B_1)$ and y defined as in (i) fulfills $y \in \ker(B)$, so (∞, y) is a generalized eigenpair of (A, B). If $\lambda \neq \infty$,

one can easily verify that $Ay = \lambda By$ for y defined as in (i).
Part (ii) follows from the definition of B and from the minimizing property of S_1:

$$\langle Bz, z\rangle = \langle B_{11} z_1, z_1\rangle \le \gamma \langle S_{11} z_1, z_1\rangle \le \gamma \langle Az, z\rangle. \qquad \square$$

Proof of Lemma 4.2. We apply the "Schur" Principle 4.4 with $V_2 := \ker(B)$ and some complementary space V_1, such that $n = \dim(V_1)$. Since A is SPSD, Lemma D.3 ensures that indeed $\ker(A_{22}) \subset \ker(A_{12})$. Now B_{11} is positive *definite*, has a well-defined inverse, and defines an inner product $(v, w)_{B_{11}} := \langle B_{11} v, w\rangle$ on V_1. Apparently, $B_{11}^{-1} S_{11} \colon V_1 \to V_1$ is self-adjoint with respect to $(\cdot,\cdot)_{B_{11}}$. The classical spectral theorem (see e.g., [36, Sect. 8.1]) yields the existence of eigenpairs $(\widetilde{\lambda}_k, \widetilde{y}_k)_{k=1}^n$ such that $0 \le \widetilde{\lambda}_1 \le \widetilde{\lambda}_2 \le \ldots \le \widetilde{\lambda}_n < \infty$ with $(\widetilde{y}_k)_{k=1}^n$ forming a basis of V_1 and

$$\langle B_{11} \widetilde{y}_k, \widetilde{y}_\ell\rangle = \delta_{k\ell}, \qquad \langle S_1 \widetilde{y}_k, \widetilde{y}_\ell\rangle = \widetilde{\lambda}_k \delta_{k\ell} \qquad \forall k, \ell = 1, \ldots, n.$$

Next, we show an auxiliary estimate. Let $k < n$ be such that $\widetilde{\lambda}_{k+1} > 0$. Let $z_1 \in V_1$ be of form $z_1 = \sum_{\ell=k+1}^{\dim(V_1)} \beta_\ell \widetilde{y}_\ell$, which is equivalent to $\langle B_{11} \widetilde{y}_\ell, z_1\rangle = 0$, $\ell = 1, \ldots, k$. Then

$$\langle B_{11} z_1, z_1\rangle \;=\; \sum_{\ell=k+1}^n \beta_\ell^2 \;\le\; \frac{1}{\widetilde{\lambda}_{k+1}} \sum_{\ell=k+1}^n \widetilde{\lambda}_\ell \beta_\ell^2 \;=\; \frac{1}{\widetilde{\lambda}_{k+1}} \langle S_1 z_1, z_1\rangle.$$

The constant cannot be improved due to the Courant-Fisher minimax principle [36, Thm. 8.1.2]. Let $(y_k)_{k=n+1}^{\dim(V)}$ be a basis of $\ker(B)$ and set

$$\lambda_k = \widetilde{\lambda}_k, \qquad y_k = \begin{bmatrix} \widetilde{y}_k \\ -A_{22}^\dagger A_{21} \widetilde{y}_k \end{bmatrix} \qquad \text{for } k = 1, \ldots, n.$$

Now all the statements follow from Principle 4.4. $\square$

The "Schur" Principle 4.4 is not only valuable for the proof of Lemma 4.2 but will be quite useful in our subsequent theory and method as it provides a way to reduce an eigenproblem by keeping all the finite eigenvalues. Conversely, Principle 4.4 can be used to unroll a Schur complement popping up in a generalized eigenproblem.

Sometimes, we want to compute with matrices but on a subspace of $\mathbb{R}^n$ for which we do not have a basis at hand. The following principle is a slight generalization of [73, Lemma 5].

Principle 4.5 (projected eigenproblem)**.** *Let A, $B \in \mathbb{R}^{n\times n}$, let $\Pi\colon \mathbb{R}^n \to \mathbb{R}^n$ be some projection onto a subspace* $\operatorname{range}(\Pi) \subset \mathbb{R}^n$*, and let $Q \in \mathbb{R}^{n\times n}$ be SPD on* $\operatorname{range}(I - \Pi)$*, e.g., $Q = tI$ with $t \in \mathbb{R} > 0$.*

(i) *For $\lambda \in [0, \infty)$,*
   (a) $\Pi^T A \Pi y = \lambda \Pi^\top B \Pi y$ *and* $y \in \operatorname{range}(\Pi)$
   if and only if
   (b) $(\Pi^T A \Pi + (I - \Pi^\top) Q (I - \Pi)) y = \lambda \Pi^T B \Pi y$.

(ii) *If A is SPD on* $\operatorname{range}(\Pi)$ *then* $\Pi^\top A \Pi + (I - \Pi^\top) Q (I - \Pi)$ *is SPD.*

Proof. Part (i): If (a) holds, then $y \in \operatorname{range}(\Pi) = \ker(I - \Pi)$ and so (b) holds. If (b) holds, then $(I - \Pi^\top) Q (I - \Pi) y \in \operatorname{range}(\Pi^\top) = \ker(I - \Pi^\top)$ and so $(I - \Pi^\top) Q (I - \Pi) y = 0$. Since Q is SPD on $\operatorname{range}(I - \Pi)$, we obtain that $(I - \Pi) y = 0$, i.e., $y \in \ker(I - \Pi) = \operatorname{range}(\Pi)$, and so (a) holds.
Part (ii): Assume that A is SPD on $\operatorname{range}(\Pi)$ and that

$$\langle (\Pi^\top A \Pi + (I - \Pi^\top) Q (I - \Pi)) y, y\rangle = 0.$$

Then $\langle A\Pi y, \Pi y\rangle = 0$ and $\langle Q(I-\Pi)y, (I-\Pi)y\rangle = 0$. Due to the assumptions on A and Q, we obtain $\Pi y = 0$ and $(I-\Pi)y = 0$, and finally $y = 0$. □

Remark 4.6. It is yet questionable whether it is easier to construct a basis for a subspace of $\mathbb{R}^n$ or a projection onto it. If the matrices S_i stem from sparse stiffness matrices, then we would like the basis transformation matrix to be sparse too, in the sense that all rows and columns have $\mathcal{O}(1)$ non-zero entries except for $\mathcal{O}(1)$ rows/columns which may be dense.

Remark 4.7 ("saddle point" eigenproblem)**.** With similar arguments as in the proof of the "Schur" Principle 4.4, one can show that the generalized eigenproblem

$$\langle Ay, z\rangle = \lambda\langle By, z\rangle \qquad \forall y, z \in V := \{v \in \mathbb{R}^n \colon Cv = 0\},$$

with surjective $C \in \mathbb{R}^{m\times n}$, $m < n$, is equivalent to

$$\begin{bmatrix} A & C^\top \\ C & 0 \end{bmatrix} \begin{bmatrix} v \\ \mu \end{bmatrix} = \lambda \begin{bmatrix} B & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} v \\ \mu \end{bmatrix},$$

up to some eigenvalues of infinity. The latter eigenproblem is posed on the simpler space $\mathbb{R}^{n+m}$.

In the following two principles, the eigenvalues might change.

Principle 4.8 (eigenproblem on larger space)**.** *Let V, A, B be as in Lemma 4.2 and let $\widetilde{V} \supset V$ be a larger space with the natural embedding operator $E\colon V \to \widetilde{V}$. Suppose that there are SPSD operators $\widetilde{A}$, $\widetilde{B}\colon \widetilde{V} \to \widetilde{V}^*$ such that $A = E^\top \widetilde{A} E$ and $B = E^\top \widetilde{B} E$, and let $(\widetilde{\lambda}_k, \widetilde{y}_k)$ be the eigenpairs of $(\widetilde{A}, \widetilde{B})$ according to Lemma 4.2. If $\widetilde{\lambda}_{k+1} \in (0,\infty)$ then for all $z \in V$ with $\langle E^\top \widetilde{B} \widetilde{y}_\ell, z\rangle = 0$, $\ell = 1,\ldots,k$,*

$$\langle Bz, z\rangle = \langle \widetilde{B}Ez, Ez\rangle \le \frac{1}{\widetilde{\lambda}_{k+1}} \langle \widetilde{A}Ez, Ez\rangle = \frac{1}{\widetilde{\lambda}_{k+1}} \langle Az, z\rangle.$$

Principle 4.9 (nearby eigenproblem)**.** *Let V, A, B be as in Lemma 4.2 and let $\widetilde{A}$, $\widetilde{B}\colon V \to V^*$ be two SPSD operators such that*

$$\widetilde{A} \le c_1 A \quad \textit{and} \quad B \le c_2 \widetilde{B},$$

and let $(\widetilde{\lambda}_k, \widetilde{y}_k)$ be the eigenpairs of $(\widetilde{A}, \widetilde{B})$ according to Lemma 4.2. If $\widetilde{\lambda}_{k+1} \in (0,\infty)$ then for all $z \in V$ with $\langle \widetilde{B}\widetilde{y}_\ell, z\rangle = 0$, $\ell = 1,\ldots,k$,

$$\langle Bz, z\rangle \le c_2 \langle \widetilde{B}z, z\rangle \le \frac{c_2}{\widetilde{\lambda}_{k+1}} \langle \widetilde{A}z, z\rangle \le \frac{c_1\, c_2}{\widetilde{\lambda}_{k+1}} \langle Az, z\rangle.$$

When A, B have block structure, a special application of Principle 4.9 allows us to decouple the eigenproblem (at the price of approximation).

Principle 4.10 (decoupling)**.** *For a finite-dimensional Hilbert space V, let A, $B\colon V^n \to (V^n)^*$ be SPSD block operators,*

$$A = \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{bmatrix}, \qquad B = \begin{bmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{n1} & \cdots & B_{nn} \end{bmatrix}.$$

and let $m \leq n$ be the maximal number of non-zero block-entries per row of B. For each $i = 1, \ldots, n$ let S_i the Schur complement of A eliminating all but the i-th block. Then

$$\begin{bmatrix} S_1 & & \\ & \ddots & \\ & & S_n \end{bmatrix} \leq n\, A, \qquad B \leq m \begin{bmatrix} B_{11} & & \\ & \ddots & \\ & & B_{nn} \end{bmatrix}.$$

So if $(\lambda_k^{(i)}, y_k^{(i)})$ are the eigenpairs of (S_i, B_{ii}), and if $\lambda_{k_i+1}^{(i)} \in (0, \infty)$, then for all $z \in V^n$ with $\langle B_{ii} y_\ell^{(i)}, z_i \rangle = 0$ for $\ell = 1, \ldots, k_i$,

$$\langle Bz, z\rangle \leq n\, m \max_{i=1,\ldots,n} \frac{1}{\lambda_{k_i+1}} \langle Az, z\rangle.$$

Of course, different choice of the space splitting (leading to the block structure) can lead to different spectra in the decoupled eigenproblem.

Proof. The first spectral inequality follows from the minimizing property of the Schur complement (Lemma D.5), while the second one is simply a consequence of the Cauchy-Bunyakovsky-Schwarz inequality. The rest follows from Principle 4.9 (nearby eigenproblem). □

We also provide a simple result to recombine decoupled eigenproblems (A_i, B_i), $i = 1, \ldots, n$.

Principle 4.11 (recombination)**.** *Let V be a finite-dimensional Hilbert space and A_i, $B_i \colon V \to V^*$, $i = 1, \ldots, n$ SPSD operators. We consider the* single *eigenproblem*

$$\langle \underbrace{(A_1 : A_2 : \ldots : A_N)}_{=:\underline{A}} y, z\rangle = \lambda \langle \underbrace{(B_1 + B_2 + \ldots + B_N)}_{=:\overline{B}} y, z\rangle \qquad \text{for } y, z \in V,$$

with eigenpairs $(\overline{y}_k, \overline{\lambda}_k)$. For $m < n$ with $\overline{\lambda}_{m+1} > 0$,

$$|z|^2_{B_i} \;\leq\; \frac{1}{\overline{\lambda}_{m+1}} |z|^2_{A_i} \qquad \forall z \in \mathbb{R}^n \colon \langle \overline{B}\overline{y}_k, z\rangle = 0 \qquad \forall i = 1, \ldots, n$$

The same result holds for any $\underline{A}$ with $\underline{A} \leq A_i$ for all $i = 1, \ldots, n$.

Proof. For i and z as above,

$$|z|^2_{B_i} \;\leq\; |z|^2_{\overline{B}} \;\leq\; \frac{1}{\overline{\lambda}_{m+1}} |z|^2_{\underline{A}} \;\leq\; \frac{1}{\overline{\lambda}_{m+1}} |z|^2_{A_i}.$$ □

Finally, we need a result for general eigenproblems of special structure.

Lemma 4.12. *Let V be a finite-dimensional Hilbert space, $A \colon V \to V^*$ a linear SPSD operator and $P \colon V \to V$ a projection ($P^2 = P$). Then for*

$$B := \beta\, P^\top A P, \qquad \text{with } \beta \in (0, \infty),$$

the following statements hold:

(i) *The eigenspace of infinite generalized eigenvalues of (A, B) is given by*

$$\ker(B) \;=\; \ker(P) \oplus (\ker(A) \cap \operatorname{range}(P)),$$

and the ambiguous eigenspace by

$$\ker(A) \cap \ker(B) \;=\; (\ker(A) \cap \ker(P)) \oplus (\ker(A) \cap \operatorname{range}(P)).$$

(ii) *If $\ker(A) \subset \ker(P)$, then (A, B) has no genuine zero eigenvalues.*

(iii) *If* $\ker(A) \cap \operatorname{range}(P) = \{0\}$ *and if* (A, B) *has no genuine zero eigenvalues then*

$$\ker(A) \;\subset\; \ker(P).$$

Proof. (i) Since P is a projection, $V = \ker(P) \oplus \operatorname{range}(P)$. Assume that

$$v = v_1 + v_2 \in \ker(B), \qquad \text{with } v_1 \in \ker(P), \quad v_2 \in \operatorname{range}(P).$$

From the definition of B we see that $Bv_1 = 0$ and so, if $v \in \ker(B)$ then

$$0 = \langle Bv, v\rangle = \langle Bv_2, v_2\rangle = \beta\,\langle APv_2, Pv_2\rangle = \beta\,\langle Av_2, v_2\rangle,$$

and so $Av_2 = 0$. Conversely, if $v_1 \in \ker(P)$ and $v_2 \in \ker(A) \cap \operatorname{range}(P)$, then $v_1 + v_2 \in \ker(B)$. The formula for $\ker(A) \cap \ker(B)$ is then straightforward.
(ii) If $\ker(A) \subset \ker(P)$ then $\ker(A) \cap \operatorname{range}(P) = \{0\}$ and so $\ker(B) = \ker(P)$. Also, $\ker(A) \cap \ker(B) = \ker(A) \cap \ker(P)$ and $\ker(A) \setminus \ker(B) = \emptyset$.
(iii) Let $\lambda_1 \leq \ldots$ be the genuine eigenvalues of (A, B) according to Lemma 4.2. If there are no genuine zero eigenvalues, then $\lambda_1 > 0$. Suppose $v \in \ker(A)$, then

$$\langle Bv, v\rangle \;\leq\; \frac{1}{\lambda_1}\langle Av, v\rangle \;=\; 0$$

and so $v \in \ker(B) = \ker(P) \oplus (\ker(A) \cap \operatorname{range}(P))$, using Part (i). Due to our assumptions, $\ker(A) \cap \operatorname{range}(P) = \{0\}$ and so $v \in \ker(P)$. □

Let us apply the "Schur" Principle 4.4 to the generalized eigenproblem $(A, \beta P^\top AP)$ and eliminate $\ker(P)$. If $\ker(A) \cap \operatorname{range}(P) = \{0\}$, then the reduced eigenproblem neither has ambiguous nor infinite eigenvalues. Under the stronger condition $\ker(A) \subset \ker(P)$ (see Lemma 4.12(ii) and (iii)), the reduced eigenproblem has only eigenvalues in $(0, \infty)$.

4.2. **Generalized eigenproblems associated with estimate** (45)**.** Let us fix a set of linearly independent primal dofs in the sense of Definition 2.15 (possibly an empty set) and let $G \in \mathcal{G}^*$. Recall the space $\widetilde{W}_{\mathcal{N}_G}$ from (39) and let $\widetilde{I}_{\mathcal{N}_G} \colon \widetilde{W}_{\mathcal{N}_G} \to W_{\mathcal{N}_G}$ denote the natural embedding. Moreover define

$$S_{\mathcal{N}_G} := \operatorname{diag}(S_i)_{i \in \mathcal{N}_G} \colon W_{\mathcal{N}_G} \to W_{\mathcal{N}_G}$$

and consider the

generalized eigenproblem associated with glob G:

$$\widetilde{\mathcal{S}}_{\mathcal{N}_G} y \;=\; \lambda\,\widetilde{\mathcal{B}}_G y \qquad (y \in \widetilde{W}_{\mathcal{N}_G}), \tag{51}$$

with

$$\widetilde{\mathcal{S}}_{\mathcal{N}_G} := \widetilde{I}_{\mathcal{N}_G}^\top S_{\mathcal{N}_G} \widetilde{I}_{\mathcal{N}_G}, \qquad \widetilde{\mathcal{B}}_G := \widetilde{P}_{D,G}^\top \widetilde{\mathcal{S}}_{\mathcal{N}_G} \widetilde{P}_{D,G} = \widetilde{I}_{\mathcal{N}_G}^\top P_{D,G}^\top S_{\mathcal{N}_G} P_{D,G} \widetilde{I}_{\mathcal{N}_G},$$

where $\widetilde{P}_{D,G}$ is the projection operator from Lemma 3.8(v). The next result immediately follows from Lemma 4.2.

Corollary 4.13. *Let* $(\lambda_{G,k}, \widetilde{y}_{G,k})_{k=1}^{\dim(\widetilde{W}_{\mathcal{N}_G})}$ *be the generalized eigenpairs of* $(\widetilde{\mathcal{S}}_{\mathcal{N}_G}, \widetilde{\mathcal{B}}_G)$ *according to Lemma 4.2 with* $0 \leq \lambda_{G,1} \leq \lambda_{G,2} \leq \ldots \leq \infty$.
(i) If there are no genuine zero eigenvalues ($\lambda_{G,1} > 0$)*, then estimate* (45) *holds with*

$$\omega_G \;=\; \frac{1}{\lambda_{G,1}}\,.$$

(ii) Let us fix a number m_G such that $0 < \lambda_{G,m_G+1} < \infty$ and let $\Phi_{G,\mathrm{add}}\colon \mathbb{R}^{m_G} \to W_{\mathcal{N}_G}$ be the matrix whose columns are the first m_G eigenvectors,

$$\Phi_{G,\mathrm{add}} = \left[\, \cdots \middle| \widetilde{I}_{\mathcal{N}_G} \widetilde{y}_{G,k} \middle| \cdots \right]_{k=1}^{m_G}.$$

Then

(52)

$$\sum_{i\in\mathcal{N}_G} |(P_{D,G}w)_i|_{S_i}^2 \;\le\; \frac{1}{\lambda_{G,m_G+1}} \sum_{i\in\mathcal{N}_G} |w_i|_{S_i}^2 \qquad \forall w \in \widetilde{W}_{\mathcal{N}_G},\ \Phi_{G,add}^\top P_{D,G}^\top S_{\mathcal{N}_G} P_{D,G} w = 0,$$

which is an improved estimate compared to (45)*.*

Lemma 4.14. *If Assumption 3.4 (D_i block diagonal) holds and Condition 3.1 (local kernel condition, p. 16) is fulfilled then* (51) *has no genuine zero eigenvalues.*

Proof. Condition 3.1 is equivalent to $\ker(\mathcal{S}_{\mathcal{N}_G}) \cap \widetilde{W}_{\mathcal{N}_G} \subset \ker(P_{D,G})$ which, by using Lemma 3.8(v), is further equivalent to

$$\ker(\widetilde{\mathcal{S}}_{\mathcal{N}_G}) \;\subset\; \ker(\widetilde{P}_{D,G}).$$

Due to Assumption 3.4 and Lemma 3.8(v), $\widetilde{P}_{D,G}$ is a projection and the statement follows from Lemma 4.12(ii). □

Remark 4.15. The converse of Lemma 4.14 does not hold in general. In Sect. 7, we will formulate additional assumptions, under which one can conclude Condition 3.1 (local kernel condition) from the positivity of the genuine eigenvalues.

One can now think of several strategies.

Strategy 1. We solve the generalized eigenproblem (51) right away.

Strategy 2. If each S_i is the Schur complement of a sparse stiffness matrix A_i, we can unroll the elimination and consider, by applying the "Schur" Principle 4.4, the associated *sparse* generalized eigenproblem which has the same spectrum up to ambiguous and infinite eigenvaues. Applying additionally Principle 4.5 (projected eigenproblem) leads to the method in [73, 76], except that the eigenproblem therein is posed on the closed faces, and that the roles of A and B are interchanged.

Strategy 3. In Strategies 1 and 2, we expect a series of infinite eigenvalues. To get rid of (some of) them, observe that

$$\begin{aligned} \ker(\widetilde{P}_{D,G}) &= \widetilde{X}_G \oplus \widehat{Y}_G, \\ \widetilde{X}_G &= \{w \in \widetilde{W}_{\mathcal{N}_G} \colon \forall i \in \mathcal{N}_G \colon R_{iG} w_i = 0\}, \\ \widehat{Y}_G &= \{w \in \widetilde{W}_{\mathcal{N}_G} \colon \forall i \in \mathcal{N}_G \colon R_{iG^c} w_i = 0 \text{ and } \forall j \in \mathcal{N}_G \colon R_{iG} w_i = R_{jG} w_j)\}, \end{aligned}$$

where R_{iG^c} is the restriction matrix extracting all dofs *not* associated with glob G, with the property

$$R_{iG}^\top R_{iG} + R_{iG^c}^\top R_{iG^c} \;=\; I. \tag{53}$$

Functions from the space $\widetilde{X}_G \subset \widetilde{W}_{\mathcal{N}_G}$ vanish on G, whereas functions from $\widehat{Y}_G$ are continuous on G and vanish on all other dofs. Using a change of basis, we can parametrize $\widetilde{W}_{\mathcal{N}_G}$ and the two subspaces above explicitly. Forming the Schur eigenproblem according to Principle 4.4 eliminating $\ker(\widetilde{P}_{D,G})$, we get rid of some ambiguous infinite eigenvalues, which may be important in practice.

Strategy 4. We apply Principle 4.8 and embed the eigenproblem into the *larger* space

$$\widetilde{W}_{\mathcal{N}_G}^G := \{w \in W_{\mathcal{N}_G} \colon \forall i, j \in \mathcal{N}_G \colon Q_G^\top(R_{iG} w_i - R_{jG} w_j) = 0\}$$

from Remark 3.12. We warn the reader that doing this, we *discard* any (good) influence of the primal constraints on the neighboring globs of G. Defining the projection operator $\widetilde{P}_{D,G}^G$ analogously as $\widetilde{P}_{D,G}$ in Lemma 3.8(v), replacing $\widetilde{W}_{\mathcal{N}_G}$ by $\widetilde{W}_{\mathcal{N}_G}^G$, we find that the eigenproblem has the form $(\widetilde{\mathcal{S}}_{\mathcal{N}_G}^G, (P_{D,G}^G)^\top \widetilde{\mathcal{S}}_{\mathcal{N}_G}^G P_{\mathcal{N}_G}^G)$. As an advantage,

$$\ker(\widetilde{P}_{D,G}^G) = X_G \oplus \widehat{Y},$$

where the first space

$$X_G = \{w \in W_{\mathcal{N}_G} \colon \forall i \in \mathcal{N}_G \colon R_{iG} w_i = 0\} = \bigotimes_{i \in \mathcal{N}_G} \{w_i \in W_i \colon R_{iG} w_i = 0\} \supset \widetilde{X}_G$$

is much simpler than $\widetilde{X}_G$. Consequently, it is much simpler to implement the Schur complement operator of $\mathcal{S}_{\mathcal{N}_G}$ on $\widetilde{W}_{\mathcal{N}_G}^G$ eliminating $X_G \oplus \widehat{Y}$. Let us also note that if no primal constraints are enforced on the neighboring globs (G' with $|\mathcal{N}_G \cap \mathcal{N}_{G'}| \geq 2$), then $\widetilde{W}_{\mathcal{N}_G} = \widetilde{W}_{\mathcal{N}_G}^G$, i.e., the two eigenproblems are identical.

For all strategies, the underlying spaces are given implicitly, as subspaces of $\mathbb{R}^n$. One can either explicitly parametrize them by $\mathbb{R}^m$, $m < n$ (i.e., constructing a basis), or construct a projection from $\mathbb{R}^n$ to the subspace and apply Principle 4.5 (projected eigenproblem). As an alternative, one can use the constraints defining the subspace in the eigenproblem (Remark 4.7). Note also that for all the Strategies 1–4, the initially chosen primal constraints on the glob G are preserved. Modifying them means changing the eigenproblem; see also Remark 4.16 below.

No matter which of the four strategies we use, we will always get the statement of Corollary 4.13 (with some of the operators replaced):

1. If the minimal eigenvalue $\lambda_{G,1}$ of the respective generalized eigenproblem is *positive*, then the local glob estimate (45) with $\omega_G = \frac{1}{\lambda_{G,1}}$.
2. We can *improve* the estimate by enforcing *additional* constraints of the form

(54) $$\Phi_{G,\mathrm{add}}^\top P_{D,G}^\top \mathcal{S}_{\mathcal{N}_G} P_{D,G} w_{\mathcal{N}_G} = 0.$$

   These constraints are of the more general form in Sect. 2.6 and fulfill the conditions (35)–(36) of locality and consistency.

Remark 4.16 (orthogonality of constraints)**.** For each of the strategies, we consider a generalized eigenproblem of the form: find eigenpairs $(y, \lambda) \in \widetilde{V} \times \mathbb{R}$:

$$\langle Ay, z \rangle \;=\; \lambda \langle By, z \rangle \qquad \forall z \in \widetilde{V} := \{v \in V \colon Cv = 0\},$$

where $Cv = 0$ correspond to initially chosen constraints. An adaptively chosen constraint reads

$$\langle q_k, w \rangle := \langle B y_k, w \rangle = 0,$$

where y_k is an eigenvector. Assume that B is SPD. Then the functionals q_k are pairwise orthogonal in the B^{-1}-inner product. Since $C y_k = 0$, it follows that

$$C B^{-1} q_k = 0,$$

so the new constraints q_k are also pairwise orthogonal to the initial constraints in the B^{-1}-inner product. This pattern also applies to the simpler eigenproblems in the coming section.

5. Adaptive choice of primal dofs

In this section, we

(i) study more in detail the structure of the glob eigenproblem (51) for subdomain faces (Sect. 5.2) and general globs (Sect. 5.3),
(ii) show how to turn the constraints (54) originating from the local generalized eigenproblems into primal dofs (Sect. 5.4),
(iii) provide a way to rewrite the glob eigenproblem using a transformation of variables and to decouple it into $(n-1)$ independent eigenproblems where n is the number of subdomains shared by the glob (Sect. 5.5),
(iv) show that recombining the $(n-1)$ into a single one leads to the eigenproblem proposed by Kim, Chung, and Wang (Sect. 5.6),
(v) comment on how the eigenproblems could be organized in an algorithm (Sect. 5.7).

To this end, we need further notation (given below) and the *parallel sum* of matrices (Sect. 5.1).

Definition 5.1. For $G \in \mathcal{G}_i$ let

$$S_{iG} := R_{iG} S_i R_{iG}^\top \tag{55}$$

denote the restriction of S_i to the dofs on G and

$$S_{iGG^c} := R_{iG} S_i R_{iG^c}, \quad S_{iG^cG} := R_{iG^c} S_i R_{iG}, \quad S_{iG^c} := R_{iG^c} S_i R_{iG^c} \tag{56}$$

the other subblocks of S_i, where R_{iG^c} is the restriction matrix from (53). Finally, we define the (generalized) Schur complement

$$S_{iG}^\star := S_{iG} - S_{iGG^c} S_{iG^c}^\dagger S_{iG^cG}\,. \tag{57}$$

Remark 5.2. In practice, the matrix $S_{kG}^\star$ is usually linked to a problem on subdomain k with fixed dofs on G and homogeneous "Neumann" conditions on the remaining boundary dofs. Figure 4 shows that it may happen that S_{kG}, S_{kG^c}, or $S_{kG}^\star$ are singular.

Remark 5.3. As we use these matrices in the subsequent eigenproblems, we spend some words on their handling in practice. Suppose that S_i is the Schur complement of a sparse matrix A_i eliminiating interior dofs. Since S_{iG} is a principal minor of S_i, its application can be realized by a subdomain solve. Some direct solvers, such as MUMPS [2] or PARDISO [62] offer the possibility of computing the dense matrix S_{iG} directly. Since G^c usually contains many more dofs than G, computing S_{iGG^c}, $S_{iG^cG^c}$ in the same way would be inefficient. Instead, following Stefano Zampini [113], one can compute $S_i^\dagger$ once and extract $S_{iG}^\star$ as a principal minor of $S_i^\dagger$, see also [81].

5.1. **The parallel sum of matrices***.

The following definition was originally introduced by Anderson and Duffin [3] for Hermitian positive semi-definite matrices.

Definition 5.4 (parallel sum of matrices [3]). For two SPSD matrices A, $B \in \mathbb{R}^{n\times n}$ the *parallel sum* of A, B is given by

$$A : B \;=\; A(A+B)^\dagger B,$$

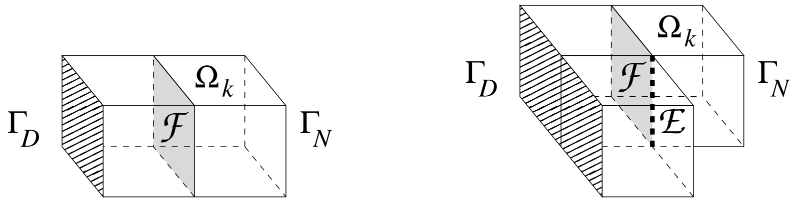

FIGURE 4. *Left:* Laplace/linear elasticity: S_{kF^c} empty, $S^\star_{kF}$ singular. *Right:* Linear elasticity, straight edge E: $S_{kE^c} = S_{kF}$ singular, $S_{kF^c} = S_{kE}$ non-singular, $S^\star_{kF}$, $S^\star_{kE}$ singular.

were $(A{+}B)^\dagger$ is a generalized inverse, i.e., $(A{+}B)(A{+}B)^\dagger f = f$ for all $f \in \operatorname{range}(A{+}B)$, cf. Def. D.1. The definition is independent of the particular choice of the generalized inverse (cf. [3, p. 579] and Proposition D.2), $A : B = B : A$ [3, Lemma 1], and $A : B$ is again SPSD [3, Lemma 2, Lemma 4]. Moreover, due to [3, Lemma 6], $(A : B) : C = A : (B : C)$.

Remark 5.5. If A and B are both SPD, then $A : B = (A^{-1} + B^{-1})^{-1}$. Therefore, up to a factor of 2, the above matrix generalizes the *harmonic mean value* $\frac{2}{a^{-1}+b^{-1}}$ of two positive scalars a, b, cf. [4]. Moreover, it can be shown that for A, B SPD,

$$x^\top (A : B)x \;=\; \inf_{x=x_1+x_2} (x_1^\top A x_1 + x_2^\top B x_2) \qquad \forall x \in \mathbb{R}^n, \tag{58}$$

i.e., $\|x\|_{A:B}$ is the natural norm on the *sum* of the Hilbert spaces $(\mathbb{R}^n, \|\cdot\|_A)$, $(\mathbb{R}^n, \|\cdot\|_B)$, see also [8] and Corollary 5.11 below. See also [106, Eqn. (4)] for a related result.

Let A, B be as in Def. 5.4. We easily see that

$$A : A = \tfrac{1}{2} A, \qquad (cA) : (cB) = c(A : B) \qquad \forall c \in \mathbb{R}_0^+ \tag{59}$$

(see also [3, Thm. 10]). Since A, B are SPSD, we have

$$\ker(A + B) \;=\; \ker(A) \cap \ker(B), \qquad \operatorname{range}(A + B) \;=\; \operatorname{range}(A) + \operatorname{range}(B),$$

and we can conclude that

$$\ker(A : B) \;=\; \ker(A) + \ker(B), \qquad \operatorname{range}(A : B) \;=\; \operatorname{range}(A) \cap \operatorname{range}(B), \tag{60}$$

cf. [3, Lemma 3]. From Definition 5.4 and Proposition D.2, one easily shows

$$A : B \;=\; A - A(A + B)^\dagger A \;=\; B - B(A + B)^\dagger B. \tag{61}$$

Next, let us consider the generalized eigenproblem

$$Ap \;=\; \lambda(A + B)p \tag{62}$$

in the sense of Sect. 4.1. With the above relations, it is straightforward to show that, if (p, λ) is an eigenpair of (62) (and $p \notin \ker(A) \cap \ker(B)$) then $\lambda \in [0, 1]$ and

$$Bp \;=\; (1 - \lambda)(A + B)p,$$

$$(A : B)p \;=\; \lambda(1 - \lambda)(A + B)p. \tag{63}$$

From (60) and (63), we easily conclude that

$$A : B \;\le\; A, \qquad A : B \;\le\; B, \tag{64}$$

which is a special case of [3, Lemma 18] (as usual, $A \le B$ stands for $y^\top A y \le y^\top B y$ for all $y \in \mathbb{R}^n$). Anderson and Duffin also show an important transitivity property:

Lemma 5.6 ([3, Corollary 21])**.** *Let D, E, $F \in \mathbb{R}^{n\times n}$ be SPSD. Then $D \le E$ implies $D : F \le E : F$.*

As the next proposition shows, the parallel sum $A : B$ is—up to a factor of two—a *sharp* "lower bound matrix" of A and B.

Proposition 5.7. *Let A, B be as in Def. 5.4 and let the matrix $C \in \mathbb{R}^{n\times n}$ be SPSD with $C \le A$ and $C \le B$. Then*

$$C \;\le\; 2(A : B).$$

Proof. Due to Lemma 5.6, $C \le A$ implies $\frac{1}{2}C = C : C \le A : C$ and $C \le B$ implies $A : C \le A : B$. □

The following result states that the parallel sum of two spectrally equivalent matrices is spectrally equivalent to the parallel sum of the original matrices.

Proposition 5.8. *Let A, $\widetilde{A}$, B, $\widetilde{B} \in \mathbb{R}^{n\times n}$ be SPSD and assume that*

$$\underline{\alpha} A \;\le\; \widetilde{A} \;\le\; \overline{\alpha} A, \qquad \underline{\beta} B \;\le\; \widetilde{B} \;\le\; \overline{\beta} B,$$

with strictly positive constants $\underline{\alpha}$, $\overline{\alpha}$, $\underline{\beta}$, $\overline{\beta}$. Then

$$\min(\underline{\alpha}, \underline{\beta})(A : B) \;\le\; \widetilde{A} : \widetilde{B} \;\le\; \max(\overline{\alpha}, \overline{\beta})(A : B).$$

Proof. Firstly, we set $\underline{\gamma} := \min(\underline{\alpha}, \underline{\beta})$, $\overline{\gamma} := \max(\overline{\alpha}, \overline{\beta})$ and observe that

$$\underline{\gamma} A \;\le\; \widetilde{A} \;\le\; \overline{\gamma} A, \qquad \underline{\gamma} B \;\le\; \widetilde{B} \;\le\; \overline{\gamma} B.$$

Secondly, from Lemma 5.6 we obtain

$$\widetilde{A} : \widetilde{B} \;\le\; (\overline{\gamma} A) : B \;\le\; (\overline{\gamma} A) : (\overline{\gamma} B) \;=\; \overline{\gamma}(A : B)$$

as well as the analogous lower bound $\widetilde{A} : \widetilde{B} \ge \underline{\gamma}(A : B)$. □

Proposition 5.9. *For non-negative constants c_1, c_2 and a SPSD matrix A,*

$$(c_1 A) : (c_2 A) = c_1 (c_1 + c_2)^\dagger c_2\, A.$$

The last lemma of this subsection appears to be new (for earlier versions see [91, 48]) and generalizes the elementary identity and inequality

$$\frac{a\, b^2}{(a+b)^2} + \frac{a^2\, b}{(a+b)^2} = \frac{a\, b}{a+b}, \qquad \frac{a\, b^2}{(a+b)^2} \le \min(a,\, b)$$

for non-negative scalars a, b with $a + b > 0$, cf. [107, (6.19), p. 141].

Lemma 5.10. *Let A, $B \in \mathbb{R}^{n\times n}$ be SPSD. Then*

$$B(A+B)^\dagger A(A+B)^\dagger B + A(A+B)^\dagger B(A+B)^\dagger A \;=\; A : B.$$

In particular,

$$\left.\begin{array}{c} B(A+B)^\dagger A(A+B)^\dagger B \\ A(A+B)^\dagger B(A+B)^\dagger A \end{array}\right\} \;\le\; A : B \;\le\; \left\{\begin{array}{l} A, \\ B. \end{array}\right.$$

Proof. Since $A : B = B(A+B)^\dagger A = A(A+B)^\dagger B$ (see Def. 5.4),

$$\begin{aligned} &\underbrace{B(A+B)^\dagger A(A+B)^\dagger B}_{=:H_1} + \underbrace{A(A+B)^\dagger B(A+B)^\dagger A}_{=:H_2} \\ &= \;(A : B)(A+B)^\dagger B + (A : B)(A+B)^\dagger A \\ &= \;(A : B)(A+B)^\dagger (A+B) \;=\; A : B. \end{aligned}$$

The last identity holds because for any $v \in \mathbb{R}^n$, $(A+B)^\dagger(A+B)v = v + v_K$ for some $v_K \in \ker(A+B) = \ker(A)\cap\ker(B) \subset \ker(A)+\ker(B) = \ker(A:B)$, cf. (125), Appendix D and (60). So $H_1 + H_2 = A : B$. Since H_1 and H_2 are both SPSD, H_1, $H_2 \le A : B$. Due to (64), $A : B \le A$, B, which concludes the proof. ☐

Corollary 5.11. *For SPSD matrices A, $B \in \mathbb{R}^n$,*

$$|x|^2_{A:B} = \inf_{x=x_1+x_2} |x_1|^2_A + |x_2|^2_B \qquad \forall x \in \mathbb{R}^n.$$

Proof. Minimization yields the first order condition $x_1^* = (A+B)^\dagger Bx + x_{1K}$ for some $x_{1K} \in \ker(A+B) = \ker(A)\cap\ker(B)$ and $x_2^* = (A+B)^\dagger Ax + x_{2K}$ for a suitable vector $x_{2K} \in \ker(A)\cap\ker(B)$. The Hessian is given by $A+B$, so all these solutions are minimizers. Due to Lemma 5.10, $|x_1^*|^2_A + |x_2^*|^2_B = x^\top(A:B)x = |x|^2_{A:B}$. ☐

Remark 5.12. Unfortunately, Lemma 5.10 *cannot* be generalized to three matrices (see also [13]), in the sense that already for SPD matrices A, B, C,

$$B(A+B+C)^{-1}A(A+B+C)^{-1}B \not\le A : B \qquad \text{in general!}$$

Our counterexample in Appendix E shows that $B(A+B+C)^{-1}A(A+B+C)^{-1}B \not\le A$. Since $A : B \le A$, the above inequality cannot hold.

5.2. **Subdomain faces.** Suppose that F is a face shared by subdomains $\mathcal{N}_F = \{i,j\}$. Firstly, we have a look at the right-hand side of eigenvalue problem (51).

Lemma 5.13. *Under Assumption 3.4, for a face F with $\mathcal{N}_F = \{i,j\}$, we have*

$$z^\top P_{D,F}^\top \mathcal{S}_{\mathcal{N}_G} P_{D,F} y = (R_{iF}z_i - R_{jF}z_j)^\top M_F (R_{iF}y_i - R_{jF}y_j) \quad \forall y,z \in W_{\mathcal{N}_F},$$

with

$$M_F := D_{jF}^\top S_{iF} D_{jF} + D_{iF}^\top S_{jF} D_{jF} \tag{65}$$

Proof. We obtain from (44) that

$$\begin{aligned}(P_{D,F}w)_i &= R_{iF}D_{jF}(R_{iF}w_i - R_{jF}w_j),\\ (P_{D,F}w)_j &= R_{jF}D_{iF}(R_{jF}w_j - R_{iF}w_i).\end{aligned}$$

Hence,

$$\begin{aligned} &z^\top P_{D,F}^\top \mathcal{S}_{\mathcal{N}_G} P_{D,F} y \\ &\quad = (R_{iF}z_i - R_{jF}z_j)^\top \underbrace{\begin{bmatrix} D_{jF}^\top & -D_{iF}^\top\end{bmatrix}\begin{bmatrix} S_{iF} & 0\\ 0 & S_{jF}\end{bmatrix}\begin{bmatrix} D_{jF}\\ -D_{iF}\end{bmatrix}}_{=(D_{jF}^\top S_{iF}D_{jF} + D_{iF}^\top S_{jF} D_{jF})}(R_{iF}y_i - R_{jF}y_j). \qquad ☐\end{aligned}$$

The lemma shows that the constraints $z^\top P_{D,G}^\top \mathcal{S}_{\mathcal{N}_G} P_{D,F} w = 0$ are *classical primal constraints* (Definition 2.15), and so for each column z of $\Phi_{G,\text{add}}$ in (54), we can use

$$M_F(R_{iF}z_i - R_{jF}z_j) \tag{66}$$

as an additional column in Q_G (after a modified Gram-Schmidt orthonormalization).

Secondly, we investigate the structure of eigenproblem (51). The next lemma reduces the eigenproblem on $\widetilde{W}^F_{\mathcal{N}_F}$ (Strategy 4) to an eigenproblem on a subspace of U_G.

Lemma 5.14. *Let F be a face shared by subdomains $\mathcal{N}_F = \{i, j\}$. Then the corresponding generalized eigenproblem of Strategy 4, i.e., finding eigenpairs $(y, \lambda) \in \widetilde{W}^F_{\mathcal{N}_F} \times \mathbb{R}$,*

$$\langle \mathcal{S}_{\mathcal{N}_F} y, z \rangle = \lambda \langle P_{D,F}^\top \mathcal{S}_{\mathcal{N}_F} P_{D,F} y, z \rangle \qquad \forall z \in \widetilde{W}^F_{\mathcal{N}_F} \tag{67}$$

is (up to infinite eigenvalues) equivalent to finding eigenpairs $(\check{y}_F, \lambda) \in U_{F\Delta} \times \mathbb{R}$,

$$\langle (S^\star_{iF} : S^\star_{jF}) \check{y}_F, \check{z}_F \rangle \;=\; \lambda \langle M_F \check{y}_F, \check{z}_F \rangle \qquad \forall \check{z}_F \in U_{F\Delta}\,,$$

where $\check{y}_F := R_{iF} y_i - R_{jF} y_j$, $\check{z}_F := R_{iF} z_i - R_{jF} z_j$, $U_{F\Delta} = \{q \in U_F \colon Q_F^\top q = 0\}$, and M_F is the matrix from (65).

Proof. Let us first rewrite (67) using Lemma 5.13:

$$\begin{bmatrix} z_i \\ z_j \end{bmatrix}^\top \begin{bmatrix} S_i & 0 \\ 0 & S_j \end{bmatrix} \begin{bmatrix} y_i \\ y_j \end{bmatrix} = \lambda (R_{iF} z_i - R_{jF} z_j)^\top M_F (R_{iF} y_i - R_{jF} y_j).$$

Due to Definition 5.1, we can write

$$y_k \;=\; R_{kF}^\top y_{kF} + R_{kF^c}^\top y_{kF^c} \quad \text{for } k \in \{i, j\}, \tag{68}$$

for some vectors y_{kF}, y_{kF^c}. Since $y \in \widetilde{W}^F_{\mathcal{N}_F}$ (not $\widetilde{W}_{\mathcal{N}_F}$) we do not get any constraints on y_{iF^c}, y_{jF^c}. Moreover, since $P_{D,F} y$ is independent of y_{iF^c}, y_{jF^c}, we can use the "Schur" Principle 4.4. With (57), we obtain that that eigenproblem (67) is (up to infinite eigenvalues) equivalent to

$$\begin{bmatrix} z_{iF} \\ z_{jF} \end{bmatrix}^\top \begin{bmatrix} S^\star_{iF} & 0 \\ 0 & S^\star_{jF} \end{bmatrix} \begin{bmatrix} y_{iF} \\ y_{jF} \end{bmatrix} = \lambda (z_{iF} - z_{jF})^\top M_F (y_{iF} - y_{jF}), \tag{69}$$

where the eigenvectors and test vectors fulfill $Q_F^\top (y_{iF} - y_{jF}) = 0$, $Q_F^\top (z_{iF} - z_{jF}) = 0$, respectively. To get the last side condition explicitly, we use a simple transformation of variables:

$$\begin{aligned} y_{iF} &= \widehat{y}_F + \tfrac{1}{2}\check{y}_F, & z_{iF} &= \widehat{z}_F + \tfrac{1}{2}\check{z}_F, \\ y_{jF} &= \widehat{y}_F - \tfrac{1}{2}\check{y}_F, & z_{jF} &= \widehat{z}_F - \tfrac{1}{2}\check{z}_F. \end{aligned} \tag{70}$$

Since

$$y_{iF} - y_{jF} \;=\; \check{y}_F\,, \qquad z_{iF} - z_{jF} = \check{z}_F\,, \tag{71}$$

the condition $y, z \in \widetilde{W}^F_{\mathcal{N}_F}$ is equivalent to

$$\widehat{y}_F,\ \widehat{z}_F \in U_F, \qquad \check{y}_F,\ \check{z}_F \in U_{F\Delta}\,.$$

A straightforward calculation shows that

$$\begin{bmatrix} z_{iF} \\ z_{jF} \end{bmatrix}^\top \begin{bmatrix} S^*_{iF} & 0 \\ 0 & S^*_{jF} \end{bmatrix} \begin{bmatrix} y_{iF} \\ y_{jF} \end{bmatrix} \;=\; \begin{bmatrix} \widehat{z}_F \\ \check{z}_F \end{bmatrix}^\top \begin{bmatrix} S^*_{iF} + S^*_{jF} & \frac{1}{2}(S^*_{iF} - S^*_{jF}) \\ \frac{1}{2}(S^*_{iF} - S^*_{jF}) & \frac{1}{4}(S^*_{iF} + S^*_{jF}) \end{bmatrix} \begin{bmatrix} \widehat{y}_G \\ \check{y}_G \end{bmatrix}. \tag{72}$$

Hence, we can use the "Schur" Principle 4.4 once again and eliminate $\widehat{y}_F$, $\widehat{z}_F$ from the eigenproblem. The corresponding Schur complement of the matrix in (72) is given by

$$\begin{aligned} &\tfrac{1}{4}[(S^\star_{iF} + S^\star_{jF}) - (S^\star_{iF} - S^\star_{jF})(S^\star_{iF} + S^\star_{jF})^\dagger (S^\star_{Fi} - S^\star_{jF})] \\ &= \tfrac{1}{4}[(S^\star_{iF} + S^\star_{jF})(S^\star_{iF} + S^\star_{jF})^\dagger (S^\star_{Fi} + S^\star_{jF}) - (S^\star_{iF} - S^\star_{jF})(S^\star_{iF} + S^\star_{jF})^\dagger (S^\star_{Fi} - S^\star_{jF})] \\ &= \tfrac{1}{4}[2\, S^\star_{iF}(S^\star_{iF} + S^\star_{jF})^\dagger S^\star_{jF} + 2\, S^\star_{jF}(S^\star_{iF} + S^\star_{jF})^\dagger S^\star_{iF}] \\ &= S^\star_{iF} : S^\star_{jF}\,, \end{aligned}$$

cf. Definition 5.4 (Sect. 5.1). □

Remark 5.15. (i) The generalized eigenproblem $(S^\star_{iF} : S^\star_{jF})v = \lambda M_F v$ has been used in [48, 50] and in [91, 13, 116, 117] for the deluxe scaling, which we further investigate in Sect. 6.1 below.

(ii) If we consider the original glob eigenproblem (51) (on $\widetilde{W}_{\mathcal{N}_G}$), we can still apply the "Schur" Principle 4.4 to the splitting (68). But the primal constraints enforced on the globs neighboring F (i.e., globs $G \neq F$ with $|\mathcal{N}_G \cap \mathcal{N}_F| \geq 2$) result in an equivalent eigenproblem of the form

$$\begin{bmatrix} z_{iF} \\ z_{jF} \end{bmatrix}^\top \begin{bmatrix} T_{iiF} & T_{ijF} \\ T_{jiF} & T_{jjF} \end{bmatrix} \begin{bmatrix} y_{iF} \\ y_{jF} \end{bmatrix} = \lambda (z_{iF} - z_{jF})^\top M_F (y_{iF} - y_{jF}),$$

in general with $T_{ijF} \neq 0$, $T_{jiF} \neq 0$. In that case, the transformation (70) will lead to a matrix different than $(S^\star_{iF} : S^\star_{jF})$.

5.3. **Globs shared by more than two subdomains.** Recall that

$$(P_{D,G} y)_i \;=\; R_{iG}^\top \sum_{j \in \mathcal{N}_G \setminus \{i\}} D_{jG} (R_{iG} y_i - R_{jG} y_j).$$

Therefore, any new constraint of the form

$$(P_{D,G} z)^\top S_{\mathcal{N}_G} P_{D,G} y \;=\; 0,$$

we wish to impose, rewrites as

$$\sum_{i \in \mathcal{N}_G} \Big(\sum_{j \in \mathcal{N}_G \setminus \{i\}} (R_{iG} z_i - R_{jG} z_j)^\top D_{jG}^\top \Big) S_{iG} \Big(\sum_{j \in \mathcal{N}_G \setminus \{i\}} D_{jG} (R_{iG} y_i - R_{jG} y_j) \Big) \;=\; 0. \tag{73}$$

(The matrix on the left-hand side is related to but substantially different from the matrix A_E in [42, Slide 10].) It is not hard to show that (73) has the form

$$\sum_{j \in \mathcal{N}_G} L_{jG} R_{jG} y_j = 0, \tag{74}$$

(Condition (35) from Sect. 2.6). From Lemma 3.8(iii), we know that $P_{D,G}$ vanishes for functions that are continuous across G, from which we obtain $\sum_{j \in \mathcal{N}_G} L_{jG} = 0$, (Condition (37) from Sect. 2.6).

Appendix C shows that such generalized primal constraints (73) can be cast into an algorithm very similar to the original BDDC method [19], leading to independent subdomain problems and a sparse SPD coarse problem. Alternatively, in a FETI-DP framework, one can enforce the generalized primal constraints by deflation [54, 38, 49], see also [42, 43]. In the next section, we suggest for BDDC to *convert* the constraints (74) into (stronger) classical primal constraints and show that this is more favorable.

5.4. **Enforcing generalized primal constraints by (stronger) classical primal constraints***. In this section, we assume that we are given generalized primal constraints of form (35) (or (74)). We show first how these can be enforced by *classical primal constraints* (cf. Def. 2.15). Although this can increase the total number of constraints, we are able to show in a second step, that the coarse problem underlying the classical constraints is *smaller or equal* in its dimension to the coarse problem underlying the generalized constraints (while the condition number bound we obtain for the generalized constraints also holds for the classical constraints).

Let G be an arbitrary but fixed glob and consider one of the rows of the equation $\sum_{j\in\mathcal{N}_G} L_{jG} R_{jG} w_j = 0$, which we rewrite as

$$\sum_{j\in\mathcal{N}_G} \ell_{jG}^\top R_{jG} w_j = 0,$$

where ℓ_{jG} is the column vector with the same entries as the selected row of L_{jG}. Since the constraint above is non-trivial and because of (37), at least two of the vectors $\{\ell_{jG}\}_{j\in\mathcal{N}_G}$ are non-zero. We select $j^* \in \mathcal{N}_G$ such that ℓ_{j^*G} is non-zero. Without loss of generality, we assume that

$$\mathcal{N}_G = \{1, \ldots, n\}, \qquad j^* = 1,$$

and introduce the simplified notation

$$w_{jG} := R_{jG} w, \qquad j \in \mathcal{N}_G\,.$$

Next, we define a transformation of variables:

$$\left\{ \begin{array}{lcll} \widehat{w}_{1G} &:=& \frac{1}{n}\sum_{j=1}^n w_{jG}, & \\ \check{w}_{jG} &:=& w_{jG} - w_{1G} & \forall j = 2, \ldots, n. \end{array} \right. \tag{75}$$

The inverse transformation is given by

$$\left\{ \begin{array}{lcll} w_{1G} &=& \widehat{w}_{1G} - \frac{1}{n}\sum_{k=2}^n \check{w}_{kG}, & \\ w_{jG} &=& \widehat{w}_{1G} - \frac{1}{n}\sum_{k=2}^n \check{w}_{kG} + \check{w}_{jG} & \forall j = 2, \ldots, n. \end{array} \right. \tag{76}$$

Using (37) one can show that $\sum_{j\in\mathcal{N}_G} \ell_{jG}^\top w_{jG} = \sum_{j=2}^n \ell_{jG}^\top \check{w}_{jG}$, and so,

$$\ell_{kG}^\top (w_{iG} - w_{jG}) = 0 \qquad \forall i, j \in \mathcal{N}_G \quad \forall k \in \mathcal{N}_G \setminus \{j^*\} \tag{77}$$

$$\implies \quad \ell_{jG}^\top \check{w}_{jG} = 0 \qquad \forall j = 2, \ldots, n$$

$$\implies \quad \sum_{j\in\mathcal{N}_j} \ell_{jG}^\top w_{jG} = 0. \tag{78}$$

The first line is in a suitable form for classical primal constraints, only that we should orthonormalize the vectors $\{\ell_{kG}\}_{k\in\mathcal{N}_G\setminus\{j^*\}}$ and possibly drop some of them. Because of (37), the space of vectors $\{w_{iG}\}_{i\in\mathcal{N}_G}$ fulfilling (77) is independent of the choice of the distinguished index j^*. If $|\mathcal{N}_G| = 2$ then (77) and (78) are equivalent.

From the development above, it becomes clear that in any case, we end up with a matrix $Q_G^\top$ of full row rank such that for some matrix T_G of full column rank,

$$L_G^C := \begin{bmatrix} \vdots \\ L_{jG} \\ \vdots \end{bmatrix}_{j\in\mathcal{N}_G} = T_G Q_G^\top, \qquad \operatorname{rank}(L_G^C) = \operatorname{rank}(Q_G^\top) \tag{79}$$

(L_G^C is a block column vector). A primal dof matrix $Q_G^\top$ fulfilling the above can be obtained in various ways. Theoretically, we just have to remove linearly dependent rows from L_G^C. In practice, one can use the (thin) *QR factorization* (either implemented via Householder, Givens, or (modified) Gram-Schmidt, cf. [36, Sect. 5.2]):

$$L_G^C = \begin{bmatrix} Q_1 \,|\, Q_2 \end{bmatrix} \begin{bmatrix} R_1 \\ \hline 0 \end{bmatrix} = Q_1 R_1, \qquad \text{set } T_G := Q_1,\ Q_G^\top := R_1\,,$$

such that $Q_G^\top$ is even upper triangular. Note that the QR factorization is also used in the algorithm proposed in [76, Sect. 5]. In any case, the number of classical primal dofs on glob G is given by

$$n_{\Pi G} = \dim(U_{\Pi G}) = \operatorname{rank}(L_G^C). \tag{80}$$

Following this construction for all globs results in classical primal dofs $\{Q_G^\top\}_{G\in\mathcal{G}}$ and the corresponding space from Definition 2.21, which we denote by $\widetilde{\widetilde{W}}$ in order to distinguish it from $\widetilde{W}$ defined by (32). From Proposition 2.23, we obtain

Corollary 5.16. *Let $\widetilde{\widetilde{W}}$ be as in Definition 2.21 based on the classical primal dofs $Q_G^\top$ from* (79) *and let*

$$\widetilde{\widetilde{W}}_\Delta = \bigotimes_{i=1}^N \widetilde{\widetilde{W}}_{i\Delta}\,, \qquad \widetilde{\widetilde{W}}_{i\Delta} := \{w_i \in W_i \colon \forall G \in \mathcal{G}_i \colon Q_G^\top R_{iG} w_i = 0\}$$

(cf. (29)*). Then for any space $\widetilde{\widetilde{W}}_\Pi$ fulfilling $\widetilde{\widetilde{W}} = \widetilde{\widetilde{W}}_\Pi \oplus \widetilde{\widetilde{W}}_\Delta$,*

$$\dim(\widetilde{\widetilde{W}}_\Pi) = n_\Pi = \dim(U_\Pi) = \sum_{G\in\mathcal{G}} n_{\Pi G} = \sum_{G\in\mathcal{G}} \operatorname{rank}(L_G^C).$$

Before we can state the main theorem of this section, we need to discuss the dimension of the more general space $\widetilde{W}$ of form (32), (35). Let $r_{\Pi G}$ denote the number of (linearly independent) constraints on G, i.e., the number of linearly independent rows of the equation $\sum_{j\in\mathcal{N}_G} L_{jG} R_{jG} w_j = 0$. Since each R_{jG} is surjective,

$$r_{\Pi G} \;=\; \operatorname{rank}(L_G^R), \qquad \text{where } L_G^R := \big[\cdots | L_{jG} | \cdots\big]_{j\in\mathcal{N}_G} \tag{81}$$

(L_G^R is a block row vector, opposed to L_G^C). Moreover, it is easily seen that

$$\dim(\widetilde{W}) \;=\; \sum_{i=1}^N \dim(W_i) - \sum_{G\in\mathcal{G}} r_{\Pi G}\,. \tag{82}$$

We define the generalized dual spaces

$$W_{i\Delta} \;:=\; \big\{w_i \in W_i \colon \forall G \in \mathcal{G}_i \colon L_{iG} R_{iG} w_i = 0\big\}, \qquad W_\Delta \;:=\; \bigotimes_{i=1}^N W_{i\Delta} \tag{83}$$

as well as the numbers

$$q_{\Pi i G} := \operatorname{rank}(L_{iG}), \qquad q_{\Pi i} := \sum_{G\in\mathcal{G}_i} q_{\Pi i}\,. \tag{84}$$

Proposition 5.17. *Let $\widetilde{W}$ be the space based on generalized primal constraints given by* (32)*, assume that* (35)*,* (37) *hold, and let W_Δ be as in* (83)*. Then*

(i) *$W_\Delta \subset \widetilde{W}$,*
(ii) *the space W_Δ in* (83) *is the maximal subspace of $\widetilde{W}$ which has the form $\bigotimes_{i=1}^N V_i$,*
(iii) *$\dim(W_{i\Delta}) \;=\; \dim(W_i) - q_{\Pi i}$ with $q_{\Pi i}$ from* (84)*,*
(iv) *for any complementary space $\widetilde{W}_\Pi$ fulfilling $\widetilde{W} \;=\; \widetilde{W}_\Pi \oplus W_\Delta$,*

$$\dim(\widetilde{W}_\Pi) \;=\; \sum_{i=1}^N q_{\Pi i} - \sum_{G\in\mathcal{G}} r_{\Pi G}\,,$$

with $r_{\Pi G}$ from (81)*.*

Proof. Parts (i)–(iii) can easily be verified. Since the sum in Part (iv) is direct, we obtain from (82) and Part (iii) that

$$\begin{aligned}\dim(\widetilde{W}_\Pi) &= \dim(\widetilde{W}) - \sum_{i=1}^N \dim(W_{i\Delta}) \\ &= \Big(\sum_{i=1}^N \dim(W_i) - \sum_{G\in\mathcal{G}} r_{\Pi G}\Big) - \sum_{i=1}^N \Big(\dim(W_i) - \sum_{G\in\mathcal{G}_i} q_{\Pi i G}\Big) \\ &= -\sum_{G\in\mathcal{G}} r_{\Pi G} + \sum_{G\in\mathcal{G}}\sum_{j\in\mathcal{N}_G} q_{\Pi j G} = -\sum_{G\in\mathcal{G}} r_{\Pi G} + \sum_{i=1}^N \sum_{G\in\mathcal{G}_i} q_{\Pi i G}\,. \qquad \square\end{aligned}$$

We next state the main result of this section.

Theorem 5.18. *Let $\widetilde{W}$ be the space based on generalized glob constraints given by* (32) *and let $\widetilde{W}_\Delta$ denote the corresponding dual space from* (83)*. Then, for $\widetilde{\widetilde{W}}$, $\widetilde{\widetilde{W}}_\Delta$ as in Corollary 5.16,*

$$\widetilde{\widetilde{W}} \subset \widetilde{W}, \qquad \dim(\widetilde{\widetilde{W}}_\Delta) \le \dim(\widetilde{W}_\Delta),$$

and for any complementary spaces $\widetilde{W}_\Pi$, $\widetilde{\widetilde{W}}_\Pi$ with $\widetilde{W} = \widetilde{W}_\Pi \oplus \widetilde{W}_\Delta$ and $\widetilde{\widetilde{W}} = \widetilde{\widetilde{W}}_\Pi \oplus \widetilde{\widetilde{W}}_\Delta$,

$$\dim(\widetilde{\widetilde{W}}_\Pi) \le \dim(\widetilde{W}_\Pi).$$

Let us first rephrase the statement of Theorem 5.18 based on the following observation. According to [19, 72] (or Appendix C), the action of $\widetilde{\widetilde{I}}\,\widetilde{\widetilde{S}}^{-1}\widetilde{\widetilde{I}}^\top$ can be performed by independent subdomain problems and a sparse SPD coarse problem of dimension $\dim(\widetilde{\widetilde{W}}_\Pi)$. Correspondingly, the operator $\tilde{I}\,\tilde{S}^{-1}\tilde{I}^\top$ involving the more general space $\widetilde{W}$ leads to a coarse problem of size at least $\dim(\widetilde{W}_\Pi)$. Actually, we show in Appendix C that the coarse problem is of size exactly equal to $\dim(\widetilde{W}_\Pi)$. So,

(i) although in $\widetilde{\widetilde{W}}$ *more constraints* are enforced than in $\widetilde{W}$, working with the space $\widetilde{\widetilde{W}}$ leads to a coarse problem of lower dimension (thus solvable more efficiently) than for $\widetilde{W}$.
(ii) At the same time, we obtain from Remark 2.10, that at high probability the smaller space $\widetilde{\widetilde{W}}$ leads to a smaller condition number as well.

Summarizing, the advantages of using the (stronger) classical primal dofs from (79) clearly prevail.

See Figure 5 for a simple example showing that this is (although counter-intuitive) indeed possible.

Remark 5.19. If the constraints are imposed by *deflation* in a FETI-DP framework [54, 38, 49, 42, 43], things turn around: Since there, the number of dofs in the second coarse problem equals the number of constraints, it is better to use the *original constraints* (35) (or (74)) in the deflation process.

Proof of Theorem 5.18. The first two statements follow from Definition 2.15, (32), and (77)–(78). The remainder of the proof is devoted to the inequality relating the primal

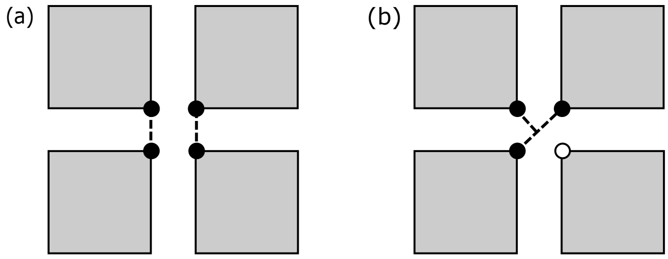

FIGURE 5. Two examples of generalized constraints on a vertex shared by four subdomains. White bullet: dual (unconstrained) dof, black bullet: primal (constrained) dof, dashed line: constraint. In example (a), the coarse space requires two basis functions, one having support on the two left subdomains and vanishing on the two right ones, the other one supported on the right. Example (b) requires one coarse basis function. For both examples the stronger constraint is simple the classical vertex constraint involving a single coarse dof.

space dimensions. Beforehand, recall the matrices L_G^C from (79). From Corollary 5.16 and Proposition 5.17, we obtain

$$\dim(\widetilde{\widetilde{W}}_\Pi) = \sum_{G\in\mathcal{G}} \operatorname{rank}(L_G^C),$$
$$\dim(\widetilde{W}_\Pi) = \sum_{G\in\mathcal{G}} \big(q_{\Pi G} - r_{\Pi G}\big), \qquad q_{\Pi G} = \sum_{j\in\mathcal{N}_G} q_{\Pi jG}\,.$$

We will show that each of the summands in the first line is less than or equal to the corresponding one in the second line. Therefore, we can consider a single glob $G\in\mathcal{G}$ at a time. For a clearer presentation, we assume that $\mathcal{N}_G = \{1,\ldots,n\}$ and omit the subscripts G and Π.

For each $j\in\mathcal{N}_G$ we consider the matrix L_{jG}, which may have incomplete row rank. However, we can find matrices $\bar{L}_{jG}$ of full row rank such that

$$L_{jG} = K_{jG}\bar{L}_{jG}, \qquad q_{\Pi jG} := \operatorname{rank}(L_{jG}) = \operatorname{rank}(\bar{L}_{jG}) \le r_{\Pi G}\,, \tag{85}$$

for some matrix $K_{jG}\in\mathbb{R}^{r_{\Pi G}\times q_{\Pi jG}}$, e.g., via the thin QR factorization [36, Sect. 5.2]. It is easy to see that

$$\operatorname{rank}(L^C) = \operatorname{rank}(\bar{L}^C), \qquad \text{where } \bar{L}^C := \begin{bmatrix}\bar{L}_1\\ \vdots\\ \bar{L}_n\end{bmatrix}.$$

Therefore, we only have to show that

$$\operatorname{rank}(\bar{L}^C) \;\le\; q - r, \quad \text{where } q = \sum_{j=1}^n q_j\,. \tag{86}$$

Recall that $L^R := [L_1|\cdots|L_n]$ and $r = \operatorname{rank}(L^R)$, cf. (81). If m is the number of dofs on glob G, then

$$\dim(\ker(L^R)) = n\,m - r.$$

A different characterization is related to the matrices $\{K_j\}_{j=1}^n$ from (85). From $L_j = K_j \bar{L}_j$ we derive

$$L^R \;=\; \underbrace{[K_1|\cdots|K_n]}_{=:K} \underbrace{\begin{bmatrix} \bar{L}_1 & & \\ & \ddots & \\ & & \bar{L}_n \end{bmatrix}}_{=:\bar{L}^D} .$$

Since each $\bar{L}_j$ is surjective, so is $\bar{L}^D$ and we can conclude that

$$\dim(\ker(L^R)) \;=\; \dim(\ker(\bar{L}^D)) + \dim(\ker(K)). \tag{87}$$

From $\operatorname{rank}(\bar{L}_j) = q_j$ it follows that $\dim(\ker(\bar{L}^D)) = n\,m - \sum_{j=1}^n q_j = n\,m - q$. Combining with (87), we obtain

$$\dim(\ker(K)) = q - r. \tag{88}$$

Finally, recall that $\sum_{j=1}^n L_j = 0$, which can be rewritten as

$$K\bar{L}^C \;=\; [K_1|\ldots|K_n] \begin{bmatrix} \bar{L}_1 \\ \vdots \\ \bar{L}_n \end{bmatrix} \;=\; 0.$$

In other words, the columns of $\bar{L}^C$ are in $\ker(K)$, and so there can only be as many linearly independent columns as the dimension of $\ker(K)$. To summarize,

$$\operatorname{rank}(L^C) \;=\; \operatorname{rank}(\bar{L}^C) \;\leq\; \dim(\ker(K)) \;=\; q - r. \qquad \square$$

5.5. **Alternative eigenproblem for subdomain edges.** In this section, we show that using the transformation of variables (75)–(76) and Principle 4.9 (nearby eigenproblem), one can decouple the glob eigenproblem of Strategy 4 into $|\mathcal{N}_G| - 1$ independent eigenproblems, similar to Principle 4.10. The price to pay is a potentially larger set of constraints because (i) we use Strategy 4 and neglect the neighboring globs (cf. Def. 2.12) and (ii) replace the coupled eigenproblem by a decoupled one.

Let G be an arbitrary but fixed glob and assume without loss of generality that $\mathcal{N}_G = \{1, \ldots, n\}$. Recall the shortcut $w_{iG} = R_{iG} w_i$ as well as the transformation (75):

$$\begin{cases} \widehat{w}_{1G} & := & \frac{1}{n} \sum_{j=1}^n w_{jG}, \\ \check{w}_{jG} & := & w_{jG} - w_{1G} \qquad \forall j = 2, \ldots, n. \end{cases}$$

Notice for $|\mathcal{N}_G| = 2$ that this transformation (up to a positive or negative sign) is not biased towards either the first or second subdomain in G. In contrast, for $|\mathcal{N}_G| > 2$, there is a clear bias towards the first subdomain.

Lemma 5.20. *Under the assumptions above,*

$$\sum_{i \in \mathcal{N}_G} |(P_{D,G} w)_i|^2_{S_i} \leq (|\mathcal{N}_G| - 1) \sum_{i=2}^n \check{w}_{iG}^\top M_{iG} \check{w}_{iG} \,,$$

where

$$M_{iG} := D_{iG}^\top \Big(\sum_{j \in \mathcal{N}_G \setminus \{i\}} S_{jG} \Big) D_{iG} + \Big(\sum_{j \in \mathcal{N}_G \setminus \{i\}} D_{jG}^\top \Big) S_{iG} \Big(\sum_{j \in \mathcal{N}_G \setminus \{i\}} D_{jG} \Big) \quad \textit{for } i = 2, \ldots, n.$$

For a face, i.e., $G = F \in \mathcal{F}$, we have equality and $M_{2F} = M_F$.

Proof. Firstly, observe that

$$
\begin{aligned}
(P_{D,G}w)_i &= R_{iG}^\top \sum_{j\in\mathcal{N}_G\setminus\{i\}} D_{jG}(w_{iG}-w_{jG}) \\
&= R_{iG}^\top \begin{cases} \sum_{j\in\mathcal{N}_G\setminus\{1\}} -D_{jG}\check{w}_{jG} & i=1, \\ \Big(D_{1G}\check{w}_{iG} + \sum_{j\in\mathcal{N}_G\setminus\{1,i\}} D_{jG}(\check{w}_{iG}-\check{w}_{jG})\Big) & i\neq 1. \end{cases}
\end{aligned} \tag{89}
$$

Using the above, we rewrite the expression

$$
\sum_{i\in\mathcal{N}_G} (P_{D,G}z)_i^\top S_i (P_{D,G}w)_i
$$

in the new variables $(\widehat{w}_{1G}, \check{w}_{2G}, \ldots, \check{w}_{nG})$, $(\widehat{z}_{1G}, \check{z}_{2G}, \ldots, \check{z}_{nG})$. The whole expression is independent of $\widehat{w}_{1G}$, $\widehat{z}_{1G}$; in particular, the diagonal entry corresponding to $\widehat{w}_{1G}$, $\widehat{z}_{1G}$ is simply zero. The diagonal entry corresponding to $\check{w}_{kG}$, $\check{z}_{kG}$ computes as

$$
D_{kG}^\top S_{1G} D_{kG} + \sum_{i=2}^n \underbrace{\Big(D_{1G}\delta_{ik} + \sum_{\substack{j=2\\ j\neq i}}^n D_{jG}(\delta_{ik}-\delta_{jk})\Big)}_{=\begin{cases}\sum_{\substack{j=1\\ j\neq i}}^n D_{jG} & k=i\\ D_{kG} & k\neq i\end{cases}}{}^\top S_{iG}\Big(D_{1G}\delta_{ik} + \sum_{\substack{j=2\\ j\neq i}}^n D_{jG}(\delta_{ik}-\delta_{jk})\Big)
$$

$$
= D_{kG}^\top\Big(\sum_{\substack{i=1\\ i\neq k}}^n S_{iG}\Big) D_{kG} + \Big(\sum_{\substack{j=1\\ j\neq k}}^n D_{jG}\Big)^\top S_{kG}\Big(\sum_{\substack{j=1\\ j\neq k}}^n D_{jG}\Big).
$$

The second inequality in Principle 4.10 yields the desired inequality. □

Applying the whole idea of Principle 4.10 (decoupling), we have to compute the Schur complement of $\mathrm{diag}(S_{iG}^\star)_{i\in\mathcal{N}_G}$ but in the transformed variables $(\widehat{w}_{1G}, \check{w}_{2G}, \ldots, \check{w}_{nG})$ eliminating $\check{w}_{kG}$ for $k = 2, \ldots, n$, which we call $\widetilde{S}_{kG}^\star$ in the sequel. From Lemma D.6, we know that $\widetilde{S}_{kG}^\star$ does not depend on the complementary space. Therefore, we may use the simpler transformation $(w_{1G}, \ldots, w_{nG}) \mapsto (w_{1G}, \ldots, w_{(k-1)G}, \check{w}_{kG}, w_{(k+1)G}, \ldots, w_{nG})$, where $w_{kG} = w_{1G} + \check{w}_{kG}$. When we write the operator $\mathrm{diag}(S_{iG}^\star)_{i\in\mathcal{N}_G}$ in the new variables, then $(w_{1G}, \check{w}_{kG})$ are decoupled from the remaining variables. So, if we form the Schur complement eliminating w_{jG}, $j = 1, \ldots, n$, $j \neq k$, it suffices to take the Schur complement of $\begin{bmatrix} S_{1G}^\star + S_{kG}^\star & S_{kG}^\star \\ S_{kG}^\star & S_{kG}^\star \end{bmatrix}$, which is

$$
\widetilde{S}_{kG}^\star = S_{kG}^\star - S_{kG}^\star (S_{1G}^\star + S_{kG}^\star)^\dagger S_{kG}^\star = S_{kG}^\star : S_{1G}^\star, \tag{90}
$$

where in the last step, we have used (61). Principle 4.10 implies

$$
\sum_{k=2}^n \check{w}_{kG}^\top (S_{kG}^\star : S_{1G}^\star)\check{w}_{kG} \;\leq\; (n-1)\sum_{j=1}^n w_{jG}^\top S_{jG}^\star w_{jG}\,, \tag{91}
$$

and we may alternatively study $(n-1)$ decoupled eigenproblems of the form

$$
\check{z}_{iG}^\top (S_{iG}^\star : S_{1G}^\star)\check{y}_{iG} \;=\; \lambda \check{z}_{iG}^\top M_{iG}\check{y}_{iG} \qquad \text{for } \check{y}_{iG},\, \check{z}_{iG} \in U_{G\Delta}\,, \tag{92}
$$

for $i = 2, \ldots, n$ and with the matrix M_{iG} from Lemma 5.20. Apparently, there is a bias towards the first subdomain.

Remark 5.21. If we compute the decoupled eigenproblems independently to form primal constraints, we have to orthonormalize eigenvectors originating from different eigenproblems. This can, however, lead to many unnecessary constraints. A more attractive strategy could be the following:

- Compute the eigenproblem for $i = 2$ and get adaptive constraints Q_{G2}
- For $i = 3, \ldots, n$:
  - *Project* the eigenproblem i onto the space orthogonal to $Q_{G2}, \ldots, Q_{G(i-1)}$
  - Compute constraints Q_{Gi}.
- Use $Q_{G2}, \ldots, Q_{Gn}$ as set of adaptive constraints.

(This corresponds to updating $U_{G\Delta}$ each time in the spirit of a Gauss-Seidel iteration.)

5.6. **A recombined edge eigenproblem.** A different recipe is to use Principle 4.11 and recombine the decoupled eigenproblems (92) into a single one:

$$\check{z}_G^\top (S_{1G}^\star : S_{2G}^\star : \ldots : S_{nG}^\star)\check{y}_G = \lambda \check{z}_G^\top (M_{2G} + \ldots + M_{nG})\check{y}_G \qquad \text{for } \check{y}_G, \check{z}_G \in U_{\Delta G}\,.$$

Due to the Cauchy-Bunyakovsky-Schwarz inequality,

$$M_{iG} \leq \sum_{j \in \mathcal{N}_G \setminus \{i\}} D_{iG}^\top S_{jG} D_{iG} + (|\mathcal{N}_G| - 1) \underbrace{\sum_{j \in \mathcal{N}_G \setminus \{i\}} D_{jG}^\top S_{iG} D_{jG}}_{=:A_{iG}}\,.$$

Therefore,

$$\sum_{i=2}^{n} M_{iG} \;\leq\; |\mathcal{N}_G| \sum_{i=1}^{n} A_{iG}\,.$$

Applying Principle 4.9 (nearby eigenproblem with constant $c_2 = |\mathcal{N}_G|$) yields the eigenproblem

$$\check{z}_G^\top (S_{1G}^\star : S_{2G}^\star : \ldots : S_{nG}^\star)\check{y}_G = \lambda \check{z}_G^\top (A_{1G} + \ldots + A_{nG})\check{y}_G \qquad \text{for } \check{y}_G, \check{z}_G \in U_{\Delta G}\,, \tag{93}$$

which is the one proposed by Kim, Chung, and Wang [42, 43].

5.7. **Comments on the adaptive algorithm.** In general, adaptively chosen constraints can be enforced in several ways. Firstly, one can just add them to the previously chosen ones (if there are any) and recompute some components of BDDC. Secondly, for FETI-DP, the newly chosen constraints can be enforced by *deflation*, see [54, 38, 49, 42, 43]. Suppose, we want to add adaptively chosen constraints to the existing primal constraints, then we fall into one of the two cases below.

(i) If the chosen glob eigenproblems discard the influence of their neighboring globs (or if the neighboring globs are all totally primal), then they can be computed independently from each other.
(ii) Otherwise, one has to make an additional choice whether after computing the adaptive constraints on a single glob, one would update at once the global set of primal constraints (in the spirit of a Gauss-Seidel iteration), or not (like a Jacobi iteration). In the first case, of course the *ordering* of the globs matters.

In several publications [73, 76, 17, 49, 50], it is proposed to use a fixed tolerance as bound for the eigenvalues and use all the corresponding eigenvectors simultaneously for constraints. A different option is to impose *one constraint* at a time and update the neighboring eigenproblems at once, see also Remark 5.21.

6. The deluxe scaling

The *deluxe scaling* was originally introduced in [22] for 3D $H(\mathrm{curl})$ problems and further used in, e.g., [22, 23, 84, 7, 16, 66, 12, 50, 6]. Recall the definition of S_{iG} from (55) and set

$$\bar{S}_G \;:=\; \sum_{j \in \mathcal{N}_G} S_{jG}\,. \tag{94}$$

The *deluxe scaling* is the following choice of the scaling matrices D_{iG} from Assumption 3.4:

$$D_{iG} \;=\; \bar{S}_G^{-1} S_{iG}\,. \tag{95}$$

It is easily seen that $\bar{S}_G$ is a principal minor of the original problem matrix $\widehat{S}$ and as such non-singular. The application of the inverse $\bar{S}_G^{-1}$ can be realized in several ways. Firstly, applying $\bar{S}_G^{-1}$ is equivalent to solving an SPD matrix problem on the subdomains $\mathcal{N}_G$ sharing glob G [7]. Secondly, some sparse direct solvers such as MUMPS [2] or PARDISO [62] offer a *Schur complement* option to compute the dense matrices S_{jG} in a complexity comparable to a direct subdomain solve (see also Remark 5.3). The latter option might be quite interesting for computations on a large number of cores [116, 117].

By construction, choice (95) fulfills the glob-wise partition of unity property (Condition 3.5). Note that it is not guaranteed that each single matrix S_{jG} is non-singular. For example, for the standard FEM-discretization of Poisson's problem or linear elasticity, the matrix S_{kF} corresponding to Figure 4(left), p. 32 is singular.

6.1. **Deluxe scaling on faces.** Recall that for a face F with $\mathcal{N}_F = \{i, j\}$,

$$z^\top P_{D,F}^\top \mathcal{S}_{\mathcal{N}_F} P_{D,F} y \;=\; (R_{iF} z_i - R_{jF} z_j)^\top M_F (R_{iF} y_i - R_{jF} y_j).$$

with

$$M_F \;=\; D_{iF}^\top S_{jF} D_{iF} + D_{jF}^\top S_{iF} D_{iF} \;=\; S_{iF} \bar{S}_F^{-1} S_{jF} \bar{S}_F^{-1} S_{iF} + S_{jF} \bar{S}_F^{-1} S_{iF} \bar{S}_F^{-1} S_{jF}$$

for the deluxe scaling.

Whereas it has been shown in many references [23, 7, 16] that $D_{iF} S_{iF} D_{jF} \leq S_{iF}$ and $D_{iF} S_{iF} D_{jF} \leq S_{iF}$. The inequality in Lemma 5.10 implies $D_{jF}^\top S_{iF} D_{jF} \leq S_{iF} : S_{jF}$, see also [49], and so

$$M_F \;\leq\; 2(S_{iF} : S_{jF}).$$

The core of Lemma 5.10, however, implies the surprising result:

Corollary 6.1. *If F is a face with $\mathcal{N}_F = \{i, j\}$, and if D_{iF}, D_{jF} are chosen according to the deluxe scaling* (95)*, then the following identity holds for M_F (defined in* (65)*):*

$$M_F \;=\; S_{iF} : S_{jF}\,.$$

Using Corollary 6.1, the eigenproblem in Lemma 5.14 (under the stated assumptions!) rewrites as

$$\check{z}_F^\top (S_{iF}^\star : S_{jF}^\star) \check{y}_F \;=\; \lambda\, \check{z}_F^\top (S_{iF} : S_{jF}) \check{y}_F \qquad \text{for } \check{y}_F, \check{z}_F \in U_{F\Delta}.$$

We warn the reader that possible constraints enforced on globs neighboring G are *ignored* in the above eigenproblem, whereas they are present in the original eigenproblem (51).

Remark 6.2. Assume that S_{kF} is spectrally equivalent to $\alpha_k S_F$, $k \in \{i,j\}$ and $S^\star_{kF}$ to $\alpha_k S^\star_F$, $k \in \{i,j\}$, with constant coefficients $\alpha_k > 0$ and with benign equivalence constants. Due to Proposition 5.9,

$$(\alpha_i S_F) : (\alpha_j S_F) = \frac{\alpha_i\,\alpha_j}{\alpha_i + \alpha_j} S_F\,, \qquad (\alpha_i S^\star_F) : (\alpha_j S^\star_F) = \frac{\alpha_i\,\alpha_j}{\alpha_i + \alpha_j} S^\star_F\,.$$

Together with Proposition 5.8 we can instead study the eigenproblem

$$\check z_F^\top S^\star_F \check y_F \;=\; \lambda\, \check z_F^\top S_F \check y_F \qquad \text{for } \check y_F,\, \check z_F \in U_{F\Delta}.$$

For the case of scalar diffusion, $S^\star_F$ corresponds to the $H^{1/2}(F)$-norm and S_F to the $H^{1/2}_{00}(F)$-norm, see [107]. The coefficient-dependent scaling $D_{kF} = \frac{\alpha_k}{\alpha_i+\alpha_j} I$ (sometimes called ρ-scaling, cf. [107, 96]) leads to the same eigenproblem.

Remark 6.3. As noted by Stefano Zampini [116, 117], if we compute the eigenproblem on the space U_F instead of $U_{F\Delta}$, and if S_{iF}, S_{jF}, $S^\star_{iF}$, $S^\star_{jF}$ are all definite, then one can apply the formula from Remark 5.5 and rewrite the eigenproblem as

$$(S_{iF}^{-1} + S_{jF}^{-1})v = \lambda({S^\star_{iF}}^{-1} + {S^\star_{jF}}^{-1})v.$$

6.2. **Optimality of the deluxe scaling for subdomain faces*.** Below $\mathrm{tr}(M) := \sum_{i=1}^n M_{ii}$ denotes the *trace* of the matrix $M \in \mathbb{R}^{n\times n}$. The following lemma can be seen as a matrix version of Corollary 5.11.

Lemma 6.4. *Let A, $B \in \mathbb{R}^{n\times n}$ be SPSD matrices with $A + B$ definite and define*

$$M_{A,B}(X) := X^\top A X + (I - X)^\top B (I - X).$$

Then for any (fixed) symmetric positive definite matrix $C \in \mathbb{R}^{n\times n}$, the functional

$$J_{A,B,C}(X) = \mathrm{tr}(C M_{A,B}(X) C)$$

attains its global minimum at

$$X_* = (A + B)^{-1} B.$$

Proof. Let us first assume that $C = I$. From the properties of the trace, we see that for any X, $Y \in \mathbb{R}^{n\times n}$,

$$J_{A,B,I}(X + Y) = J_{A,B,I}(X) + 2\,\mathrm{tr}(Y^\top A X + Y^\top B(X - I)) + \mathrm{tr}(Y^\top (A + B) Y).$$

Since $\langle M_1, M_2\rangle_F := \mathrm{tr}(M_1^\top M_2)$ is an inner product on $\mathbb{R}^{n\times n}$, we find that the gradient of $J_{A,B,I}$ at X is given by $AX + B(X - I)$. The gradient vanishes if and only if

$$(A + B)X = B.$$

Since the expression $\mathrm{tr}(Y^\top (A + B)Y)$ is positive unless $Y = 0$, we have the global minimum. For a general SPD matrix C, one easily sees that

$$C M_{A,B}(X) C \;=\; M_{\widetilde A,\widetilde B}(\widetilde X)$$

where $\widetilde A = CAC$, $\widetilde B = CBC$, and $\widetilde X = C^{-1} X C$. From the earlier case, the minimum of $J_{A,B,C}(X) = J_{\widetilde A,\widetilde B,I}(\widetilde X)$ is attained at $\widetilde X_* = (\widetilde A + \widetilde B)^{-1}\widetilde B$. Transforming back reveals the formula for X_*. □

Corollary 6.5. *Let F be a subdomain face and let $0 \le \lambda_1(X) \le \cdots \le \lambda_n(X) \le \infty$ denote the generalized eigenvalues of*

$$(S_{iF} : S_{jF})y \;=\; \lambda\, M_{S_{iF},S_{jF}}(X) y \qquad \textit{for } y \in U_F\,,$$

so for $X = D_{jF}$ and $I - X = D_{iF}$, the matrix on the right-hand side equals M_F from Lemma 5.14. Assume further that $S_{iF} : S_{jF}$ is non-singular such that $\lambda_1(X) > 0$. Then the choice $X = D_{jF} = (S_{iF} + S_{jF})^{-1} S_{jF}$ according to the deluxe scaling minimizes

$$\mathcal{J}(X) := \sum_{i=1}^{n} \lambda_i(X)^{-1}.$$

Proof. We set $C = (S_{iF} : S_{jF})^{-1/2}$, where $(S_{iF} : S_{jF})^{1/2}$ is the SPD matrix square root. Then $0 \leq \lambda_n(X)^{-1} \leq \cdots \leq \lambda_1(X)^{-1} < \infty$ are the regular eigenvalues of the matrix $C M_{S_{iF},S_{jF}}(X) C$ (recall that we have set $\infty^{-1} := 0$) and,

$$\mathcal{J}(X) = \operatorname{tr}(C M_{S_{iF},S_{jF}}(X) C).$$

The rest follows from Lemma 6.4. □

In a practical algorithm, one would actually like to minimize the number m of outliers where $\lambda_1(X) \leq \cdots \leq \lambda_m(X) \ll \lambda_{m+1}(X)$, but this would lead to a *non-quadratic* optimization problem. But under the outlier assumption,

$$\sum_{i=1}^{m} \lambda_i(X)^{-1} \approx \sum_{i=1}^{n} \lambda_i(X)^{-1} = \mathcal{J}(X).$$

The term on the left-hand side is the sum over factors that we could potentially obtain in the condition number bound, so minimizing the *quadratic* functional $\mathcal{J}(X)$ appears to be a good alternative.

Remark 6.6. The case of singular $(S_{iF} : S_{jF})$ is harder and left for future research.

6.3. **Economic deluxe scaling on faces*.** *Economic* versions of the deluxe scaling have been proposed in [23, 50]. Recall that in the typical application, the matrix S_i and the derived matrices S_{iF}, $S_{iF}^\star$ stem from the elimination of *interior* subdomain dofs. Replacing the original stiffness matrix K_i by the one just assembled over the elements at a distance $\leq \eta$ from the face F, one arrives at matrices $S_{iF\eta}$, $S_{iF\eta}^\star$ with the properties

$$S_{iF} \leq S_{iF\eta}, \qquad S_{iF\eta}^\star \leq S_{iF}^\star\,, \tag{96}$$

for details see [50]. The *economic deluxe scaling* (on face F shared by subdomains i and j) is given by

$$D_{iF} := (S_{iF\eta} + S_{jF\eta})^{-1} S_{iF\eta}\,.$$

For sufficiently small η, the computation of this matrix or its application to a vector is much cheaper than for the original deluxe scaling. In [23], only one layer of elements is used ($\eta = h$). From (96) and Lemma 5.10, we obtain

$$M_F = D_{iF}^\top S_{jF} D_{iF} + D_{jF}^\top S_{iF} D_{jF} \leq D_{iF}^\top S_{jF\eta} D_{iF} + D_{jF}^\top S_{iF\eta} D_{jF} = S_{iF\eta} : S_{jF\eta}\,. \tag{97}$$

From (96) and Proposition 5.8, we obtain

$$(S_{iF\eta}^\star : S_{jF\eta}^\star) \leq (S_{iF}^\star : S_{jF}^\star). \tag{98}$$

In [50], it is proposed to consider the face eigenproblem

$$(S_{iF\eta}^\star : S_{jF\eta}^\star) v = \lambda (S_{iF\eta} : S_{jF\eta}) v.$$

In view of (96)–(98), this is an implicit application of Principle 4.9 (nearby eigenproblem).

6.4. **Deluxe scaling on edges.** For arbitrary globs, we consider the eigenproblem

$$\mathcal{S}_{\mathcal{N}_G} = \lambda\, P_{D,G}^\top \mathcal{S}_{\mathcal{N}_G} P_{D,G} \qquad \text{in } W_{\mathcal{N}_G},$$

here discarding *any* influence of primal constraints and let the weight matrices $\{D_{jG}\}_{j\in\mathcal{N}_G}$ vary subject to the condition $\sum_{j\in\mathcal{N}_G} D_{jG} = I$. One can show that the trace of the matrix on the right-hand side attains a minimum if the weight matrices are chosen according to the deluxe scaling.

Next, we investigate the decoupled eigenproblem from Sect. 5.5. Suppose again that $\mathcal{N}_G = \{1,\ldots,n\}$ and set $S_{iG}^\sharp := \sum_{j\in\mathcal{N}_G\setminus\{i\}} S_{jG} = \bar{S}_G - S_{iG}$. Then, due to Lemma 5.10,

$$M_{iG} = S_{iG}\bar{S}_G^{-1}S_{iG}^\sharp\bar{S}_G^{-1}S_{iG} + S_{iG}^\sharp\bar{S}_G^{-1}S_{iG}\bar{S}_G^{-1}S_{iG}^\sharp = S_{iG} : S_{iG}^\sharp$$

Hence, the $(n-1)$ decoupled eigenproblems from (92) rewrite as

$$\check{z}_{iG}^\top(S_{iG}^\star : S_{1G}^\star)\check{y}_{iG} \;=\; \lambda\check{z}_{iG}^\top(S_{iG} : S_{iG}^\sharp)\check{y}_{iG} \quad \text{for } \check{y}_{iG},\ \check{z}_{iG}\in U_{G\Delta}\,, \quad \forall i = 2,\ldots,n. \tag{99}$$

Applying Principle 4.11 (recombination), we obtain the *single* eigenproblem

$$\check{z}_G^\top(S_{1G}^\star : S_{2G}^\star : \ldots : S_{nG}^\star)\check{y}_G \;=\; \lambda\check{z}_G^\top(T_{2G} + \ldots + T_{nG})\check{y}_G \quad \text{for } \check{y}_{iG},\ \check{z}_{iG}\in U_{G\Delta}\,,$$

where $T_{iG} := S_{iG} : S_{iG}^\sharp$. Applying Principle 4.9 (nearby eigenproblem) replacing the matrix on the right-hand side by $T_{1G} + \ldots + T_{nG}$ results in the eigenproblem proposed by Calvo and Widlund [111, 13].

Remark 6.7. Recall the eigenproblem (93),

$$\check{z}_G^\top(S_{1G}^\star : S_{2G}^\star : \ldots : S_{nG}^\star)\check{y}_G \;=\; \lambda\check{z}_G^\top(A_{1G} + \ldots + A_{nG})\check{y}_G \quad \text{for } \check{y}_{iG},\ \check{z}_{iG}\in U_{G\Delta}\,,$$

proposed by Kim, Chung, and Wang [42, 43], where $A_{iG} = \sum_{j=1,j\neq i}^n D_{jG}^\top S_{iG} D_{jG}$. For the deluxe scaling,

$$\sum_{i=1}^n A_{iG} = \sum_{i=1}^n \sum_{j=1,j\neq i}^n S_{jG}\bar{S}_G^{-1}S_{iG}\bar{S}_G^{-1}S_{jG} = \sum_{j=1}^n S_{jG}\bar{S}_G^{-1}S_{jG}^\sharp\bar{S}_G^{-1}S_{jG} \leq \sum_{j=1}^n T_{jG}\,, \tag{100}$$

where in the last step, we have used Lemma 5.10. That means, for the deluxe scaling, one can get from the Kim-Chung-Wang eigenproblem to the Calvo-Widlund eigenproblem by Principle 4.9 (nearby eigenproblem) using the spectral inequality (100).

7. Achieving definiteness of $\widetilde{S}$

In this section, we show that under the following mild assumptions, we can guarantee the definiteness of $\widetilde{S}$ algorithmically.

Assumption 7.1. *Each substructure has at least one face.*

Assumption 7.2. *If F is a face of substructure k then*

$$(S_k w_k = 0, \quad R_{kF} w_k = 0) \implies w_k = 0.$$

Assumption 7.3. *For each $k = 1,\ldots,N$ either*

1. $\ker(S_k) = \{0\}$, *or*
2. *substructure k has two faces, or*
3. *substructure k has only one face F, $\mathcal{N}_F = \{k,\ell\}$ and the matrix*

$$M_F = D_{kF}^T S_{\ell F} D_{kF} + D_{\ell F}^T S_{kF} D_{\ell F}$$

is definite on $U_{F\Delta} := \{u \in U_F \colon Q_F^T u = 0\}$.

Lemma 7.4. *If Assumptions 7.1–7.3 hold, then for each $G \in \mathcal{G}^*$,*

$$\ker(S_{\mathcal{N}_G}) \cap \operatorname{range}(P_{D,G}) \cap \widetilde{W}_{\mathcal{N}_G} = \{0\}.$$

Proof. Throughout the proof, let $w \in \ker(S_{\mathcal{N}_G}) \cap \operatorname{range}(P_{D,G}) \cap \widetilde{W}_{\mathcal{N}_G}$ be arbitrary but fixed. From $w \in \operatorname{range}(P_{D,G}) \cap \widetilde{W}_{\mathcal{N}_G}$ and Lemma 3.8, we obtain that

$$w = P_{D,G}\, y \qquad \text{for some } y \in \widetilde{W}_{\mathcal{N}_G}\,. \tag{101}$$

We treat two cases. Firstly, assume that G is a *face* shared by substructures i and j, such that

$$\begin{aligned} w_i &= (P_{D,G}\,y)_i = R_{iG}^T D_{jG} (R_{iG} y_i - R_{jG} y_j) \\ w_j &= (P_{D,G}\,y)_j = -R_{jG}^T D_{iG} (R_{iG} y_i - R_{jG} y_j) \end{aligned} \tag{102}$$

Assume now that $S_i w_i = 0$ and $S_j w_j = 0$. For $k \in \{i, j\}$ we apply Assumption 7.3:

1. If $\ker(S_k) = \{0\}$ then $w_k = 0$.
2. If substructure k has two faces, namely G and F' then we see from (102) that $R_{kF'} w_k = 0$ and Assumption 7.2 implies that $w_k = 0$.
3. Finally, if substructure k has only one face (namely G) and if M_G is definite on $U_{G\Delta}$, we have (using (102) and the fact that $S_{iG} = R_{iG} S_i R_{iG}^T$ etc.)

$$0 \;=\; |w_i|_{S_i}^2 + |w_j|_{S_j}^2 \;=\; (R_{iG} y_i - R_{jG} y_j)^T \underbrace{(D_{jG}^T S_{iG} D_{iG} + D_{iG}^T S_{jG} D_{iG})}_{=M_G} (R_{iG} y_i - R_{jG} y_j).$$

Since $R_{iG} y_i - R_{jG} y_i \in U_{G\Delta}$ and M_G is definite on that space, we conclude that $R_{iG} y_i - R_{jG} y_j = 0$. This is sufficient to conclude (from (102)) that $w_i = w_j = 0$.

Secondly, assume that $G \in \mathcal{G}^* \setminus \mathcal{F}$. Due to our assumptions, $S_k w_k = 0$ for all $k \in \mathcal{N}_G$. For any such k, since substructure k has a face F (cf. Assumption 7.1), we see from (101) and the formula for $P_{D,G}$ that $R_{kF} w_k = 0$. Assumption 7.2 implies that $w_k = 0$. □

Theorem 7.5. *Let Assumptions 7.1–7.3 hold. Assume further that for each glob $G \in \mathcal{G}^*$ the glob eigenproblem*

$$(\widetilde{\mathcal{S}}_{\mathcal{N}_G}, \underbrace{\widetilde{P}_{D,G}^\top \widetilde{S}_{\mathcal{N}_G} \widetilde{P}_{D,G}}_{=\widetilde{\mathcal{B}}_G}) \qquad \text{on } \widetilde{W}_{\mathcal{N}_G}$$

has no zero eigenvalues. Then S is definite on $\widetilde{W}$.

Proof. Let $G \in \mathcal{G}^*$ be arbitrary but fixed and set $A = \widetilde{\mathcal{S}}_{\mathcal{N}_G}$, $P = \widetilde{P}_{D,G}$ and $B = \widetilde{\mathcal{B}}_G$. Thanks to Lemma 7.4,

$$\ker(A) \cap \operatorname{range}(P) = \{0\},$$

and due to our assumptions, (A, B) has no genuine zero eigenvalues. Lemma 4.12(iii) implies that $\ker(A) \subset \ker(P)$, which means

$$\forall w \in \widetilde{W}_{\mathcal{N}_G} \colon \big(\forall j \in \mathcal{N}_G \colon S_j w_j = 0 \quad \Longrightarrow \quad \widetilde{P}_{D,G} w = 0\big).$$

Due to Lemma 3.8(iii) the last identity implies

$$R_{iG} w_i - R_{jG} w_j = 0 \qquad \forall i, j \in \mathcal{N}_G\,.$$

Since $G \in \mathcal{G}^*$ was arbitrary, Condition 3.1 is fulfilled and Lemma 3.2 concludes the proof. □

Remark 7.6. (i) Assumption 7.1 usually holds in practice, otherwise we would have substructures joined to the rest only by an edge or a vertex, which is somewhat unphysical.

(ii) Assumption 7.2 is fulfilled for the typical finite element discretizations and for the typical differential operators, provided that
- the face F is large enough and
- each subdomain is *connected*.

Note that *connectivity* is a geometric concept that can, nevertheless, be made accessible via the matrix graph of the underlying sparse matrix, cf. [114].

(iii) Should neither Item 1 nor Item 2 of Assumption 7.3 hold, then Item 3 can be fulfilled by computing the eigenproblem

$$M_F = \lambda I$$

first, and converting any zero modes into primal constraints.

Acknowledgement

We would like to thank Walter Zulehner for helpful hints that have led us to the parallel sum of matrices. We are also grateful to Stefano Zampini, who provided us many hints and suggestions that improved the manuscript in a late stage; in particular he motivated us to introduce Sect. 5.6 and the recombined edge eigenproblem in Sect. 6.4. Furthermore, we wish to thank Olof Widlund for fruitful discussions and helpful hints on the whole topic, Robert Scheichl and Marcus Sarkis for early discussions on FETI-DP and multiscale problems, and Johannes Kraus for detailed explanations and discussions on [61]. Finally, the first author is grateful for the good atmosphere at the Institute of Numerical Mathematics (JKU Linz) and the RICAM (Austrian Academy of Sciences, Linz) where parts of our ideas were developed.

Appendix A. Proof of Theorem 2.8 based on the fictitious space lemma

We first show that (18) and (19) are equivalent. From the properties of E_D and P_D, we find that there exists a projection $\widetilde{E}_D\colon \widetilde{W} \to \widetilde{W}$ onto $\widehat{W}$ such that $RE_D\tilde{I} = \tilde{I}\widetilde{E}_D$ and $P_D\tilde{I} = \tilde{I}(I - \widetilde{E}_D)$. So (18) is equivalent to $\|\widetilde{E}_D\|_{\widetilde{S}}^2 \le \omega$, and (19) to $\|I - \widetilde{E}_D\|_{\widetilde{S}}^2 \le \omega$, where $\|\cdot\|_{\widetilde{S}}$ is the norm on $\widetilde{W}$ induced by $\widetilde{S}$. Since $\widetilde{E}_D$ is a non-trivial projection in a Hilbert space, $\|\widetilde{E}_D\|_{\widetilde{S}} = \|I - \widetilde{E}_D\|_{\widetilde{S}}$. This useful result is often ascribed to Kato (cf. [39, Appendix, Lemma 4], [110, Lemma 3.6]) but has been proved several times in the literature, see Szyld's concise presentation [105] with further references.

For the condition number bound, we use Sergei Nepomnyashikh's fictitious space lemma [82], [83, Lemma 2.3]; see also [61]. Here, we have rewritten it in terms of duality products rather than inner products.

Lemma A.1 (Fictitious space lemma)**.** *Let H, $\widetilde{H}$ be finite-dimensional Hilbert spaces and $A\colon H \to H^*$, $\widetilde{A}\colon \widetilde{H} \to \widetilde{H}^*$ bounded, self-adjoint and positive definite linear operators. Moreover, let $\Pi\colon \widetilde{H} \to H$ be a bounded linear operator. Then*

$$\lambda_{\max}(\Pi\widetilde{A}^{-1}\Pi^T A) \;=\; \sup_{\widetilde{v}\in\widetilde{H}\setminus\{0\}} \frac{\langle A\Pi\widetilde{v}, \Pi\widetilde{v}\rangle}{\langle \widetilde{A}\widetilde{v}, \widetilde{v}\rangle} \;=:\; \gamma_2\,. \tag{103}$$

In addition, let $T\colon H \to \widetilde{H}$ be a linear operator such that

$$\Pi T v \;=\; v \qquad \text{and} \qquad \gamma_1\,\langle \widetilde{A}Tv, Tv\rangle \;\le\; \langle Av, v\rangle \qquad \forall v \in H, \tag{104}$$

for some constant $\gamma_1 > 0$*. Then* $\lambda_{\min}(\Pi\widetilde{A}^{-1}\Pi^\top A) \geq \gamma_1$*. Summarizing,*

$$\kappa(\Pi\widetilde{A}^{-1}\Pi^\top A) \leq \gamma_2/\gamma_1\,.$$

Proof. With $\|v\|_B := \langle Bv, v\rangle^{1/2}$ for positive definite B and basic functional analysis, we obtain $\|\psi\|_{B^{-1}} = \sup_{v\in V\setminus\{0\}} \frac{\langle\psi,v\rangle}{\|v\|_B}$ and $\langle\psi, v\rangle \leq \|\psi\|_{B^{-1}}\|v\|_B$. Since the operator $\Pi\widetilde{A}^{-1}\Pi^T A$ is self-adjoint with respect to the inner product $\langle Av, v\rangle$, its spectrum is real. We show (103) using the Rayleigh quotient and simply omit "$\setminus\{0\}$" in all suprema:

$$\begin{aligned}\lambda_{\max}(\Pi\widetilde{A}^{-1}\Pi^T A) &= \sup_{v\in H}\frac{\langle\Pi\widetilde{A}^{-1}\Pi^T Av, Av\rangle}{\langle Av, v\rangle} \overset{v=A^{-1}\psi}{=} \sup_{\psi\in H^*}\frac{\|\Pi^T\psi\|^2_{\widetilde{A}^{-1}}}{\|\psi\|^2_{A^{-1}}}\\ &= \sup_{\psi\in H^*}\sup_{\widetilde{v}\in\widetilde{H}}\frac{\langle\psi,\Pi\widetilde{v}\rangle^2}{\|\psi\|^2_{A^{-1}}\|\widetilde{v}\|^2_{\widetilde{A}}} = \sup_{\widetilde{v}\in\widetilde{H}}\frac{\|\Pi\widetilde{v}\|^2_A}{\|\widetilde{v}\|^2_{\widetilde{A}}}\,.\end{aligned}$$

If (104) holds then

$$\|\psi\|^2_{A^{-1}} = \sup_{v\in H}\frac{\langle\psi,\overbrace{\Pi Tv}^{=v}\rangle^2}{\|v\|^2_A} = \sup_{v\in H}\frac{\langle\Pi^\top\psi, Tv\rangle^2}{\|v\|^2_A} \leq \|\Pi^T\psi\|^2_{\widetilde{A}^{-1}}\sup_{v\in H}\frac{\|Tv\|^2_{\widetilde{A}}}{\|v\|^2_A} \leq \frac{1}{\gamma_1}\|\Pi^T\psi\|^2_{\widetilde{A}^{-1}}\,.$$

Using the Rayleigh quotient we obtain the lower bound for $\lambda_{\min}(\Pi\widetilde{A}^{-1}\Pi^T A)$. □

To get the BDDC condition number bound, we set $H := U$, $\widetilde{H} := \widetilde{W}$, $A := \widehat{S}$, $\widetilde{A} = \widetilde{S}$ and $\Pi := E_D\tilde{I}$. Then bound (18) is equivalent to $\lambda_{\max}(M^{-1}_{\text{BDDC}}\widehat{S}) \leq \omega$. To get (104), we first define $T\colon U \to \widetilde{W}$ by $Tv := Rv$ for $v \in U$ which is well-defined since range$(R) \subset \widetilde{W}$. From $E_D R = I$ we conclude that $\Pi T = E_D\tilde{I}T = I$. Finally, since RE_D is a projection,

$$\langle\widetilde{A}Tv, Tv\rangle = \langle SRv, Rv\rangle = \langle\widehat{S}v, v\rangle = \langle Av, v\rangle \qquad \forall v \in H = U,$$

so the inequality in (104) holds with $\gamma_1 = 1$ and $\lambda_{\min}(M^{-1}_{\text{BDDC}}\widehat{S}) \geq 1$.

Appendix B. The related FETI-DP method

Let Λ be a Euclidean space (usually called space of Lagrange multipliers) and $B\colon W \to \Lambda$ be a matrix (usually called the jump operator) such that

$$\widehat{W} = \ker(B).$$

Remark B.1. Identity (12) already implies the existence of a matrix B with $\widehat{W} = \ker(B)$. For standard choices of B see, e.g., [107, 33]. Furthermore, $\widehat{W} \subset \widetilde{W} \subset W$ (Condition 2.5) implies the existence of a matrix $\bar{L}$ of full rank such that $\widetilde{W} = \ker(\bar{L}B)$, see also [73, Sect. 2.3] and Remark 2.29.

With $\widetilde{B} := B\,\tilde{I}\colon \widetilde{W} \to \Lambda$, problem (8) can be rewritten as

$$\text{find } (\widetilde{u}, \lambda) \in \widetilde{W}\times\Lambda\colon \quad \begin{bmatrix}\widetilde{S} & \widetilde{B}^\top\\ \widetilde{B} & 0\end{bmatrix}\begin{bmatrix}\widetilde{u}\\ \lambda\end{bmatrix} = \begin{bmatrix}\widetilde{g}\\ 0\end{bmatrix}, \tag{105}$$

where $\widetilde{g} := \tilde{I}^\top g$. Since the restriction of $\widetilde{S}$ to $\ker(\widetilde{B})$ is isomorphic to $\widehat{S}$, which was assumed to be definite, problem (105) is uniquely solvable up to adding an element from $\ker(\widetilde{B}^\top)$ to λ. If S is definite on $\widetilde{W}$ (Condition 2.6), we can eliminate the variable $\widetilde{u}$ and obtain the *dual equation*

$$F\,\lambda \;=\; d, \tag{106}$$

where $F := B\,\tilde{I}\widetilde{S}^{-1}\tilde{I}^\top B^\top$ and $d := B\,\tilde{I}\widetilde{S}^{-1}\tilde{I}^\top g$. We assume that there exists a matrix $B_D\colon W \to \Lambda$ such that

$$B_D^\top B \;=\; P_D \;=\; I - R\,E_D\,.$$

Remark B.2. Under Assumption 3.4 (p. 17) and for *fully redundant* Lagrange multipliers, B_D indeed exists. For the fully redundant setting, $\Lambda = \bigotimes_{G\in\mathcal{G}}\bigotimes_{i,j\in\mathcal{N}_G, i>j} U_G$. We denote the components of $\lambda \in \Lambda$ by $\lambda_{G,ij}$ for $G \in \mathcal{G}$, $i > j \in \mathcal{N}_G$ and define $(Bu)_{G,ij} := R_{iG}u_i - R_{jG}u_j$ (cf. (26)). The definition of B_D then reads $(B_D w)_{G,ij} := D_{jG}R_{iG}w_i - D_{iG}R_{jG}w_j$. This generalizes the well-known formula for diagonal matrices D_i, see [107, Sect. 6.3.3] or [89, Sect. 2.2.4.2]. The transpose is given by

$$(B_D^T\mu)_i = \sum_{G\in\mathcal{G}_i}\sum_{j\in\mathcal{N}_G\setminus\{i\}} \operatorname{sign}(i-j)\, R_{iG}^T D_{jG}\mu_{G,ij}$$

from which one can infer that $B_D^\top B = P_D$.

The FETI-DP preconditioner (for problem (106)) is defined as

$$M_{\text{FETI-DP}}^{-1} \;:=\; B_D\,S\,B_D^\top\colon \Lambda \to \Lambda. \tag{107}$$

In [72, 10, 69, 74] it was shown that bound (19) (or equally (18)) implies

$$\kappa_{\text{FETI-DP}} := \kappa(M_{\text{FETI-DP}}^{-1}F_{|\Lambda_{/\ker(\widetilde{B}^\top)}}) \;\le\; \omega,$$

and that the spectra of BDDC and FETI-DP (with corresponding components) are identical except for possible eigenvalues equal to one.

Appendix C. Realization of $\tilde{I}\widetilde{S}^{-1}\tilde{I}^\top$

The method in Sect. C.1–C.2 treats the case of classical primal dofs (Sect. 2.5) and was introduced in [19]. For similar approaches see, e.g., [32], [107, Sect. 6.4], [69], [58, Sect. 4.2], and [89, Sect. 5.3]. In Sect. C.3, we extend the method to the generalized primal constraints from Sect. 2.6.

C.1. **The energy minimizing basis of $\widetilde{W}_\Pi$ for classical primal dofs.** Let the matrices $C_i\colon W_i \to U_{\Pi i}$ fulfill $\ker(C_i^\top) = \{0\}$ (Condition 2.18), let $\widetilde{W}$ be defined via (31), i.e.,

$$\widetilde{W} \;=\; \{w \in W\colon \exists u_\Pi \in U_\Pi\ \forall i = 1,\ldots,N\colon C_i w_i = R_{\Pi i}u_\Pi\},$$

and $W_{i\Delta} = \{w_i \in W_i\colon C_i w_i = 0\}$, $W_\Delta := \bigotimes_{i=1}^N W_{i\Delta}$. Let $\Psi_i\colon W_{i\Pi} \to W_i$ fulfill

$$C_i\Psi_i \;=\; I. \tag{108}$$

Such matrices Ψ_i exist because C_i is surjective, e.g., we could use $\Psi_i = C_i^\top(C_iC_i^\top)^{-1}$. A distinguished choice is defined by the linear saddle point system

$$\begin{bmatrix} S_i & C_i^\top \\ C_i & 0 \end{bmatrix}\begin{bmatrix}\Psi_i \\ \Lambda_i\end{bmatrix} \;=\; \begin{bmatrix}0 \\ I\end{bmatrix}, \tag{109}$$

with Lagrange parameters $\Lambda_i\colon W_{\Pi i} \to W_{\Pi i}$. Assume that S_i is definite on $\ker(C_i) = W_{i\Delta}$ (cf. Condition (38), p. 16). Due to $\ker(C_i^\top) = \{0\}$ (Condition 2.18)), problem (109) is guaranteed to have a unique solution.

The columns of Ψ_i can be regarded as shape functions on subdomain i. Condition (108) states that primal dof k of shape function j evaluates to δ_{kj}.

Proposition C.1. (i) Ψ_i *has full column rank,*
(ii) $\operatorname{range}(\Psi_i) \cap W_{i\Delta} = \{0\}$,
(iii) *if* (109) *holds then even* $\langle S_i z_i, w_i\rangle = 0 \quad \forall z_i \in \operatorname{range}(\Psi_i),\ w_i \in W_{i\Delta}$.

Proof. Part (i) follows directly from (108).
Part (ii). If $w_i = \Psi_i v \in W_{i\Delta}$, then $0 = C_i w_i = C_i \Psi_i v = v$, so $v = 0$ and $w_i = 0$.
Part (iii). From the first line of (109) we derive that for any $w_i \in W_{i\Delta}$,

$$w_i^\top S_i \Psi_i = -w_i^\top C_i^\top \Lambda_i = -\Lambda_i^\top \underbrace{C_i w_i}_{=0} = 0. \qquad \square$$

For each $i = 1, \ldots, N$, choose $\Psi_i \colon W_{i\Pi} \to W_i$ such that (108) holds. We set $\Psi := \operatorname{diag}(\Psi_i)_{i=1}^N \colon W_\Pi \to W$ and define, in a finite element spirit, the *assembled basis*

$$\widetilde{\Psi} \colon U_\Pi \to W, \quad \widetilde{\Psi} := \Psi R_\Pi\,, \tag{110}$$

where $R_\Pi \colon U_\Pi = \mathbb{R}^{n_\Pi} \to W_\Pi$ is the matrix from (28) and has full column rank.

Lemma C.2. *Let* $\widetilde{\Psi}$ *be given as in* (110). *Then*
(i) $\widetilde{\Psi}$ *has full column rank, in particular,* $\dim(\operatorname{range}(\widetilde{\Psi})) = n_\Pi$,
(ii) $\operatorname{range}(\widetilde{\Psi}) \subset \widetilde{W}$,
(iii) $\widetilde{W} = \operatorname{range}(\widetilde{\Psi}) \oplus W_\Delta$.
(iv) *If for each* $i = 1, \ldots, N$ (109) *holds, then even*

$$\langle Sw, z\rangle = 0 \quad \forall w \in W_\Delta,\ z \in \operatorname{range}(\widetilde{\Psi}).$$

Proof. Part (i). Due to Proposition C.1(i), Ψ is injective. Since R_Π is injective, the composition $\widetilde{\Psi}$ is injective too.
Part (ii). Due to (108), for any $G \in \mathcal{G}$ and $i \in \mathcal{N}_G$:

$$Q_G^T R_{iG} (\widetilde{\Psi})_i \;=\; \sum_{G' \in \mathcal{G}_i} \underbrace{R_{i\Pi G} R_{\Pi i G'}^\top}_{=\delta_{GG'} I} Q_{G'}^\top R_{iG'} \Psi_i R_{\Pi i} \;=\; R_{i\Pi G} \underbrace{C_i \Psi_i}_{=I} R_{\Pi i} \;=\; \widehat{R}_{\Pi G}\,,$$

and so $Q_G^\top R_{iG}(\widetilde{\Psi})_i = Q_G^\top R_{jG}(\widetilde{\Psi})_j$ for all $i, j \in \mathcal{N}_G$.
Part (iii). From Proposition C.1(ii) we obtain $\operatorname{range}(\Psi) \cap W_\Delta = \{0\}$ so the sum is direct. Thanks to Part (i) and Proposition 2.23,

$$\dim(\operatorname{range}(\widetilde{\Psi})) + \dim(W_\Delta) = n_\Pi + \dim(W_\Delta) = \dim(\widetilde{W}),$$

so together with Part (ii), the direct sum must equal $\widetilde{W}$.
Part (iv) follows directly from Proposition C.1(iii). $\square$

C.2. **Realization of $\tilde{I}\,\tilde{S}^{-1}\tilde{I}^\top$.** For this section, we only make two assumptions. Firstly,

$$\widetilde{W} \;=\; \operatorname{range}(\widetilde{\Psi}) \oplus W_\Delta, \tag{111}$$

where $\widetilde{\Psi} \colon U_\Pi \to \widetilde{W}$ is injective and $W_\Delta = \bigotimes_{i=1}^N W_{i\Delta}$ with $W_{i\Delta} = \{w_i \in W_i \colon C_i w_i = 0\}$. Secondly, we assume that $\operatorname{range}(\widetilde{\Psi})$ and W_Δ are $\widetilde{S}$-orthogonal (see Remark C.6 for the non-orthogonal case). Since the sum is direct, we can identify $\widetilde{W}$ with the *product space* $\widetilde{\boldsymbol{W}} := U_\Pi \times W_\Delta$ and obtain

$$\widetilde{\boldsymbol{I}} \colon \widetilde{\boldsymbol{W}} \to W \colon \begin{bmatrix} \boldsymbol{w}_\Pi \\ w_\Delta \end{bmatrix} \mapsto \widetilde{\Psi} \boldsymbol{w}_\pi + w_\Delta, \qquad \widetilde{\boldsymbol{I}}^\top \colon W^* \to \widetilde{\boldsymbol{W}}^* \colon f \mapsto \begin{bmatrix} \widetilde{\Psi}^\top f \\ f \end{bmatrix}.^4$$

The operator $\widetilde{S}$ can then be identified with $\widetilde{\boldsymbol{S}} \colon \widetilde{\boldsymbol{W}} \to \widetilde{\boldsymbol{W}}^*$, given by

$$\begin{bmatrix} \boldsymbol{v}_\Pi \\ v_\Delta \end{bmatrix}^\top \widetilde{\boldsymbol{S}} \begin{bmatrix} \boldsymbol{w}_\Pi \\ w_\Delta \end{bmatrix} \;=\; \boldsymbol{v}_\Pi^\top (\widetilde{\Psi}^\top S \widetilde{\Psi}) \boldsymbol{w}_\Pi + v_\Delta^T S w_\Delta,$$

which is a block-diagonal operator. Its inverse is given by

$$\widetilde{\boldsymbol{S}}^{-1} \begin{bmatrix} \boldsymbol{r}_\Pi \\ r \end{bmatrix} \;=\; \begin{bmatrix} (\widetilde{\Psi}^\top S \widetilde{\Psi})^{-1} \boldsymbol{r}_\Pi \\ z_\Delta \end{bmatrix}$$

where $z_\Delta \in W_\Delta$ is such that $\langle S z_\Delta, v_\Delta \rangle = \langle r, v_\Delta \rangle$ for all $v_\Delta \in W_\Delta$. The latter can be obtained by solving the saddle point problem

$$\begin{bmatrix} S & C^\top \\ C & 0 \end{bmatrix} \begin{bmatrix} z_\Delta \\ \mu \end{bmatrix} \;=\; \begin{bmatrix} r \\ 0 \end{bmatrix},$$

whose system matrix is block-diagonal with blocks identical to (109).

To summarize, the application $v = \widetilde{I}\widetilde{S}^{-1}\widetilde{I}^\top r$, $r \in W$ is now realized by

$$v \;=\; \widetilde{\Psi} \boldsymbol{w}_\Pi + z_\Delta, \tag{112}$$

where $\boldsymbol{w}_\Pi \in \mathbb{R}^{n_P}$ solves the (global) coarse problem

$$(\widetilde{\Psi}^\top S \widetilde{\Psi}) \boldsymbol{w}_\Pi \;=\; \widetilde{\Psi}^\top r, \tag{113}$$

and the components z_i of z_Δ solve the local (and independent) saddle point problems

$$\begin{bmatrix} S_i & C_i^\top \\ C_i & 0 \end{bmatrix} \begin{bmatrix} z_i \\ \mu_i \end{bmatrix} \;=\; \begin{bmatrix} r_i \\ 0 \end{bmatrix}. \tag{114}$$

Remark C.3. Certainly, the saddle point problems (109), (114) can either (i) be solved as they are, (ii) be reformulated by penalty techniques, or (iii), using a transformation of basis [51, 69], one can enforce the constraints explicitly, eliminate some dofs, and reduce the saddle point problem to an SPD problem.

Remark C.4. For the energy minimizing construction (109), the coarse matrix in (113) can be assembled from the subdomain contributions $\Psi_i^\top S_i \Psi_i = -\Psi_i^\top C_i^\top \Lambda_i = -\Lambda_i$, cf. [89, Sect. 5.3.4.2].

Remark C.5. If S_i is a Schur complement of a matrix K_i eliminating *interior* dofs, then the saddle point problems (109) and (114) can easily be rewritten in terms of K_i and are thus amenable to sparse direct solvers. In that context, however, it is recommended to suitably scale the second line and to check for the right parameters, such that the solver can cope with the zero block on the lower right (e.g., *weighted matching* [97] in case of PARDISO).

Remark C.6. Based on the block Cholesky factorization, a similar algorithm can also be given for the case that range($\widetilde{\Psi}$) is not S-orthogonal to W_Δ. Then, however, the coarse and the local problems are not anymore independent, and *two* local problems have to be solved, see [69] and [89, Sect. 5.3].

[4] To be strict, we actually add the embedded function $w_\Delta \in W_\Delta \subset W$ and correspondingly, in the second component of $\widetilde{\boldsymbol{I}}^\top f$, we would have to write the embedding of $f \in W^* \subset W_\Delta^*$.

C.3. **A basis of $\widetilde{W}_\Pi$ for generalized primal constraints.** Let $\widetilde{W}$ be a space generated from generalized primal constraints, i.e., (32), (35). We give an algorithm computing a basis of $\widetilde{W}_\Pi$ that has local support, such that $\widetilde{W} = \widetilde{W}_\Pi \oplus W_\Delta$, with W_Δ defined in (83). We only require that S is definite on $\widetilde{W}$ (Condition 2.6).

Step 1. For each subdomain i and glob $G \in \mathcal{G}_i$ we construct a matrix $\bar{L}_{iG} \in \mathbb{R}^{r_{\Pi G} \times q_{\Pi iG}}$ of full row rank such that

$$L_{iG} = K_{iG} \bar{L}_{iG}\,, \qquad q_{\Pi iG} = \operatorname{rank}(\bar{L}_{iG}) = \operatorname{rank}(L_{iG}). \tag{115}$$

This can, e.g., be achieved by the *QR factorization* [36, Sect. 5.2] (see also the proof of Theorem 5.18). We collect them into a subdomain constraint matrix

$$\bar{L}_i = \begin{bmatrix} \vdots \\ \bar{L}_{iG} R_{iG} \\ \vdots \end{bmatrix}_{G \in \mathcal{G}_i}, \tag{116}$$

which again has full row rank $q_{\Pi i} := \sum_{G \in \mathcal{G}_i} q_{\Pi iG}$. The space from (83) rewrites as

$$W_{i\Delta} \;=\; \{ w_i \in W_i \colon \bar{L}_i w_i = 0 \}. \tag{117}$$

Step 2. For each subdomain i, we construct a matrix $\Psi_i \colon \mathbb{R}^{q_{\Pi i}} \to W_i$ such that

$$\bar{L}_i \Psi_i \;=\; I, \tag{118}$$

e.g., we could use $\Psi_i = \bar{L}_i^\top (\bar{L}_i \bar{L}_i^\top)^{-1}$. A distinguished choice are the energy-minimizing functions given by the solution of the saddle point system

$$\begin{bmatrix} S_i & \bar{L}_i^\top \\ \bar{L}_i & 0 \end{bmatrix} \begin{bmatrix} \Psi_i \\ \Lambda_i \end{bmatrix} \;=\; \begin{bmatrix} 0 \\ I \end{bmatrix} \tag{119}$$

with Lagrange multipliers $\Lambda_i \in \mathbb{R}^{q_{\Pi i} \times q_{\Pi i}}$.

Proposition C.7. *For a matrix Ψ_i fulfilling* (118)*, the following statements hold:*

(i) *The columns of Ψ_i are linearly independent.*
(ii) *The system matrix in* (119) *is invertible.*
(iii) *If Ψ_i is constructed via* (119)*, then* $\quad \langle S_i \Psi_i, z_i \rangle = 0 \quad \forall z_i \in W_{i\Delta}$.

Proof. Part (i) follows immediately from (118).
Part (ii). S_i is definite on $\ker(\bar{L}_i) = W_{i\Delta}$ (cf. (38), p. 16) and $\ker(\bar{L}_i^\top) = \{0\}$.
Part (iii). From the first line in (119) and from (117) we derive for $z_i \in W_{i\Delta}$,

$$\langle S_i \Psi_i, z_i \rangle \;=\; -\langle \bar{L}_i^\top \Lambda_i, z_i \rangle \;=\; -\langle \Lambda_i, \bar{L}_i z_i \rangle \overset{(117)}{=} 0.$$

□

Step 3. Corresponding to (116), the shape functions are arranged into groups corresponding to the globs:

$$\Psi_i = \big[\cdots \big| \Psi_i^{(G)} \big| \cdots \big]_{G \in \mathcal{G}_i}\,. \tag{120}$$

One easily shows the property

$$\bar{L}_{iG} R_{iG} \Psi_i^{(G')} = \delta_{GG'} I. \tag{121}$$

Step 4. Next, we loop over all globs $G \in \mathcal{G}$ and return to the original constraint matrices $\{L_{jG}\}_{j\in\mathcal{N}_G}$. We form the matrix

$$K_G = \big[\cdots \big| L_{jG} R_{jG} \Psi_j^{(G)} \big| \cdots \big]_{j\in\mathcal{N}_G} = \big[\cdots \big| K_{jG} \big| \cdots \big]_{j\in\mathcal{N}_G} \in \mathbb{R}^{r_{\Pi G}\times q_{\Pi G}}$$

and compute a coefficient matrix

$$Y_G := \begin{bmatrix} \vdots \\ Y_{jG} \\ \vdots \end{bmatrix}_{j\in\mathcal{N}_G} \in \mathbb{R}^{q_{\Pi G}\times n_{\Pi G}},$$

whose columns form a basis of $\ker(K_G)$, i.e.,

$$K_G Y_G = 0, \qquad n_{\Pi G} = \operatorname{rank}(Y_G) = \dim(\ker(K_G)). \tag{122}$$

This can, e.g., be done by a singular value decomposition (SVD), see [36, Sect. 2.5]. As we have shown in (88) in the proof of Theorem 5.18,

$$\dim(\ker(K_G)) = q_{\Pi G} - r_{\Pi G}\,. \tag{123}$$

Step 5. The number $n_{\Pi G}$ will be the number of coarse basis functions used on glob G. Therefore, the global space of coarse dofs given by $U_\Pi := \mathbb{R}^{n_\Pi}$ with $n_\Pi = \sum_{G\in\mathcal{G}} n_{\Pi G}$. The coarse basis itself is given by

$$\widetilde{\Psi}\colon U_\Pi \to W,\ \widetilde{\Psi} := \big[\cdots \big| \widetilde{\Psi}^{(G)} \big| \cdots \big]_{G\in\mathcal{G}},$$

where

$$\widetilde{\Psi}^{(G)}\colon \mathbb{R}^{n_{\Pi G}} \to W\colon \quad \widetilde{\Psi}_i^{(G)} := \begin{cases} \Psi_i^{(G)} Y_{iG} & i \in \mathcal{N}_G\,, \\ 0 & \text{otherwise.} \end{cases}$$

Theorem C.8. *For the construction above the following statements hold:*

(i) $\operatorname{range}(\widetilde{\Psi}) \subset \widetilde{W}$,
(ii) *the columns of* $\widetilde{\Psi}$ *are linearly independent and* $\dim(\operatorname{range}(\widetilde{\Psi})) = n_\Pi$,
(iii) $\widetilde{W} = \operatorname{range}(\widetilde{\Psi}) \oplus W_\Delta$,
(iv) *If all matrices* Ψ_i *are constructed via* (119) *then*

$$\langle Sw, z\rangle = 0 \qquad \forall w \in \operatorname{range}(\widetilde{\Psi}),\ z \in W_\Delta.$$

Proof. Part (i). We simply show that $\operatorname{range}(\widetilde{\Psi}^{(G)}) \in \widetilde{W}$ for an arbitrary but fixed glob $G \in \mathcal{G}$. From the definition of $\widetilde{\Psi}^{(G)}$ and property (121) we derive that for any glob $G' \in \mathcal{G}$ and any $j \in \mathcal{N}_{G'}$,

$$\bar{L}_{jG'} R_{jG'} \widetilde{\Psi}_j^{(G)} = \begin{cases} \bar{L}_{jG'} R_{jG'} \Psi_j^{(G)} Y_{jG} = \delta_{GG'} Y_{jG} & \text{if } j \in \mathcal{N}_G\,, \\ 0 & \text{otherwise.} \end{cases} \tag{124}$$

From (115) and the above we conclude that

$$\begin{aligned} \sum_{j\in\mathcal{N}'_G} L_{jG'} R_{jG'} \widetilde{\Psi}_j^{(G)} &= \sum_{j\in\mathcal{N}'_G} \begin{cases} \delta_{GG'} K_{jG'} Y_{jG} & \text{if } j \in \mathcal{N}_G \\ 0 & \text{otherwise} \end{cases} \\ &= \begin{cases} \sum_{j\in\mathcal{N}_G} K_{jG} Y_{jG} & \text{if } G' = G, \\ 0 & \text{otherwise,} \end{cases} \end{aligned}$$

but due to (122), this expression always evaluates to zero.
Part (ii). Firstly, we define

$$\overline{\Psi}^{(G)} := \operatorname{diag}(\Psi_i^{(G)})_{i=1}^N \colon \mathbb{R}^{q_{\Pi G}} \to W, \qquad \text{where } \Psi_i^{(G)} := 0 \in \mathbb{R}^{\dim(W_i)\times 0} \text{ if } i \notin \mathcal{N}_G\,,$$
$$\overline{\Psi} := [\cdots | \overline{\Psi}^{(G)} | \cdots]_{G\in\mathcal{G}}\,,$$

such that we can write

$$\widetilde{\Psi} \;=\; \overline{\Psi}\operatorname{diag}(Y_G)_{G\in\mathcal{G}}\,.$$

From (120), we observe that the columns of $\overline{\Psi}$ are just columns of some matrix Ψ_i extended by zero to the remaining subdomains. Hence, Proposition C.7 implies that $\overline{\Psi}$ is injective. Since each Y_G is injective, $\widetilde{\Psi}$ is injective as well.
Part (iii). Let $\overline{\Psi}$ be as above. From Proposition C.7 we obtain that $\operatorname{range}(\overline{\Psi}) \cap W_\Delta = \{0\}$, which implies that $\operatorname{range}(\widetilde{\Psi}) \cap W_\Delta = \{0\}$, so the sum $\operatorname{range}(\widetilde{\Psi}) + W_\Delta$ is direct and

$$\dim(\operatorname{range}(\widetilde{\Psi}) + W_\Delta) = n_\Pi + \dim(W_\Delta).$$

From (123) and Proposition 5.17 we obtain that $\dim(\widetilde{W}) = \dim(W_\Delta) + n_\Pi$, therefore the sum must equal $\widetilde{W}$.
Part (iv). Proposition C.7(iii) implies that for $z_i \in W_{\Delta i}$,

$$\langle S_i \widetilde{\Psi}_i, z_i\rangle \;=\; \langle S_i \sum_{G\in\mathcal{G}_i} \Psi_i^{(G)} R_{\Pi G}, z_i\rangle \;=\; 0. \qquad \square$$

Based on the direct sum $\widetilde{W} = \operatorname{range}(\widetilde{\Psi}) \oplus W_\Delta$, the operator $\tilde{I}\,\widetilde{S}^{-1}\tilde{I}^\top$ can be realized as in Sect. C.2.

Appendix D. Generalized inverse and Schur complement

Throughout this section, V is a finite-dimensional vector space and $A\colon V \to V^*$ a linear operator.

Definition D.1 (generalized inverse)**.** $A^\dagger\colon V^* \to V$ is a *generalized inverse*[5] of A if

$$A\,A^\dagger f \;=\; f \qquad \forall f \in \operatorname{range}(A).$$

From this definition, one easily derives

$$A^\dagger A x = x + v^K \text{ for some } v^K \in \ker(A) \qquad \forall x \in V, \tag{125}$$

as well as the following statement.

Proposition D.2. *For linear operators A, C, $D\colon V \to V^*$ with with* $\ker(A) \subset \ker(C)$ *and* $\operatorname{range}(D) \subset \operatorname{range}(A)$*, the expression $CA^\dagger D$ is invariant under the particular choice of the generalized inverse $A^\dagger$. Moreover, if $D = A$ then $CA^\dagger A = C$, and if $C = A$ then $AA^\dagger D = D$.*

For the following, let $V = V_1 \times V_2$ and

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}. \tag{126}$$

Lemma D.3. *If A is SPSD then* $\ker(A_{22}) \subset \ker(A_{12})$ *and* $\operatorname{range}(A_{21}) \subset \operatorname{range}(A_{22})$*. In particular, $A_{22}A_{22}^\dagger A_{21} = A_{21}$.*

[5]If, additionally, $A^\dagger A A^\dagger = A^\dagger$ then $A^\dagger$ is called *reflexive* generalized inverse, but we do not need this property.

Proof. Suppose that there exists an element $v_2 \in \ker(A_{22}) \setminus \{0\}$ with $A_{12}v_2 \neq 0$. Then there exists $v_1 \in V_1$ with $\langle A_{12}v_2, v_1\rangle < 0$. From the assumption on A we get for *any* $\beta \in \mathbb{R}^+$,

$$0 \leq \left\langle A \begin{bmatrix} v_1 \\ \beta v_2 \end{bmatrix}, \begin{bmatrix} v_1 \\ \beta v_2 \end{bmatrix} \right\rangle \;=\; \underbrace{\langle A_{11}v_1, v_1\rangle}_{\geq 0} + 2\beta \underbrace{\langle A_{12}v_2, v_1\rangle}_{<0},$$

which is a contradiction. From functional analysis we know that $\overline{\mathrm{range}(A^\top)} = \ker(A)^\circ$ where $W^\circ := \{\psi \in V^*\colon \langle \psi, w\rangle = 0\ \forall w \in W$ (for $W \subset V$}) is the annihilator (see, e.g., [80, p. 23]). This shows $\mathrm{range}(A_{22})^\circ \subset \mathrm{range}(A_{21})^\circ$ which implies the second assertion. □

Definition D.4. Let A, V_1, V_2 be as in (126). Then the *generalized Schur complement* (eliminating the components in V_2) is given by

$$S_1 \;:=\; A_{11} - A_{12}A_{22}^\dagger A_{21}$$

where $A_{22}^\dagger$ is a generalized inverse of A_{22}. If $\ker(A_{22}) \subset \ker(A_{12})$ and $\mathrm{range}(A_{21}) \subset \mathrm{range}(A_{22})$, this definition is independent of the particular choice of $A_{22}^\dagger$.

Lemma D.5. *Let A, V_1, V_2 be as in* (126) *and assume that A is SPSD. Then the generalized Schur complement S_1 has the following properties:*

$$\langle S_1v_1, v_1\rangle \leq \langle Av, v\rangle \qquad \forall v = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \in V, \tag{127}$$

$$\langle S_1v_1, v_1\rangle = \langle Av, v\rangle \qquad \forall v = \begin{bmatrix} v_1 \\ -A_{22}^\dagger A_{21}v_1 + v_2^K \end{bmatrix},\ v_1 \in V_1,\ v_2^K \in \ker(A_{22}). \tag{128}$$

Proof. Minimization of the quadratic functional $\langle Av, v\rangle$ with respect to v_2 for fixed v_1 leads to the first-order condition

$$A_{22}v_2 + A_{21}v_1 \;=\; 0. \tag{129}$$

By Lemma D.3, $A_{21}v_1 \in \mathrm{range}(A_{22})$, and so all solutions of (129) have the form

$$v_2 \;=\; -A_{22}^\dagger A_{21}v_1 + v_2^K, \qquad \text{with } v_2^K \in \ker(A_{22}).$$

The Hessian is given by A_{22} and by assumption positive semi-definite, so all these solutions are minimizers. We verify (128):

$$\begin{aligned} \langle Av, v\rangle \;&=\; \langle A_{11}v_1, v_1\rangle + \langle -A_{12}A_{22}^\dagger A_{21}v_1, v_1\rangle + \langle A_{12}v_2^K, v_1\rangle + \langle A_{21}v_1, -A_{22}^\dagger A_{21}v_1\rangle \\ &\quad + \langle A_{21}v_1, v_2^K\rangle + \langle A_{22}(A_{22}^\dagger A_{21}v_1 + v_2^K), A_{22}^\dagger A_{21}v_1 + v_2^K\rangle \;=\; \langle S_1v_1, v_1\rangle, \end{aligned}$$

where we have used Lemma D.3 and Definition D.1. Now (127) follows. □

The next lemma shows that the Schur complement $S_1\colon V_1 \to V_1^*$ is independent of the particular choice of the complementary space V_2.

Lemma D.6. *Let $A\colon V \to V^*$ be SPSD and let $V = V_1 \oplus V_2 = V_1 \oplus V_2'$ be two (direct) space splittings. Let S_1, S_1' be the generalized Schur complements corresponding to the first and second splitting, respectively. Then $S_1 = S_1'$.*

Proof. For $v \in V$ let (v_1, v_2), (v_1, v_2') be the components corresponding to the first and second splitting, respectively. From the properties of the direct sum, we see that there exists mappings T_1, T_2 with T_2 non-singular such that $v_2' = T_1v_1 + T_2v_2$ and $v_2 = T_2^{-1}(v_2' - T_1v_1)$. Let A_{11}, A_{12}, A_{21}, A_{22} be the components of A corresponding to the first space splitting, such that the components corresponding to the second splitting are given by

$$\begin{bmatrix} A_{11} - A_{12}T_2^{-1}T_1 - T_1^\top T_2^{-\top}A_{21} & A_{12}T_2^{-1} - T_1^\top T_2^{-\top}A_{22}T_2^{-1} \\ T_2^{-\top}A_{21} + T_2^{-\top}A_{22}T_2^{-1}T_1 & T_2^{-\top}A_{22}T_2^{-1} \end{bmatrix}.$$

Computing the generalized Schur complement eliminating the second component (v_2') and using Lemma D.3, one can easily verify that $S_1' = S_1$. □

Appendix E. Counterexample: $B(A+B+C)^{-1}A(A+B+C)^{-1}B \not\leq A$

We set

$$A = I, \quad B = \begin{bmatrix} 2.5 \cdot 10^{-5} & 0.0275 \\ 0.0275 & 838.6 \end{bmatrix}, \quad C = \begin{bmatrix} 7.2 & -29 \\ -29 & 225 \end{bmatrix}$$

Clearly, A, B, and C are SPD, as the diagonal entries are strictly positive and

$$\det(B) = 0.0134025, \quad \det(C) = 779.$$

However,

$$\sigma(A - B(A+B+C)^{-1}A(A+B+C)^{-1}B) = \{-9.26834, 1\}$$
$$\sigma(10A - B(A+B+C)^{-1}A(A+B+C)^{-1}B) = \{-0.248337, 10\}$$

So, for this particular example,

$$B(A+B+C)^{-1}A(A+B+C)^{-1}B \;\not\leq\; A$$
$$B(A+B+C)^{-1}A(A+B+C)^{-1}B \;\not\leq\; 10\,A.$$

However, from Lemma 5.10 we obtain

$$B(A+B+C)^{-1}A(A+B+C)^{-1}B \;\leq\; B(A+B+C)^{-1}(A+C)(A+B+C)^{-1}B \;\leq\; B:(A+C) \;\leq\; B.$$

So it is really the inequality with A on the right-hand side that fails to hold in general.

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