



ČESKÉ VYSOKÉ UČENÍ TECHNICKÉ V PRAZE
Fakulta stavební

Doktorský studijní program: **STAVEBNÍ INŽENÝRSTVÍ**
Studijní obor: **Matematika ve stavebním inženýrství**

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SROVNÁNÍ NĚKTERÝCH METOD DOMAIN DECOMPOSITION

COMPARISON OF SOME DOMAIN DECOMPOSITION METHODS

DISERTAČNÍ PRÁCE K ZÍSKÁNÍ AKADEMICKÉHO TITULU Ph.D.

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Praha, červen 2008

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Poděkování

Přestože předkládaná práce je psána v anglickém jazyce, rád bych úvodem česky poděkoval všem, kteří mne provázeli v doktorském studiu.

Můj dík patří Prof. Pavlu Burdovi a Dr. Jaroslavu Novotnému, kteří mne uvedli do numerické matematiky a matematického modelování. Dále děkuji svému školiteli Prof. Ivo Markovi a neméně Doc. Jozefu Bobokovi, vedoucímu katedry matematiky na fakultě stavební, ČVUT, za vstřícnost a ochotu, s jakou mne v průběhu studia podporovali a také za trpělivost a toleranci, se kterou snášeli mé časté zahraniční cesty. Velký dík patří mému školiteli specialistovi Prof. Janu Mandelovi za laskavost s jakou mne na univerzitě v Denveru přijal a za podmínky, které mi poskytl k nerušené a soustředěné práci. Chtěl bych také poděkovat svému příteli Dr. Jakubovi Šístkovi za příjemnou a plodnou spolupráci na nové formulaci a implementaci metody BDDC.

Závěrem, ale o to více, děkuji svým rodičům za výchovu a trvalou podporu, bez nichž by tato práce nemohla být sepsána.

Disertační práce byla vypracována s laskavou podporou programu Informační společnosti Akademie věd ČR 1ET400300415, Grantovou agenturou České republiky GA ČR 106/08/0403, a výzkumným projektem CEZ MSM 6840770003.

Výzkum během pobytů na University of Colorado Denver byl uskutečněn s podporou National Science Foundation granty CNS-0325314, CNS-0719641, a DMS-0713876.

Acknowledgement

Even though the thesis is written in English, I would like to thank in Czech to all, who have supported me during doctoral studies.

First, I thank to Prof. Pavel Burda and Dr. Jaroslav Novotný, for introducing me into the numerical mathematics and the mathematical modeling. Next, I would like to thank my advisor Prof. Ivo Marek as well as Doc. Jozef Bobok, the head of the Department of Mathematics at the Faculty of Civil Engineering, Czech Technical University in Prague, for their help and support of my studies as well as for their toleration of my frequent travels abroad. A large debt of gratitude goes to my second advisor Prof. Jan Mandel for his hospitality in accommodating me in Denver, and for the working conditions he created for my focused and uninterrupted work. I would also like to thank my friend Dr. Jakub Šístek for a pleasant and fruitful joint research on a new formulation and implementation of the BDDC method.

Last but not least I thank my parents for bringing me up the way they did and for continuing support, without which the thesis could never be written.

The doctoral dissertation has been kindly supported by the program of the Information Society of the Czech Academy of Sciences 1ET400300415, Grant Agency of the Czech Republic GA ČR 106/08/0403, and by the research project CEZ MSM 6840770003.

The research completed during my visit at the University of Colorado Denver has been kindly supported by the National Science Foundation under grants CNS-0325314, CNS-0719641, and DMS-0713876.

1. INTRODUCTION

Tremendous progress in the design and availability of parallel computers over the last several decades has motivated active and progressive research in many areas including the *domain decomposition methods*. By domain decomposition we will in our context understand the processes of separation of physical domain into regions typically called *substructures* or *subdomains*. The basic idea is that the problem formulated on the whole domain can be divided into a set of smaller problems formulated on individual substructures, each one assigned typically to a different processor on a parallel computer, allowing subsequently the solution of problems with significantly larger number of unknown and/or significant shortening of the computational time. An important class of methods, that we will in particular focus on, is *iterative substructuring* class characterized by non-overlapping division into subdomains. These methods are used for the construction of preconditioners in the iterative loop of conjugate gradients (or other Krylov subspace method). First, we provide a short overview of some of these iterative substructuring methods centered on works connected to the theory that motivated our research. For a more complete survey of the theory and implementation, we refer the reader to the monographs, e.g., [33, 57, 60].

Let us consider a second order, self-adjoint, positive definite problem obtained from an elliptic partial differential equation, such as Laplace equation or linearized elasticity, given on a physical domain in two or three spatial dimensions and discretized by finite elements with characteristic element size h . Given sufficient boundary conditions, the global stiffness matrix is nonsingular, and its condition number grows as $O(h^{-2})$ for $h \rightarrow 0$. However, if the domain is divided into substructures consisting of disjoint unions of elements and the interior degrees of freedom of each substructure are eliminated, the resulting matrix on the boundary degrees of freedom has condition that grows only as $O(H^{-1}h^{-1})$ where $H \gg h$ is the characteristic size of the substructure. This fact has been known early on (Keyes and Gropp [25]); for a recent rigorous treatment, see Brenner [4]. The elimination of the interior degrees of freedom is also called *static condensation*, and the resulting reduced matrix is called the *Schur complement*. Because of the significant decrease of the condition number, one can substantially accelerate iterative methods by investing some work up front in the Choleski decomposition of the stiffness matrix on the interior degrees of freedom and then just run back substitution in each iteration. The finite element matrix is assembled separately in each substructure. This process is called *subassembly*. The elimination of the interior degrees of freedom in each substructure can be done independently, which is important for parallel computing: each substructure can be assigned to an independent processor. The substructures are then treated as large elements, with the Schur complements playing the role of the local stiffness matrices of the substructures. See [25, 57] for more details.

The process just described is the background of *primal iterative substructuring methods*. Here, the condition that the values of degrees of freedom common to several substructures coincide is enforced strongly, by using a single variable to represent them. The improvement of the condition number from $O(h^{-2})$ to $O(H^{-1}h^{-1})$, straightforward implementation, and the potential for parallel computing, explain the early popularity of iterative substructuring methods [25]. However, further preconditioning is needed. Perhaps the most basic preconditioner for the reduced problem is a diagonal one. Preconditioning of a matrix by its diagonal helps to take out the dependence on scaling and variation of coefficients and grid sizes. But the diagonal of the Schur complement is expensive to obtain. It is usually better to avoid explicit computation of the Schur complement and use only multiplication by the reduced substructure matrices, which can be implemented by solving a *Dirichlet* problem on each substructure. Probing methods (Chan and Mathew [6]) use such matrix-vector multiplication to estimate the diagonal entries of the Schur complement.

In *dual iterative substructuring methods*, also called FETI methods, the condition that the values of degrees of freedom common to several substructures coincide is enforced weakly, by Lagrange multipliers. The original degrees of freedom are then eliminated, resulting in a system for the Lagrange multipliers, with the system operator consisting essentially of an assembly of the inverses of the Schur complements. Multiplication by the inverses of the Schur complements can be implemented by solving a *Neumann* problem on each substructure. The assembly process is modified to ensure that the Neumann problems are consistent, giving rise to a natural coarse problem. The system for the Lagrange multipliers is solved again iteratively. This is the essence of the FETI method by Farhat and Roux [19], later called FETI-1. The condition number of the FETI-1 method with diagonal preconditioning grows as $O(h^{-1})$ and is bounded independently of the number of substructures (Farhat, Mandel, and Roux [18]). For a small number of substructures, the distribution of the eigenvalues of the iteration operator is clustered at zero, resulting in superconvergence of conjugate gradients; however, for more than a handful of substructures, the superconvergence is lost and the speed of convergence is as predicted by the $O(h^{-1})$ growth of the condition number [18].

For large problems and large number of substructures, *asymptotically optimal preconditioners* are needed. These preconditioners result typically in condition number bounds of the form $O(\log^\alpha(1 + H/h))$ (the number 1 is there only to avoid the value $\log 1 = 0$). In particular, the condition number is bounded independently of the number of substructures and the bound grows only slowly with the substructure size. Such preconditioners require a *coarse problem*, and *local preconditioning* that inverts approximately (but well enough) the diagonal submatrices associated with segments of the interfaces between the substructures or the substructure matrices themselves. The role of the local preconditioning is to slow down the growth of the condition number as $h \rightarrow 0$, while the role of the coarse problem is to provide global exchange of information in order to bound the condition number independently of the number of substructures. Many such asymptotically optimal primal methods were designed in the 1980s and 1990s, e.g., Bramble, Pasciak, and Schatz [2, 3], Dryja [12], Dryja, Smith, and Widlund [14], Dryja and Widlund [15], and Widlund [62]. However, those algorithms require additional assumptions and information that may not be

readily available from finite element software, such as an explicit assumption that the substructures form a coarse triangulation, and that one can build coarse linear functions from its vertices.

Practitioners desire methods that work algebraically with arbitrary substructures (even if a theory may be available only in special cases), and are formulated in terms of the substructure matrices only, with minimal additional information. In addition, the methods should be robust with respect to various irregularities of the problem. Two such methods have emerged in early 1990s: the Finite Element Tearing and Interconnecting (FETI) method by Farhat and Roux [19], and the Balancing Domain Decomposition (BDD) by Mandel [42]. Essentially, the FETI method (with the Dirichlet preconditioner) preconditions assembly of the inverses of the Schur complements by an assembly of the Schur complements, and the BDD method preconditions assembly of Schur complements by an assembly of the inverses, with a suitable coarse problem added. Of course, the assembly weights and other details play an essential role.

The BDD method added a coarse problem to the local Neumann-Neumann preconditioner by DeRoeck and Le Tallec [55], which consisted of the assembly (with weights) of pseudoinverses of the local matrices of the substructures. Assembling the inverses of the local matrices is an idea similar to the Element-by-Element (EBE) method by Hughes et al. [23]. The method was called Neumann-Neumann because the preconditioner requires solution of Neumann problems on all substructures, in contrast to an earlier Neumann-Dirichlet method, which, for a problem with two substructures, required the solution of a Neumann problem on one and a Dirichlet problem on the other [62]. The coarse problem in BDD was constructed from the natural nullspace of the problem (constant for the Laplace equation, rigid body motions for elasticity) and solving the coarse problem guaranteed consistency of local problems in the preconditioner. The coarse correction was then imposed variationally, just as the coarse correction in multigrid methods. The $O(\log^2(1 + H/h))$ bound was then proved [42].

In the FETI method, solving the local problems on the substructures to eliminate the original degrees of freedom has likewise required working in the complement of the nullspace of the substructure matrices, which gave a rise to a natural coarse problem. Since the operator employs inverse of the Schur complement (solving a Neumann problem), an optimal preconditioner employs multiplication by the Schur complement (solving a Dirichlet problem), hence the preconditioner was called the Dirichlet preconditioner. The $O(\log^3(1 + H/h))$ bound was proved by Mandel and Tezaur [50], and $O(\log^2(1 + H/h))$ for a certain variant of the method by Tezaur [59].

Because the interface to the BDD and FETI methods required only the multiplication by the substructure Schur complements, solving systems with the substructure Schur complements, and information about the substructure nullspace, the methods got quite popular and widely used. Cowsar, Mandel, and Wheeler [7], implemented the multiplications as solutions of mixed problems on substructures. However, neither BDD nor the FETI method worked well for 4th order problems (plate bending). The reason was essentially that both methods involve “tearing” a vector of degrees of freedom reduced to the interface, and, for 4th order problems, the “torn” function has energy that grows as negative power of h , unlike for 2nd order problems, where the energy grows

only as a positive power of $\log(1/h)$ by the so-called discrete Sobolev inequality [43]. The solution was to prevent the “tearing” by fixing the function at the substructure corners; then only its derivative along the interface gets “torn”, which has energy again only of the order $\log(1/h)$. Preventing such “tearing” can be generally accomplished by increasing the coarse space, since the method runs in the complement to the coarse space. For the BDD method, this was relatively straightforward, because the algebra of the BDD method allows arbitrary enlargement of the coarse space. The coarse space that does the trick contains additional functions with spikes at corners, defined by fixing the value at the corner and minimizing the energy. With this improvement, $O(\log^2(1 + H/h))$ condition number bound was proved and fast convergence was recovered for 4th order problems (Le Tallec, Mandel, and Vidrascu [36, 37]). In the FETI method, unfortunately, the algebra requires that the coarse space is made of exactly the nullspace of the substructure matrices, so a simple enlargement of the coarse space is not possible. Therefore, a version of FETI, called FETI-2, was developed by Mandel, Tezaur, and Farhat [52], with a second correction by coarse functions concentrated at corners, wrapped around the original FETI method variationally much like BDD, and the $O(\log^3(1 + H/h))$ bound was proved again. However, the BDD and FETI methods with the modifications for 4th order problems were rather unwieldy (especially FETI-2), and, consequently, not as widely used. On the other hand, certain variants of the original FETI method has been successfully applied to composite materials [34, 35].

The breakthrough came with the FETI-DP method by Farhat et al. [16], which enforced the continuity of the degrees of freedom on a substructure corner as in the primal method by representing them by one common variable, while the remaining continuity conditions between the substructures are enforced by Lagrange multipliers. The primal variables are again eliminated and the iterations run on the Lagrange multipliers. The elimination process can be organized as solution of sparse system and it gives rise to a natural coarse problem, associated with substructure corners. In 2D, the FETI-DP method was proved to have condition number bounded as $O(\log^2(1 + H/h))$ both for 2nd order and 4th order problems by Mandel and Tezaur [51]. However, the method does not converge as well in 3D and averages over edges or faces of substructures need to be added as coarse variables for fast convergence (Klawonn, Widlund, and Dryja [30], Farhat, Lesoinne, and Pierson [17]), and the $O(\log^2(1 + H/h))$ bound can then be proved again ([30]).

The Balancing Domain Decomposition by Constraints (BDDC) was developed by Dohrmann [9] as a primal alternative the FETI-DP method. The BDDC method uses imposes the equality of coarse degrees of freedom on corners and of averages by constraints. In the case of only corner constraints, the coarse basis functions are the same as in the BDD method for 4th order problems from [36, 37]. The bound $O(\log^2(1 + H/h))$ for BDDC was first proved by Mandel and Dohrmann [44].

The BDDC and the FETI-DP are currently the most advanced versions of the BDD and FETI families of methods. Their convergence properties were quite similar, yet it came as a surprise when Mandel, Dohrmann, and Tezaur [45] proved that the spectra of their preconditioned operators are in fact identical, once all the components are same. This result came at the end of a long chain of ties discovered between the BDD and FETI type methods. Algebraic relations between the FETI and BDD methods were pointed out by Rixen et al. [54],

Klawonn and Widlund [27], and Fragakis and Papadrakakis [21]. An important common bound on the condition number of both the FETI and the BDD method in terms of a single inequality was given Klawonn and Widlund [27]. Fragakis and Papadrakakis [21], who derived certain primal versions of the FETI and FETI-DP methods (called P-FETI-1 and P-FETI-DP), have also observed that the eigenvalues of BDD and a certain version of FETI are identical, along with the proof that the primal version of this particular FETI algorithm gives a method same as BDD. The proof of equality of eigenvalues of BDD and this particular version of FETI was given just recently in more abstract framework by Fragakis [20]. Mandel, Dohrmann, and Tezaur [45] have proved that the eigenvalues of BDDC and FETI-DP are identical and they have obtained a simplified and fully algebraic version (i.e., with no undetermined constants) of a common condition number estimate for BDDC and FETI-DP, similar to the estimate by Klawonn and Widlund [27] for BDD and FETI. Simpler proofs of the equality of eigenvalues of BDDC and FETI-DP were obtained later by Li and Widlund [41], and by Brenner and Sung [5], who also gave an example when BDDC has an eigenvalue equal to one but FETI-DP does not. Another primal preconditioner inspired by FETI-DP was independently proposed by Cros [8]. This later gave raise to a conjecture that P-FETI-DP and BDDC are in fact the same method, which was first shown in our recent works [48, 58].

It is interesting to note that the choice of assembly weights in the BDD preconditioner was known at the very start from the work of DeRoeck and Le Tallec [55] and before, while the choice of weights for a FETI type method is much more complicated. A correct choice of weights is essential for the robustness of the methods with respect to scaling the matrix in each substructure by an arbitrary positive number (the “independence of the bounds on jumps in coefficients”). For the BDD method, such convergence bounds were proved by Mandel and Brezina [43], using a similar argument as in Sarkis [56] for Schwarz methods; see also Dryja, Sarkis, and Widlund [13]. For FETI methods, a proper choice of weights was discovered only much later - see Farhat, Lesoinne and Pierson [17] for a special case, Klawonn and Widlund [27] for a more general case and convergence bounds, and a detailed discussion in Mandel, Dohrmann, and Tezaur [45].

The main goal of this thesis is to present some of the connections between the primal and dual iterative substructuring methods as they appeared in our research, in particular in [46, 47, 48, 58]. It is organized as follows. In Chapter 2 we introduce the notation and a small set of algebraic assumptions needed in the formulation of all studied methods. The chapter is concluded by a short section on substructuring that has been motivated by two main reasons: first, to clarify how the spaces and operators arise in the standard substructuring theory and second, although we tried to derive all preconditioners in a simple abstract form, for the historical reasons and references to older version of some of the preconditioners, we could not avoid using some substructuring components. In Chapter 3 we formulate several (the most frequently used) primal and dual substructuring methods. In the first part of this chapter we derive two dual methods from the FETI family: the original (one-level) FETI method by Farhat and Roux [19] denoted from now on as FETI-1, and the FETI-DP method by Farhat et al. [16, 17] which is currently the most advanced method from this family. For both methods we also formulate their primal versions,

denoted respectively as P-FETI-1 and P-FETI-DP, introduced by Fragakis and Papadrakakis [21]. The P-FETI-DP method is derived at two different levels of detail: first, it is derived from a particularly simple formulation of FETI-DP as in our recent work [48] and then from the original FETI-DP formulation [16] - in order to complete the derivation of P-FETI-DP omitted in [20, 21]. In the second part of this chapter, we formulate two primal methods from the BDD family: the original BDD by Mandel [42] and the BDDC by Dohrmann [9]. Again, the BDDC method is derived at two levels of detail: first we state a simple variational formulation from [47], which allows us to see immediately that the BDDC and P-FETI-DP preconditioners are in fact the same. Then, we rederive the BDDC algorithm in order to show that it is the same as a version of P-FETI-DP from [21], which also immediately shows that the preconditioner by Cros [8] can be interpreted as either P-FETI-DP or BDDC. In Chapter 4, we focus on connections between the introduced primal and dual methods. In the first part of the chapter, we present the condition number bound and the proof of the equality of eigenvalues of BDDC and FETI-DP in the abstract minimalist settings from Section 2.2. In the second part of this chapter, we recall from [21] that for a particular variant of FETI-1, the P-FETI-1 method gives the same algorithm as BDD, and also apply a recent abstract result by Fragakis [20] to show that the eigenvalues of BDD and the particular variant of FETI-1 are the same. It is notable that this is the variant of FETI-1 devised to deal with difficult, heterogeneous problems [1]. One useful aspect is the translation of the abstract ideas from [20, 21] into the framework usual in the domain decomposition community. Finally in Chapter 5, based on our previous work [47], we build on the algebraic estimate from [45] to develop an adaptive fast method with FETI-DP or BDDC as preconditioners. This estimate can be computed from the matrices in the method as the solution of a generalized eigenvalue problem. By restricting the eigenproblems onto pairs of adjacent substructures, we obtain a reliable heuristic indicator of the condition number. We also show how to use the eigenvectors, which are supported on subsets of the intersections of adjacent substructures, to build coarse degrees of freedom that result in an optimal decrease of the heuristic condition number indicator. We show on numerical examples that the indicator is quite close to the actual condition number and that our adaptive approach can result in the concentration of computational work in a small troublesome part of the problem, which leads to a good convergence behavior at a small added cost. We note that related work on adaptive coarse space selection has focused on the global problem of selecting the smallest number of corners to prevent coarse mechanisms by Lesoinne [38], and the smallest number of (more general) coarse degrees of freedom to assure asymptotically optimal convergence estimates by Klawonn and Widlund [28]. This required considering potentially large chains of substructures, based on the global behavior of the structure. Our goal is different. We assume that the starting coarse degrees of freedom (i.e., those present before the adaptive selection of additional ones) are already sufficient to prevent relative rigid body motions of any two adjacent substructures that are used to compute the indicator and additional coarse degrees of freedom. Our methodology is quite general, local in nature, involving only two substructures at a time and also dimension independent. The chapter is concluded by several numerical examples in two and three spatial dimensions illustrating the effectiveness of the proposed adaptive method.

2. CONCEPTS AND SUBSTRUCTURING

We begin with preliminaries and an overview of notation used throughout the thesis. Next, we list a set of minimalist assumptions including the introduction of the spaces and linear operators used in the formulation of the studied methods. Finally, we illustrate on a model problem how the spaces and operators arise in the standard substructuring theory.

2.1 Notation and preliminaries

All considered spaces are finite dimensional linear spaces. The dual space of a space V is denoted by V' and $\langle \cdot, \cdot \rangle$ is the duality pairing. For a linear operator $L : W \rightarrow V$ we define its transpose $L^T : V' \rightarrow W'$ by $\langle v, Lw \rangle = \langle L^T v, w \rangle$ for all $v \in V'$, $w \in W$, and $\|v\|_K = \sqrt{\langle Kv, v \rangle}$ denotes the norm associated with a symmetric and positive definite operator $K : V \rightarrow V'$, i.e., such that $\langle Kv, v \rangle > 0$ for all $v \in V$, $v \neq 0$. The norm of a linear operator $E : V \rightarrow V$ subordinate to this vector norm is defined by $\|E\|_K = \max_{v \in V, v \neq 0} \|Ev\|_K / \|v\|_K$. The notation I_V denotes the identity operator on the space V .

Mappings from a space to its dual arise naturally in the variational setting of systems of linear algebraic equations. An example, consider an $n \times n$ matrix A and the system of equations $Ax = b$. The variational form of this system is

$$x \in V : (Ax, y) = (b, y) \quad \forall y \in V,$$

where $V = \mathbb{R}^n$ and (\cdot, \cdot) is the usual Euclidean inner product on \mathbb{R}^n . For a fixed x , instead of the value Ax , we find it convenient to consider the linear mapping $y \mapsto (Ax, y)$. This mapping is an element of the dual space V' . Denote this mapping by Kx and its value at y by $\langle Kx, y \rangle$; then $K : V \rightarrow V'$ is a linear operator from V to its dual that corresponds to A . This setting involving dual spaces is convenient and compact when dealing with multiple nested spaces, or with dual methods (such as FETI). Restricting a linear functional to a subspace is immediate, while the equivalent notation without duality requires introducing new operators, namely projections or transposes of injections. Also, this setting allows us to make a clear distinction between an approximate solution and its residual, which is in the dual space. It is beneficial to have approximate solutions and residuals in different spaces, because they need to be treated differently.

We wish to solve a system of linear algebraic equations

$$Ku = f,$$

where $K : V \rightarrow V'$, by a preconditioned conjugate gradient method. Here, a preconditioner is a mapping $M : V' \rightarrow V$. In iteration k the method computes the residual

$$r^{(k)} = Ku^{(k)} - f \in V',$$

and the preconditioner computes the increment to the approximate solution $u^{(k)}$ as a linear combination of the preconditioned residual $Mr^{(k)} \in V$ with preconditioned residuals in earlier iterations. Convergence properties of the method can be established from the eigenvalues λ of the *preconditioned operator* MK ; the condition number

$$\kappa = \frac{\lambda_{\max}(MK)}{\lambda_{\min}(MK)},$$

gives a well-known bound on the error reduction, cf., e.g., [22],

$$\|e^{(k)}\|_K \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \|e^{(0)}\|_K,$$

where $e^{(k)} = u^{(k)} - u$ is the error of the solution in iteration k .

2.2 Minimalist settings and assumptions

We now list a minimalist set of spaces, linear operators, and assumptions needed in formulation of the methods and to prove their properties. To see how these spaces and operators arise in the substructuring, we refer to the next section. Let W be a finite dimensional space and let $a(\cdot, \cdot)$ be a symmetric positive semidefinite bilinear form on W . Let $\widehat{W} \subset W$ be a subspace such that a is positive definite on \widehat{W} , and $f \in \widehat{W}'$. We wish to solve a variational problem

$$u \in \widehat{W} : a(u, v) = \langle f, v \rangle \quad \forall v \in \widehat{W}. \quad (2.1)$$

All the methods we are interested in are characterized by a selection of linear operators E , B , and B_D . The operator E is a projection onto \widehat{W} ,

$$E : W \rightarrow \widehat{W}, \quad E^2 = E, \quad \text{range } E = \widehat{W}. \quad (2.2)$$

The role of the operator B is to enforce the condition $u \in \widehat{W}$ by

$$Bu = 0 \iff u \in \widehat{W}, \quad (2.3)$$

and

$$B : W \rightarrow \Lambda, \quad \text{null } B = \widehat{W}, \quad \text{range } B = \Lambda. \quad (2.4)$$

The operator B_D^T is a generalized inverse of B ,

$$B_D^T : \Lambda \rightarrow W, \quad BB_D^T = I_\Lambda. \quad (2.5)$$

In the construction of the FETI-DP and BDDC preconditioners, the role of the space W is completely taken by an intermediate space \widetilde{W} ,

$$\widehat{W} \subset \widetilde{W} \subset W, \quad (2.6)$$

such that

$$a(\cdot, \cdot) \text{ is positive definite on } \widetilde{W}. \quad (2.7)$$

The properties (2.2) – (2.5) and eventually (2.7) are enough for the theories of the methods separately, and they will be assumed from now on. To relate the methods, denote by

$$R : \widehat{W} \rightarrow W, \quad R : w \in \widehat{W} \mapsto w \in W, \quad (2.8)$$

the natural injection from \widehat{W} to W . Clearly,

$$ER = I_{\widehat{W}}, \quad (2.9)$$

and

$$BR = 0. \quad (2.10)$$

We shall also assume that

$$B_D^T B + RE = I \quad (2.11)$$

when needed. No further assumptions are necessary to formulate and relate all studied methods in Chapters 3 and 4. The only exceptions are, for the historical reasons, the more detailed formulations of the P-FETI-DP and BDDC methods; to derive them we had to make few references to substructuring in Sec. 2.3.

Remark 1: *In the literature, esp. [45] and references therein, the projection E is often written in the form $E = R^T D_P$, where R is a mapping of another space (isomorphic to \widehat{W}) into W . In the abstract settings of Chapters 2-4, we choose to formulate the methods directly in the space \widehat{W} . It turns out that the space W is needed only in the theory of the FETI-1 and BDD methods and its role in the theory of the FETI-DP and BDDC methods is completely taken by \widehat{W} , and so the space W is not needed for the theory of the latter methods at all. The operator R thus becomes the identity embedding of \widehat{W} into W . Next, we remark that the equation (2.11) is found already in [54, Lemma 1] in the special case, when the construction of the equation is based on the multiplicity of interfaces. It was extended to the form used presently and to cover more general algorithms, and also used to obtain important connections between dual and primal substructuring methods, in [21, 27]. Finally, note that the assumption (2.5) allows the case when B is a matrix that does not have full row rank. All that is needed is to define Λ as $\text{range } B$.*

Finally, we need to define the linear operators \widehat{S} , \widetilde{S} and S associated with the bilinear form a on the spaces \widehat{W} , \widetilde{W} and W , respectively, by

$$\widehat{S} : \widehat{W} \rightarrow \widehat{W}', \quad \langle \widehat{S}v, w \rangle = a(v, w) \quad \forall v, w \in \widehat{W}. \quad (2.12)$$

$$\widetilde{S} : \widetilde{W} \rightarrow \widetilde{W}', \quad \langle \widetilde{S}v, w \rangle = a(v, w) \quad \forall v, w \in \widetilde{W}, \quad (2.13)$$

$$S : W \rightarrow W', \quad \langle Sv, w \rangle = a(v, w) \quad \forall v, w \in W, \quad (2.14)$$

From (2.12), the variational problem (2.1) becomes

$$\widehat{S}u = f. \quad (2.15)$$

Further, it follows from (2.12), (2.14), and (2.8), that

$$\widehat{S} = R^T S R. \quad (2.16)$$

Finally, we note that the problem (2.1) is equivalent to the minimization

$$\frac{1}{2}a(u, u) - \langle f, u \rangle \rightarrow \min \text{ subject to } u \in \widehat{W},$$

and using

$$\langle f, u \rangle = \langle f, Eu \rangle = \langle E^T f, u \rangle, \quad u \in \widehat{W},$$

we can rewrite (2.1) as

$$\frac{1}{2}a(u, u) - \langle E^T f, u \rangle \rightarrow \min \text{ subject to } u \in \widehat{W}. \quad (2.17)$$

2.3 Substructuring for a model problem

To clarify ideas, we show how the spaces and operators introduced in the previous section arise in the standard substructuring theory for a model problem obtained by a discretization of a second order elliptic problem. Consider a bounded domain $\Omega \subset \mathbb{R}^d$, where $d = 2$ or 3 , decomposed into nonoverlapping subdomains Ω_i , $i = 1, \dots, N$, which form a conforming triangulation of the domain Ω . Each subdomain Ω_i is a union of Lagrangean $P1$ or $Q1$ finite elements, and the nodes of the finite elements between the substructures coincide. In the scalar case, each node is associated with one degree of freedom and in the case of linearized elasticity each node is associated with d degrees of freedom. The nodes contained in the intersection of at least two substructures are called boundary nodes. The union of all boundary nodes of all substructures is called the interface, denoted by Γ , and Γ_i is the interface of substructure Ω_i . The interface Γ may also be classified as the union of three different types of sets: *faces*, *edges* and *corners*. We will adopt here a simple (geometric) definition: a *face* contains all nodes shared by the same two subdomains, an *edge* contains all nodes shared by same set of more than two subdomains, and a *corner* is a degenerated edge with only one node; for a more general definition see, e.g., [29]. We just remark that in 2D, we will commonly call faces as edges (as there are none according to our definition) and that these entities are understood to be relatively open, i.e., an edge does not contain its endpoints or a face does not contain its boundaries. Also, similarly to [43], we will call in 2D an edge or in the 3D a face as a *glob*.

The space of all vectors of local degrees of freedom on Γ_i is denoted by W_i . Let $S_i : W_i \rightarrow W_i$ be the Schur complement operator obtained from the stiffness matrix of the substructure Ω_i by eliminating all interior degrees of freedom of Ω_i , i.e., those that do not belong to Γ_i . We assume that the matrices S_i are symmetric positive semidefinite. Let

$$W = W_1 \times \dots \times W_N, \quad (2.18)$$

and write vectors and matrices in the block form

$$w = \begin{bmatrix} w_1 \\ \vdots \\ w_N \end{bmatrix}, \quad w \in W, \quad S = \begin{bmatrix} S_1 & & \\ & \ddots & \\ & & S_N \end{bmatrix}. \quad (2.19)$$

The bilinear form a is then given by

$$a(u, v) = u^T S v. \quad (2.20)$$

The solution space \widehat{W} of the problem (2.1) is a subspace of W such that all subdomain vectors of degrees of freedom are continuous across the interfaces, which here means that their values on all the substructures sharing an interface nodes coincide.

The BDDC and FETI-DP preconditioners are characterized by selection of *coarse degrees of freedom*, such as values at the corners and averages over edges or faces of subdomains. The space is then given by the requirement that the coarse degrees of freedom on adjacent substructures coincide; for this reason, the terms coarse degree of freedom and *constraint* may be used interchangeably.

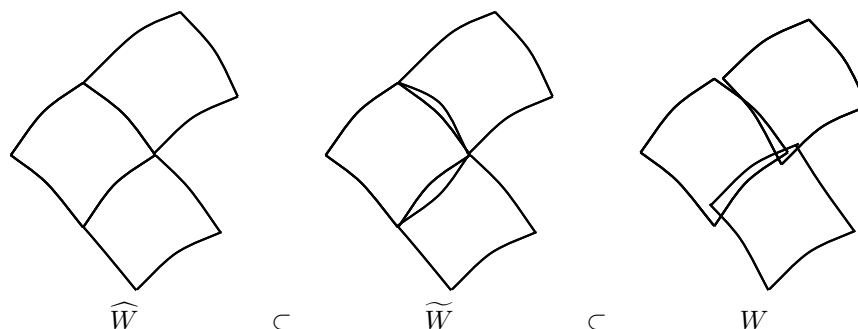


Fig. 2.1: Schematic drawing of continuity conditions between substructures, in the case of corner coarse degrees of freedom only: all degrees of freedom continuous (the space \widehat{W}), only the coarse degrees of freedom need to be continuous (the space \widetilde{W}), and no continuity conditions (the space W).

In the present setting, this becomes the selection of the subspace $\widetilde{W} \subset W$, defined as the subspace of all functions such that coarse degrees of freedom are continuous across the interfaces, cf., Fig. 2.1. There needs to be enough constraints so that the variational problem on \widetilde{W} is coercive, i.e., (2.7) is satisfied. Creating the stiffness matrix on the space \widetilde{W} is called subassembly [41].

The last ingredient of the methods is the selections of the linear operators E , B and B_D . We note that the operators E and B are defined on the whole space W . The operator $E : W \rightarrow \widehat{W}$ is an averaging of the values of degrees of freedom between the substructures. The averaging weights are often taken proportional to the diagonal entry of the stiffness matrices in the substructures. The matrix B enforces the continuity across substructure interfaces by the condition $Bw = 0$. Each row B has only two nonzero entries, one equal to $+1$ and one equal to -1 , corresponding to the two degrees of freedom whose value should be same. So, Bw is the jump of the value of w between substructures. Redundant Lagrange multipliers are possible; then B does not have full row rank and $\Lambda = \text{range } B$ is not the whole Euclidean space. Finally, B_D is a matrix such that a vector λ of jumps between the substructures is made into a vector of degrees of freedom $B_D^T \lambda$ that exhibits exactly those jumps. That is, $BB_D^T = I$. The construction of B_D involves weights, related to those in the operator E , so that $B_D^T B + RE = I$. Such construction was done first for FETI-1 in [30] in order to obtain estimates independent of the jump of coefficients between substructures, and then adopted for FETI-DP. We only note that in many cases of practical relevance, the matrix B_D is determined from the properties (2.2) – (2.11) uniquely as the Moore-Penrose pseudoinverse in a special inner product given by the averaging weights in the operator E [45, Theorem 14].

3. FORMULATION OF THE METHODS

3.1 Methods from the FETI family

We formulate two FETI methods: the FETI-1 method by Farhat and Roux [19] and the FETI-DP by Farhat et al. [16, 17]. In both cases we also derive the primal versions of these methods, proposed originally by Fragakis and Papadrakakis [21], and denoted as P-FETI-1 and P-FETI-DP, respectively.

3.1.1 FETI-1

We can write (2.17) as a constrained minimization problem posed on W ,

$$\frac{1}{2}a(w, w) - \langle E^T f, w \rangle \rightarrow \min \quad \text{subject to } w \in W \quad \text{and} \quad Bw = 0, \quad (3.1)$$

Introducing the Lagrangean

$$\mathcal{L}(w, \lambda) = \frac{1}{2}a(w, w) - \langle E^T f, w \rangle + \langle B^T \lambda, w \rangle, \quad (3.2)$$

where $\lambda \in \Lambda'$ are the Lagrange multipliers, we obtain that problem (3.1) is equivalent to solving the saddle-point problem, cf., e.g. [53],

$$\min_{w \in W} \max_{\lambda \in \Lambda'} \mathcal{L}(w, \lambda). \quad (3.3)$$

Since

$$\min_{w \in W} \max_{\lambda \in \Lambda'} \mathcal{L}(w, \lambda) = \max_{\lambda \in \Lambda'} \min_{w \in W} \mathcal{L}(w, \lambda),$$

it follows that (3.1) is equivalent to the dual problem

$$\frac{\partial \mathcal{C}(\lambda)}{\partial \lambda} = 0, \quad (3.4)$$

where

$$\mathcal{C}(\lambda) = \min_{w \in W} \mathcal{L}(w, \lambda). \quad (3.5)$$

Problem (3.4) is equivalent to stationary conditions for the Lagrangean \mathcal{L} ,

$$\begin{aligned} \frac{\partial}{\partial w} \mathcal{L}(w, \lambda) &\perp W, \\ \frac{\partial}{\partial \lambda} \mathcal{L}(w, \lambda) &= 0, \end{aligned} \quad (3.6)$$

which is the same as solving for $w \in W$ and $\lambda \in \Lambda'$ from the system

$$\begin{aligned} Sw + B^T \lambda &= E^T f, \\ Bw &= 0. \end{aligned} \quad (3.7)$$

We note that the operator S is not in general invertible on the whole space W . Also, since S is invertible on null B and λ is unique up to a component in null B^T , the space Λ in (2.4) is selected to be range B . Next, let Z be a matrix with linearly independent columns, such that

$$\text{range } Z = \text{null } S. \quad (3.8)$$

Since S is semidefinite, it must hold for the first equation in (3.7) that

$$E^T f - B^T \lambda \in \text{range } S = (\text{null } S^T)^\perp = (\text{range } Z^T)^\perp = \text{null } Z^T,$$

so equivalently,

$$Z^T(E^T f - B^T \lambda) = 0. \quad (3.9)$$

Eliminating w from the first equation in (3.7) as

$$w = S^+(E^T f - B^T \lambda) + Za, \quad (3.10)$$

substituting in the second equation in (3.7) and rewriting (3.9), we get

$$\begin{aligned} BS^+B^T\lambda - BZa &= BS^+E^T f, \\ -Z^TB^T\lambda &= -Z^TE^T f. \end{aligned}$$

Denoting $G = BZ$ and $F = BS^+B^T$ this system becomes

$$\begin{aligned} F\lambda - Ga &= BS^+E^T f, \\ -G^T\lambda &= -Z^TE^T f. \end{aligned} \quad (3.11)$$

Multiplying the first equation by $(G^T QG)^{-1} G^T Q$, where Q is some symmetric and positive definite scaling matrix, cf., e.g. [60, p. 147], we can compute a as

$$a = (G^T QG)^{-1} G^T Q(BS^+E^T f - F\lambda). \quad (3.12)$$

The first equation in (3.11) thus becomes

$$F\lambda - G(G^T QG)^{-1} G^T Q(BS^+E^T f - F\lambda) = G^T QBS^+E^T f. \quad (3.13)$$

Introducing

$$P = I - QG(G^T QG)^{-1} G^T, \quad (3.14)$$

as the Q -orthogonal projection onto null G^T , we get that (3.13) corresponds to the first equation in (3.11) multiplied by P^T . So, the system (3.11) can be written in the decoupled form as

$$\begin{aligned} P^T F\lambda &= P^T BS^+E^T f, \\ G^T \lambda &= Z^T E^T f. \end{aligned}$$

The initial value of λ is chosen to satisfy the second equation in (3.11), so

$$\lambda_0 = QG(G^T QG)^{-1} Z^T E^T f. \quad (3.15)$$

Substituting λ_0 into (3.12) gives initial value of a as

$$a_0 = (G^T QG)^{-1} G^T Q(BS^+E^T f - F\lambda_0). \quad (3.16)$$

Since we are looking for $\lambda \in \text{null } G^T$, the FETI-1 method is a preconditioned conjugate gradient method applied to the system

$$P^T F P \lambda = P^T B S^+ E^T f, \quad (3.17)$$

with the Dirichlet preconditioner

$$M_{FETI-1} = B_D S B_D^T. \quad (3.18)$$

The FETI-1 method solves for the Lagrange multiplier λ . The corresponding primal solution is found as the minimizer of w in (3.5). Equivalently, from (3.6), which is the same as the first equation in (3.7), we have expressed w in (3.10). If λ is the exact solution of the dual problem (3.4), then $w \in \widehat{W}$ and so $u = w$ is the desired solution of the primal minimization problem (3.1). However, for approximate solution $\widehat{\lambda}$, in general $w \notin \widehat{W}$, and so the primal solution needs to be projected onto \widehat{W} . We use the operator E for this purpose. So, for an arbitrary Lagrange multiplier λ , the corresponding approximate solution of the original problem is

$$u = Ew = ES^+(E^T f - B^T \lambda) + Za,$$

with a determined from (3.12). Note that the operator E does not play any role in FETI-1 iterations themselves. It only serves to form the right-hand side of the constrained problem (3.7), and to recover the primal solution in the space \widehat{W} .

3.1.2 P-FETI-1

The P-FETI-1 preconditioner is based on the first step of FETI-1; the averaged solution u is obtained from (3.10) with $f = r$ and using (3.15)-(3.16) as

$$\begin{aligned} u &= Ew \\ &= E \left[S^+(E^T r - B^T \lambda_0) + Za_0 \right] \\ &= E \left[S^+(E^T r - B^T \lambda_0) + Z (G^T Q G)^{-1} G^T Q (F \lambda_0 - BS^+ E^T r) \right] \\ &= E \left[S^+(E^T r - B^T \lambda_0) + Z (G^T Q G)^{-1} G^T Q (BS^+ B^T \lambda_0 - BS^+ E^T r) \right] \\ &= E \left[I - Z (G^T Q G)^{-1} G^T Q B \right] S^+(E^T r - B^T \lambda_0) \\ &= E \left[\left(I - Z (G^T Q G)^{-1} G^T Q B \right) S^+ \left(I - B^T Q G (G^T Q G)^{-1} Z^T \right) \right] E^T r \\ &= E H^T S^+ H E^T r \\ &= M_{P-FETI-1} r, \end{aligned}$$

where we have denoted by

$$H = I - B^T Q G (G^T Q G)^{-1} Z^T, \quad (3.19)$$

and so

$$M_{P-FETI-1} = E H^T S^+ H E^T, \quad (3.20)$$

is the associated primal P-FETI-1 preconditioner, same as [21, eq. (79)].

3.1.3 FETI-DP

We can also write (2.17) as a constrained minimization problem posed on \widetilde{W} ,

$$\frac{1}{2}a(w, w) - \langle E^T f, w \rangle \rightarrow \min \text{ subject to } w \in \widetilde{W} \quad \text{and} \quad Bw = 0. \quad (3.21)$$

By essentially the same procedure as (3.2)-(3.7), we obtain that solving (3.21) is the same as solving for $w \in \widetilde{W}$ and $\lambda \in \Lambda'$ from the system

$$\begin{aligned} \widetilde{S}w + B^T \lambda &= E^T f, \\ Bw &= 0. \end{aligned} \quad (3.22)$$

The situation is now much favorable that in the case of the FETI-1 method: by (2.7) and (2.13) the operator \widetilde{S} is invertible on \widetilde{W} . So, expressing w from the first equation in (3.22) and substituting into the second equation, we get the dual problem in an operator form,

$$B\widetilde{S}^{-1}B^T \lambda = B\widetilde{S}^{-1}E^T f. \quad (3.23)$$

The FETI-DP method is the method of preconditioned conjugate gradients applied to the problem (3.23), with the Dirichlet preconditioner given by

$$M_{FETI-DP} = B_D \widetilde{S} B_D^T. \quad (3.24)$$

The FETI-DP method solves for the Lagrange multiplier λ . The corresponding primal solution is found from the first equation in (3.22) as

$$w = \widetilde{S}^{-1} (E^T f - B^T \lambda).$$

Again, if λ is the exact solution of the dual problem, then $w \in \widehat{W}$ and so $u = w$ is the desired solution of the primal minimization problem (3.21). However, for approximate solution λ we use, as for the FETI-1 method, the operator E to project the primal solution onto \widehat{W} as

$$u = E\widetilde{S}^{-1} (E^T f - B^T \lambda). \quad (3.25)$$

Note that the operator E serves again only to form the right-hand side of the constrained problem (3.22), and to recover the primal solution $u \in \widehat{W}$.

3.1.4 P-FETI-DP

We derive the P-FETI-DP preconditioner at two distinct levels of abstraction, first on the more abstract level. The preconditioner is based on the approximate solution from the first step of FETI-DP, starting from $\lambda = 0$ (which can be used, cf., e.g., [60, Section 6.4]), and with the residual r as the right-hand side. The primal solution corresponding to the result of this step is the output of the preconditioner. Thus, from (3.25) with $\lambda = 0$ and $f = r$, we have

$$M_{P-FETI-DP} r = E\widetilde{S}^{-1}E^T r, \quad (3.26)$$

where $M_{P-FETI-DP}$ is the associated primal P-FETI-DP preconditioner.

Next, we will derive the P-FETI-DP preconditioner using the original paper on FETI-DP by Farhat et. al. [16], in order to verify and complete the derivation of the P-FETI-DP algorithm given in [21, eq. (90)] for the corner constraints. So, we need to make here a direct reference to substructuring and Section 2.3. Let us split the set of interface nodes into corners and remaining nodes and decompose the space \widetilde{W} , cf. also [45, Remark 5], as

$$\widetilde{W} = \widetilde{W}_c \oplus \widetilde{W}_r. \quad (3.27)$$

The space \widetilde{W}_c consists of functions that are continuous across interfaces, have a nonzero value at one corner degree of freedom at a time and zero at others, and the space \widetilde{W}_r consists of functions with corner degrees of freedom equal to zero. The solution splits into the solution of the global coarse problem in the space \widetilde{W}_c and the solution of independent subdomain problems in the space \widetilde{W}_r .

Remark 2: *As in Li and Widlund [41], we could perform a change of basis in order to make also all other primal constraints (such as averages over edges or faces) explicit and refer to \widetilde{W}_c as the space of coarse basis functions. The change of basis and its generalization will be described in detail in Section 5.3.*

Let $R_c^{(i)}$ be a map of global coarse variables to its subdomain component,

$$R_c^{(i)} w_c = w_c^{(i)}, \quad R_c = \begin{pmatrix} R_c^{(1)} \\ \vdots \\ R_c^{(N)} \end{pmatrix},$$

let B_r be an operator enforcing the interface continuity of w_r by

$$B_r w_r = 0, \quad B_r = \begin{pmatrix} B_r^{(1)} & \dots & B_r^{(N)} \end{pmatrix},$$

and define projections $E_r : \widetilde{W}_r \rightarrow \widehat{W}$ and $E_c : \widetilde{W}_c \rightarrow \widehat{W}$, so that their transposes distribute the primal residual r to the so called subdomain forces $f_r = E_r^T r$ and to the global coarse problem right-hand side $f_c = E_c^T r$.

The equations of equilibrium can now be written, cf. [16, eq. (9)-(10)], as

$$\begin{aligned} S_{rr} w_r &+ S_{rc} R_c w_c &+ B_r^T \lambda &= f_r, \\ \sum_{i=1}^N R_c^{(i)T} S_{rc}^{(i)T} w_r^{(i)} &+ \sum_{i=1}^N R_c^{(i)T} S_{cc}^{(i)} R_c^{(i)} w_c &&= f_c, \\ B_r w_r &&&= 0, \end{aligned}$$

where the first equation corresponds to independent subdomain problems, the second corresponds to the global coarse problem, and the third enforces the continuity of local problems. This system can be rewritten as

$$\begin{pmatrix} S_{rr} & S_{rc} R_c & B_r^T \\ (S_{rc} R_c)^T & \widetilde{S}_{cc} & 0 \\ B_r & 0 & 0 \end{pmatrix} \begin{pmatrix} w_r \\ w_c \\ \lambda \end{pmatrix} = \begin{pmatrix} f_r \\ f_c \\ 0 \end{pmatrix}, \quad (3.28)$$

and the blocks are defined as

$$\widetilde{S}_{cc} = \sum_{i=1}^N R_c^{(i)T} S_{cc}^{(i)} R_c^{(i)}, \quad S_{rr} = \begin{pmatrix} S_{rr}^{(1)} & & \\ & \ddots & \\ & & S_{rr}^{(N)} \end{pmatrix}, \quad S_{rc} R_c = \begin{pmatrix} S_{rc}^{(1)} R_c^{(1)} \\ \vdots \\ S_{rc}^{(N)} R_c^{(N)} \end{pmatrix}.$$

Remark 3: The system (3.28) is just expanded system (3.22).

Expressing w_r from the first equation in (3.28), we get

$$w_r = S_{rr}^{-1} (f_r - S_{rc} R_c w_c - B_r^T \lambda).$$

Substituting for w_r into the second equation in (3.28) gives

$$\tilde{S}_{cc}^* w_c - (S_{rc} R_c)^T S_{rr}^{-1} B_r^T \lambda = f_c - (S_{rc} R_c)^T S_{rr}^{-1} f_r,$$

where $\tilde{S}_{cc}^* = \tilde{S}_{cc} - R_c^T S_{rc}^T S_{rr}^{-1} S_{rc} R_c$. Inverting \tilde{S}_{cc}^* , we get that

$$w_c = \tilde{S}_{cc}^{*-1} \left[f_c - (S_{rc} R_c)^T S_{rr}^{-1} f_r + (S_{rc} R_c)^T S_{rr}^{-1} B_r^T \lambda \right].$$

After initialization with $\lambda = 0$ which [21, 20] does not say but it can be used, cf. the first derivation of the method, the assembled and averaged solution is

$$\begin{aligned} u &= E_r w_r + E_c w_c \\ &= E_r S_{rr}^{-1} \left\{ f_r - S_{rc} R_c \tilde{S}_{cc}^{*-1} \left(f_c - (S_{rc} R_c)^T S_{rr}^{-1} f_r \right) \right\} + \\ &\quad + E_c \tilde{S}_{cc}^{*-1} \left(f_c - (S_{rc} R_c)^T S_{rr}^{-1} f_r \right) \\ &= E_r S_{rr}^{-1} f_r - E_r S_{rr}^{-1} S_{rc} R_c \tilde{S}_{cc}^{*-1} f_c + \\ &\quad + E_r S_{rr}^{-1} S_{rc} R_c \tilde{S}_{cc}^{*-1} (S_{rc} R_c)^T S_{rr}^{-1} f_r + \\ &\quad + E_c \tilde{S}_{cc}^{*-1} f_c - E_c \tilde{S}_{cc}^{*-1} (S_{rc} R_c)^T S_{rr}^{-1} f_r \\ &= E_r S_{rr}^{-1} f_r + \\ &\quad + (E_c - E_r S_{rr}^{-1} S_{rc} R_c) \tilde{S}_{cc}^{*-1} \left(f_c - (S_{rc} R_c)^T S_{rr}^{-1} f_r \right) \\ &= E_r S_{rr}^{-1} E_r^T r + \\ &\quad + (E_c - E_r S_{rr}^{-1} S_{rc} R_c) \tilde{S}_{cc}^{*-1} \left(E_c^T r - (S_{rc} R_c)^T S_{rr}^{-1} E_r^T r \right) \\ &= M_{P-FETI-DP}, \end{aligned}$$

where

$$\begin{aligned} M_{P-FETI-DP} &= E_r S_{rr}^{-1} E_r^T + \\ &\quad + (E_c - E_r S_{rr}^{-1} S_{rc} R_c) \tilde{S}_{cc}^{*-1} (E_c^T - R_c^T S_{rc}^T S_{rr}^{-1} E_r^T) \end{aligned} \quad (3.29)$$

is the associated P-FETI-DP preconditioner, and we have verified [21, eq. (90)].

3.2 Methods from the BDD family

We recall two primal methods from the Balancing Domain Decomposition (BDD) family by Mandel in [42]; namely the original BDD and Balancing Domain Decomposition by Constraints (BDDC) introduced by Dohrmann [9].

3.2.1 BDD

The BDD is a Neumann-Neumann algorithm, cf., e.g., [15], with a simple coarse grid correction, introduced by Mandel [42]. The name of the preconditioner comes from an idea to *balance* the residual. We say that $v \in \widehat{W}$ is balanced if

$$Z^T E^T v = 0.$$

Let us denote the “balancing” operator as

$$C = EZ, \quad (3.30)$$

so the columns of C are equal to the weighted sum of traces of the subdomain zero energy modes. Next, let us denote by $S_C \widehat{S}$ the \widehat{S} – orthogonal projection onto the range of C , so that

$$S_C = C \left(C^T \widehat{S} C \right)^{-1} C^T,$$

and by P_C the complementary projection to $S_C \widehat{S}$, defined as

$$P_C = I - S_C \widehat{S}. \quad (3.31)$$

The BDD preconditioner [42, Lemma 3.1], can be written in our settings as

$$\begin{aligned} M_{BDD} &= \left[\left(I - S_C \widehat{S} \right) E S^+ E^T \widehat{S} \left(I - S_C \widehat{S} \right) + S_C \widehat{S} \right] \widehat{S}^{-1} \\ &= \left[\left(I - S_C \widehat{S} \right) E S^+ E^T \left(\widehat{S} \widehat{S}^{-1} - \widehat{S} S_C \widehat{S} \widehat{S}^{-1} \right) + S_C \widehat{S} \widehat{S}^{-1} \right] \\ &= P_C E S^+ E^T P_C^T + S_C \end{aligned} \quad (3.32)$$

where S_C serves as the coarse grid correction. See [42, 43], and [21] for details.

3.2.2 BDDC

First, we formulate the BDDC method in a particularly simple abstract variational form following our work in [47], which was inspired by a view of the Neumann-Neumann methods going back to [15]. It is essentially same as the approach of [5], and it is also related to the concept of subassembly in [41].

Algorithm 4: *The abstract BDDC preconditioner M_{BDDC} is defined by*

$$M_{BDDC} : r \longmapsto u = Ew, \quad w \in \widetilde{W} : \quad a(w, z) = \langle r, Ez \rangle, \quad \forall z \in \widetilde{W}. \quad (3.33)$$

From the definitions of \widetilde{S} in (2.13) and R in (2.8), it follows that the operator form of the BDDC preconditioner is

$$M_{BDDC} = E \widetilde{S}^{-1} E^T. \quad (3.34)$$

Comparing (3.34) with P-FETI-DP in (3.26), we have immediately:

Theorem 5: *The P-FETI-DP and the BDDC preconditioners are the same.*

Next, we introduce another mathematically equivalent formulation of the BDDC algorithm. Following Li and Widlund [41], we will assume that each constraint can be represented by an explicit degree of freedom, cf. Remark 2, and that we can decompose the space \widetilde{W} as in (3.27). The preconditioner M_{BDDC} is defined in this formulation by, cf. [41, eq. (27)],

$$M_{BDDC} = \mathcal{T}_{sub} + \mathcal{T}_{coarse},$$

where $\mathcal{T}_{sub} = E_r S_{rr}^{-1} E_r^T$ is the subdomain correction obtained by solving independent problems on subdomains, and $\mathcal{T}_{coarse} = E\Psi (\Psi^T S\Psi)^{-1} \Psi^T E^T$ is the coarse grid correction. Here Ψ are the coarse basis functions defined by energy minimization,

$$\text{tr } \Psi^T S\Psi \rightarrow \min.$$

Since we assume that each constraint corresponds to an explicit degree of freedom, the coarse basis functions Ψ can be easily determined via the analogy to the discrete harmonic functions, discussed, e.g., in [60, Section 4.4]; Ψ are equal to 1 in the coarse degrees of freedom and have energy minimal extension with respect to the remaining degrees of freedom u_r , so they are precisely given as

$$\Psi = \begin{pmatrix} R_c \\ -S_{rr}^{-1} S_{rc} R_c \end{pmatrix}.$$

Then, we can compute

$$\begin{aligned} \Psi^T S\Psi &= \begin{pmatrix} R_c^T & -R_c^T S_{rc}^T S_{rr}^{-1} \end{pmatrix} \begin{pmatrix} S_{cc} & S_{rc}^T \\ S_{rc} & S_{rr} \end{pmatrix} \begin{pmatrix} R_c \\ -S_{rr}^{-1} S_{rc} R_c \end{pmatrix} \\ &= R_c^T S_{cc} R_c - R_c^T S_{rc}^T S_{rr}^{-1} S_{rc} R_c \\ &= \widetilde{S}_{cc} - R_c^T S_{rc}^T S_{rr}^{-1} S_{rc} R_c \\ &= \widetilde{S}_{cc}^*, \end{aligned}$$

followed by

$$\begin{aligned} &E\Psi [\Psi^T S\Psi]^{-1} \Psi^T E^T \\ &= E \begin{pmatrix} R_c \\ -S_{rr}^{-1} S_{rc} R_c \end{pmatrix} \widetilde{S}_{cc}^{*-1} \begin{pmatrix} R_c^T & -R_c^T S_{rc}^T S_{rr}^{-1} \end{pmatrix} E^T \\ &= (E_c - E_r S_{rr}^{-1} S_{rc} R_c) \widetilde{S}_{cc}^{*-1} (E_c^T - R_c^T S_{rc}^T S_{rr}^{-1} E_r^T). \end{aligned}$$

So, the BDDC preconditioner takes the form

$$\begin{aligned} M_{BDDC} &= E_r S_{rr}^{-1} E_r^T + \\ &+ (E_c - E_r S_{rr}^{-1} S_{rc} R_c) \widetilde{S}_{cc}^{*-1} (E_c^T - R_c^T S_{rc}^T S_{rr}^{-1} E_r^T). \end{aligned} \tag{3.35}$$

Comparing now the definitions of both, P-FETI-DP in eq. (3.29) and BDDC in eq. (3.35) we again immediately see on another level of detail that these two preconditioners are the same. Moreover:

Theorem 6: *The preconditioner proposed by Cros [8, eq. 4.8] can be interpreted as either the P-FETI-DP preconditioner by Fragakis and Papadrakakis [21], or the BDDC preconditioner by Dohrmann [9].*

4. CONNECTIONS BETWEEN THE METHODS

We will now study some relations between the FETI-DP and BDDC methods, and between the (P-)FETI-1 and BDD methods. We would like to premise that even though we will observe some similar relations between (P-)FETI and BDD as between FETI-DP and BDDC, cf., e.g., Lemmas 7 and 16, we have decided to split the comparison into two sections for the following reason. The action of the FETI-DP and BDDC preconditioners is defined on space \widetilde{W} , where by assumption (2.7) the operator \widetilde{S} defined by (2.13) is invertible. On the other hand, the FETI and BDD algorithms are defined on the whole space W , where the operator S defined by (2.14) is in general only positive semidefinite, and more delicate analysis is necessary. This also explains why we have decided to begin with the analysis of the FETI-DP and BDDC methods, which is simpler.

The next two simple observations, following directly from the assumptions in Section 2.2, will be useful in both sections of this chapter:

$$EB_D^T B = E(I - RE) = E - ERE = 0, \quad (4.1)$$

$$REB_D^T = (I - B_D^T B) B_D^T = B_D^T - B_D^T B B_D^T = 0. \quad (4.2)$$

We note that, since R is an injection, in fact it also holds that $EB_D^T = 0$.

4.1 FETI-DP and BDDC

We have already shown in Theorems 5 and 6 that the P-FETI-DP, the BDDC, and the preconditioner by Cros are the same. We will focus now on the condition number bound and the spectral properties of the FETI-DP and BDDC preconditioned operators. Our starting point in this section is as follows:

Lemma 7: *The two preconditioned operators can be written as*

$$P_{FETI-DP} = \left(B_D \widetilde{S} B_D^T \right) \left(B \widetilde{S}^{-1} B^T \right), \quad (4.3)$$

$$P_{BDDC} = \left(E \widetilde{S}^{-1} E^T \right) \left(R^T \widetilde{S} R \right). \quad (4.4)$$

Proof. The forms of the preconditioned operators follow for FETI-DP from (3.23)-(3.24), and for BDDC from (2.16) and (3.34). ■

Clearly, both preconditioned operators have the same general form

$$(LA^{-1}L^T) (T^T AT), \quad (4.5)$$

where A is symmetric, positive definite, and L and T are some linear operators such that, because of (2.5) and (2.9),

$$LT = I. \quad (4.6)$$

This important observation was made in [41] in the equivalent form that $P\tilde{S}^{-1}P\tilde{S} : \text{range } P \rightarrow \text{range } P$, where P is a projection, and in the present form in [5].

It is interesting that the fundamental eigenvalue bound can be proved for arbitrary operators of the form (4.5) – (4.6). The following lemma was proved in terms of the BDDC preconditioner in [45, Theorem 25], and the proof carries over to the FETI-DP. Because the translation between the two settings is time consuming, the proof (with some simplifications but no substantial differences) is included here for completeness, in the general form.

Lemma 8: *Let U and V be finite dimensional vector spaces and $A : V \rightarrow V'$ be an SPD operator. If $L : V \rightarrow U$ and $T : U \rightarrow V$ are linear operators such that $LT = I$ on U , then all eigenvalues λ of the operator $(LA^{-1}L^T)(T^TAT)$ satisfy*

$$1 \leq \lambda \leq \|TL\|_A^2. \quad (4.7)$$

Proof. The operator $(LA^{-1}L^T)(T^TAT)$ is selfadjoint with respect to the inner product $\langle T^TATu, v \rangle$. So, it is sufficient to bound $\langle (LA^{-1}L^T)(T^TAT)u, u \rangle$ in terms of $\langle (T^TAT)u, u \rangle$.

Let $u \in U$. Then

$$(LA^{-1}L^T)(T^TAT)u = Lw, \quad (4.8)$$

where $w = A^{-1}L^T T^T ATu$ satisfies

$$w \in V, \quad \langle Aw, v \rangle = \langle T^TATu, Lv \rangle \quad \forall v \in V. \quad (4.9)$$

In particular, from (4.9) with $v = w$ and (4.8)

$$\langle Aw, w \rangle = \langle T^TATu, Lw \rangle = \langle T^TATu, (LA^{-1}L^T)(T^TAT)u \rangle, \quad (4.10)$$

and using $LT = I$, (4.9) with $v = Tu$, Cauchy inequality, the definition of transpose, and (4.10),

$$\begin{aligned} \langle T^TATu, u \rangle^2 &= \langle T^TATu, LTu \rangle^2 \\ &= \langle Aw, Tu \rangle^2 \\ &\leq \langle Aw, w \rangle \langle ATu, Tu \rangle \\ &= \langle Aw, w \rangle \langle T^TATu, u \rangle \\ &= \langle T^TATu, (LA^{-1}L^T)(T^TAT)u \rangle \langle T^TATu, u \rangle. \end{aligned}$$

Dividing by $\langle T^TATu, u \rangle$, we get

$$\langle T^TATu, u \rangle \leq \langle T^TATu, (LA^{-1}L^T)(T^TAT)u \rangle \quad \forall u \in U,$$

which gives the left inequality in (4.7).

To prove the right inequality in (4.7), let again $u \in U$. Then it follows, from (4.8), Cauchy inequality in the T^TAT inner product, definition of the A norm,

properties of the norm, and (4.10), that

$$\begin{aligned}
& \langle T^T ATu, (LA^{-1}L^T) (T^T AT) u \rangle^2 \\
&= \langle T^T ATu, Lw \rangle^2 \\
&\leq \langle T^T ATu, u \rangle \langle T^T ATLw, Lw \rangle \\
&= \langle T^T ATu, u \rangle \langle ATLw, TLw \rangle \\
&= \langle T^T ATu, u \rangle \|TLw\|_A^2 \\
&\leq \langle T^T ATu, u \rangle \|TL\|_A^2 \|w\|_A^2 \\
&= \langle T^T ATu, u \rangle \|TL\|_A^2 \langle T^T ATu, (LA^{-1}L^T) (T^T AT) u \rangle.
\end{aligned}$$

Dividing by $\langle T^T ATu, (LA^{-1}L^T) (T^T AT) u \rangle$, we get

$$\langle T^T ATu, (LA^{-1}L^T) (T^T AT) u \rangle \leq \|TL\|_A^2 \langle T^T ATu, u \rangle \quad \forall u \in U. \quad \blacksquare$$

The lower bound in Lemma 8 was proved in a different way in [5, Lemma 3.4].

Condition number bounds formulated as the next theorem now follow immediately from Lemma 8. These bounds will also play an essential role in the design of adaptive FETI-DP and BDDC preconditioners, studied in Chapter 5.

Theorem 9: *The eigenvalues of the preconditioned operators of FETI-DP and BDDC satisfy $1 \leq \lambda \leq \omega_{FETI-DP}$ and $1 \leq \lambda \leq \omega_{BDDC}$, respectively, where*

$$\omega_{BDDC} = \|RE\|_S^2, \quad \omega_{FETI-DP} = \|B_D^T Bw\|_S^2. \quad (4.11)$$

In addition, if $\widetilde{W} \neq \widehat{W}$ and (2.11) holds, then also

$$\omega_{BDDC} = \omega_{FETI-DP}. \quad (4.12)$$

Proof. The eigenvalue bounds with (4.11) follows from the form of the preconditioned operators (4.3)-(4.4) and Lemma 8. The equality (4.12) follows from the fact that E and $B_D B$ are complementary projections by (2.11), and the norm of a nontrivial projection depends only on the angle between its range and its nullspace [24]. \blacksquare

The result in Theorem 9 was proved in a different way in [44] for BDDC and in [51] for FETI-DP. For a simple proof of the bound for BDDC directly from the variational formulation (3.33), see [47, Theorem 2].

The next abstract lemma is the main tool in the comparison of the eigenvalues of the BDDC and FETI-DP preconditioned operators.

Lemma 10 ([5, Lemmas 3.6 – 3.8]): *Let V and U_i , $i = 1, 2$, be finite dimensional vector spaces and $A : V \rightarrow V'$ be an SPD operator. If $L_i : V \rightarrow U_i$ and $T_i : U_i \rightarrow V$ are linear operators such that*

$$L_i T_i = I \text{ on } U_i, \quad i = 1, 2, \quad (4.13)$$

$$T_1 L_1 + T_2 L_2 = I \text{ on } V, \quad (4.14)$$

then all eigenvalues (except equal to one) of the operators $(L_1 A^{-1} L_1^T) (T_1^T A T_1)$ and $(T_2^T A T_2) (L_2 A^{-1} L_2^T)$ are the same, and their multiplicities are identical.

Clearly, the assumptions in Lemma 10 correspond to (2.1)-(2.11). The proof can be found in [5], and its main ideas are as follows. First, we need to show that the eigenvectors of one operator can be transformed into (nonzero) eigenvectors of the other operator, and that they correspond to the same eigenvalues. Next step is to show that the eigenvectors can get mapped to zero only if they correspond to the eigenvalue(s) equal to one. Finally, because the nonzero mapping of the eigenvectors is one-to-one, the eigenspace of one operator gets mapped into the eigenspace of the other operator, and because this mapping can be reversed, we conclude that all eigenvalues greater than one must be the same and they also must have the same multiplicities. For completeness, we translate this abstract result in the case of FETI-DP and BDDC, which is formulated as the next lemma and theorem. We note, that this translation has been also inspired by the recent abstract result of Fragakis [20, Theorem 4].

So, the next lemma corresponds to [5, Lemma 3.6] and also, this lemma and the next theorem are particular versions of [20, Theorem 4].

Lemma 11: *The following identities are valid:*

$$\begin{aligned} \mathcal{T}_D P_{FETI-DP} &= P_{BDDC} \mathcal{T}_D, & \mathcal{T}_D &= E \tilde{S}^{-1} B^T, \\ \mathcal{T}_P P_{BDDC} &= P_{FETI-DP} \mathcal{T}_P, & \mathcal{T}_P &= B_D \tilde{S} R. \end{aligned}$$

Proof. Using (4.1) and (2.10) we derive the first identity as

$$\begin{aligned} \mathcal{T}_D P_{FETI-DP} &= E \tilde{S}^{-1} B^T B_D \tilde{S} B_D^T B \tilde{S}^{-1} B^T \\ &= E \tilde{S}^{-1} (I - E^T R^T) \tilde{S} (I - RE) \tilde{S}^{-1} B^T \\ &= E \tilde{S}^{-1} \tilde{S} (I - RE) \tilde{S}^{-1} B^T - E \tilde{S}^{-1} E^T R^T \tilde{S} \tilde{S}^{-1} B^T \\ &\quad + \left(E \tilde{S}^{-1} E^T \right) (R^T S R) E \tilde{S}^{-1} B^T \\ &= E B_D^T B \tilde{S}^{-1} B^T - E \tilde{S}^{-1} E^T R^T B^T + P_{BDDC} \mathcal{T}_D \\ &= P_{BDDC} \mathcal{T}_D, \end{aligned}$$

and using (4.2) and (2.10), we derive the second identity as

$$\begin{aligned} \mathcal{T}_P P_{BDDC} &= B_D \tilde{S} R E \tilde{S}^{-1} E^T R^T \tilde{S} R \\ &= B_D \tilde{S} (I - B_D^T B) \tilde{S}^{-1} (I - B^T B_D) \tilde{S} R \\ &= B_D \tilde{S} \tilde{S}^{-1} (I - B^T B_D) \tilde{S} R \\ &\quad - B_D \tilde{S} B_D^T B \tilde{S}^{-1} \tilde{S} R \\ &\quad + \left(B_D \tilde{S} B_D^T \right) \left(B \tilde{S}^{-1} B^T \right) B_D \tilde{S} R \\ &= B_D E^T R^T \tilde{S} R - B_D \tilde{S} B_D^T B R + P_{FETI-DP} \mathcal{T}_P \\ &= P_{FETI-DP} \mathcal{T}_P. \quad \blacksquare \end{aligned}$$

Theorem 12: *The spectra of the two preconditioned operators $P_{FETI-DP}$ and P_{BDDC} are the same except possibly for eigenvalues equal to one. Moreover, the multiplicity of any common eigenvalue $\lambda \neq 1$ is identical for both operators.*

Proof. By Theorem 9, the lower bound on eigenvalues is equal to one. Let u_D be a (nonzero) eigenvector of the preconditioned FETI-DP operator corresponding to the eigenvalue λ_D . By Lemma 11, it holds that $\mathcal{T}_D u_D$ is an eigenvector of the preconditioned BDDC operator corresponding to the eigenvalue λ_D , provided that $\mathcal{T}_D u_D \neq 0$. So, assume that $\mathcal{T}_D u_D = 0$. But then it also must be true that

$$\begin{aligned} 0 &= \mathcal{T}_P \mathcal{T}_D u_D = B_D \tilde{S} R E \tilde{S}^{-1} B^T u_D \\ &= B_D \tilde{S} (I - B_D^T B) \tilde{S}^{-1} B^T u_D = B_D B^T u_D - (B_D \tilde{S} B_D^T) (B \tilde{S}^{-1} B^T) u_D \\ &= B_D B^T u_D - P_{FETI-DP} u_D \\ &= B_D B^T u_D - \lambda_D u_D, \end{aligned}$$

but since $B_D B^T$ is a projection, λ_D could be equal only to (0 or) 1.

Next, let u_P be a (nonzero) eigenvector of the preconditioned BDDC operator corresponding to the eigenvalue λ_P . Then, by Lemma 11, it holds that $\mathcal{T}_P u_P$ is an eigenvector of the preconditioned FETI-DP operator corresponding to the eigenvalue λ_P , provided that $\mathcal{T}_P u_P \neq 0$. So, assume that $\mathcal{T}_P u_P = 0$. But then it also must be true that

$$\begin{aligned} 0 &= \mathcal{T}_D \mathcal{T}_P u_P = E \tilde{S}^{-1} B^T B_D \tilde{S} R u_P \\ &= E \tilde{S}^{-1} (I - E^T R^T) \tilde{S} R u_P = E R u_P - (E \tilde{S}^{-1} E^T) (R^T S R) u_P \\ &= E R u_P - P_{BDDC} u_P \\ &= E R u_P - \lambda_P u_P, \end{aligned}$$

but since ER is a projection, λ_P could be equal only to (0 or) 1.

Finally, let $\lambda \neq 1$ be an eigenvalue of the operator P_{BDDC} with the multiplicity m . From the previous arguments, the eigenspace corresponding to λ is mapped by the operator \mathcal{T}_P into an eigenspace of $P_{FETI-DP}$ and since this mapping is one-to-one, the multiplicity of λ corresponding to $P_{FETI-DP}$ is $n \geq m$. By the same argument, we can prove the opposite inequality and the conclusion follows. ■

Remark 13: *The equality of spectra in Theorem 12 was proved in [45] in a different way, and an elegant simplified proof was given in [41]. The equality of multiplicities of all common eigenvalues greater than one was proved in [5], where it has been also shown that the multiplicity of the eigenvalue equal to one for FETI-DP is less than or equal to the multiplicity for BDDC. However, in practice, there are other eigenvalues very close to one, and the performance of the FETI-DP and BDDC methods is essentially identical [45].*

Remark 14: *It is notable, that the definition of the space \tilde{W} with corner constraints has been already used for a variant of the BDD preconditioner designed for plates by Le Tallec et al. [37, equation (39)]. Their spaces V_i° and \bar{Z}_i correspond, respectively, to the spaces \tilde{W}_r and \tilde{W}_c defined by (3.27). The only difference between the algorithm there and BDDC (in case of corners only) is that the coarse correction is applied multiplicatively rather than additively.*

4.2 (P-)FETI-1 and BDD

In the remainder of this chapter, we will revisit the result from [21] that a certain version of the P-FETI-1 method gives exactly the same algorithm as BDD, and we will also translate the recent abstract proof relating the spectra of primal and dual methods [20, Theorem 4] in the case of FETI-1 and BDD.

Theorem 15 ([21, Section 8]): *If Q is chosen to be the Dirichlet preconditioner (3.18), the P-FETI-1 and the BDD preconditioners are the same.*

Proof. We will show that $M_{P\text{-FETI-1}}$ in (3.20) with $Q = B_D S B_D^T$ is the same as M_{BDD} in (3.32). So, similarly as in [21, pp. 3819-3820], we begin with (3.19) as

$$\begin{aligned} H &= I - B^T Q G (G^T Q G)^{-1} Z^T \\ &= I - B^T B_D S B_D^T B Z (Z^T B^T B_D S B_D^T B Z)^{-1} Z^T \\ &= I - A_R (Z^T A_R)^{-1} Z^T, \end{aligned}$$

where

$$A_R = B^T B_D S B_D^T B Z.$$

Using (2.11), definitions of C in (3.30), \widehat{S} in (2.16), and because $SZ = 0$ by (3.8),

$$\begin{aligned} A_R &= (I - E^T R^T) S (I - R E) Z \\ &= SZ - SREZ - E^T R^T SZ + E^T R^T SREZ \\ &= SZ - SRC - E^T R^T SZ + E^T \widehat{S} C \\ &= (E^T \widehat{S} - SR) C, \end{aligned}$$

and similarly

$$\begin{aligned} Z^T A_R &= Z^T (E^T \widehat{S} - SR) C \\ &= C^T \widehat{S} C - Z^T SREZ \\ &= C^T \widehat{S} C. \end{aligned}$$

Using the two previous results, (3.31), and symmetries of \widehat{S} and S_C , we get

$$\begin{aligned} HE^T &= \left(I - A_R (Z^T A_R)^{-1} Z^T \right) E^T \\ &= E^T - A_R (Z^T A_R)^{-1} Z^T E^T \\ &= E^T - (E^T \widehat{S} - SR) C (C^T \widehat{S} C)^{-1} C^T \\ &= E^T - (E^T \widehat{S} - SR) S_C \\ &= E^T - E^T \widehat{S} S_C + SRS_C \\ &= E^T (I - \widehat{S} S_C) + SRS_C \\ &= E^T P_C^T + SRS_C. \end{aligned}$$

Next, the matrix S_C satisfies the relation

$$\begin{aligned} S_C R^T S S^+ S R S_C &= S_C R^T S R S_C = S_C \widehat{S} S_C \\ &= C \left(C^T \widehat{S} C \right)^{-1} C^T \widehat{S} C \left(C^T \widehat{S} C \right)^{-1} C^T \\ &= C \left(C^T \widehat{S} C \right)^{-1} C^T = S_C. \end{aligned}$$

Because by definition $P_C C = 0$, using (2.9) we get for some Y that

$$\begin{aligned} P_C E S^+ S R S_C &= P_C E (I + ZY) R S_C \\ &= P_C E R S_C + P_C E Z Y R S_C \\ &= P_C S_C + P_C C Y R S_C \\ &= P_C S_C \\ &= \left(I - S_C \widehat{S} \right) S_C \\ &= S_C - S_C = 0, \end{aligned}$$

and the same is true for the transpose, so $S_C R^T S S^+ E^T P_C^T = 0$.

Using these results, the P-FETI-1 preconditioner from (3.20) becomes

$$\begin{aligned} M_{P-FETI-1} &= E H^T S^+ H E^T \\ &= \left(S_C R^T S + P_C E \right) S^+ \left(E^T P_C^T + S R S_C \right) \\ &= S_C R^T S S^+ E^T P_C^T + S_C R^T S S^+ S R S_C \\ &\quad + P_C E S^+ E^T P_C^T + P_C E S^+ S R S_C \\ &= P_C E S^+ E^T P_C^T + S_C, \end{aligned} \tag{4.15}$$

and we see that (4.15) is the same as the definition of M_{BDD} in (3.32). \blacksquare

Now we focus on the equality of eigenvalues of the BDD and FETI-1 preconditioned operators, with Q being the Dirichlet preconditioner (3.18). We begin with an analogy to Lemma 7, this time relating FETI-1 and BDD:

Lemma 16: *The two preconditioned operators can be written as*

$$\begin{aligned} P_{FETI-1} &= M_{FETI} \mathcal{F} = \left(B_D S B_D^T \right) \left(B S_H^+ B^T \right), \\ P_{BDD} &= M_{BDD} \widehat{S} = \left(E S_H^+ E^T \right) \left(R^T S R \right), \end{aligned}$$

where

$$S_H^+ = H^T S^+ H,$$

and H is defined by (3.19).

Proof. First, $M_{FETI-1} = B_D S B_D^T$, which is the Dirichlet preconditioner (3.18). From (3.17), using the definition of H by (3.19), we get

$$\begin{aligned} \mathcal{F} &= P^T F P \\ &= P^T B S^+ B^T P \\ &= \left(I - G \left(G^T Q G \right)^{-1} G^T Q^T \right) B S^+ B^T \left(I - Q G \left(G^T Q G \right)^{-1} G^T \right) \\ &= \left(B - B Z \left(G^T Q G \right)^{-1} G^T Q^T B \right) S^+ \left(B^T - B^T Q G \left(G^T Q G \right)^{-1} Z^T B^T \right) \\ &= B \left(I - Z \left(G^T Q G \right)^{-1} G^T Q B \right) S^+ \left(I - B^T Q G \left(G^T Q G \right)^{-1} Z^T \right) B^T \\ &= B H^T S^+ H B^T = B S_H^+ B^T. \end{aligned}$$

Next, \widehat{S} is defined by (2.16). By Theorem 15 we can use (3.20) for M_{BDD} , i.e.,

$$M_{BDD} = EH^T S^+ HE^T = ES_H^+ E^T. \quad \blacksquare$$

Before proceeding to the main result, we need to prove two technical lemmas relating the operators S and S_H^+ . The first lemma establishes [20, Assumptions (13) and (22)] as well as [20, Lemma 3] for FETI-1 and BDD.

Lemma 17: *The operators S , S_H^+ , defined by (2.19) and Lemma 16, satisfy*

$$S_H^+ SR = R, \quad (4.16)$$

$$S_H^+ SS_H^+ = S_H^+. \quad (4.17)$$

Moreover, the following relations are valid

$$BS_H^+ SR = 0, \quad (4.18)$$

$$S_H^+ B^T B_D SS_H^+ E^T = 0. \quad (4.19)$$

Proof. First, from (3.8) and symmetry of S it follows that

$$\begin{aligned} HS &= \left(I - B^T QG (G^T QG)^{-1} Z^T \right) S \\ &= S - B^T QG (G^T QG)^{-1} Z^T S = S. \end{aligned}$$

Using $H^T = I - Z (G^T QG)^{-1} G^T QB$ we get

$$\begin{aligned} H^T S^+ S &= H^T (I + ZY) = H^T + H^T ZY \\ &= H^T + \left[I - Z (G^T QG)^{-1} G^T QB \right] ZY \\ &= H^T + ZY - Z (G^T QG)^{-1} G^T QGY \\ &= H^T + ZY - ZY = H^T, \end{aligned}$$

so

$$S_H^+ S = H^T S^+ HS = H^T S^+ S = H^T.$$

Finally, from previous and (2.10), we get (4.16) as

$$S_H^+ SR = H^T R = \left(I - Z (G^T QG)^{-1} G^T QB \right) R = R,$$

and since H^T is a projection, we immediately get also (4.17) as

$$S_H^+ SS_H^+ = H^T S_H^+ = H^T H^T S^+ H = S_H^+.$$

Next, (4.18) follows directly from (4.16) noting (2.10).

Using (2.11), (4.16)-(4.17) and (4.1), we get (4.19) as

$$\begin{aligned} S_H^+ B^T B_D SS_H^+ E^T &= S_H^+ (I - E^T R^T) SS_H^+ E^T \\ &= S_H^+ SS_H^+ E^T - S_H^+ E^T R^T SS_H^+ E^T \\ &= S_H^+ E^T - S_H^+ E^T R^T E^T \\ &= S_H^+ (I - E^T R^T) E^T \\ &= S_H^+ B^T B_D E^T = 0. \quad \blacksquare \end{aligned}$$

Next lemma establishes similar identities as Lemma 11. Again, it is a particular version of [20, Theorem 4], or it can be also eventually viewed as a generalization of the result for FETI-DP and BDDC [5, Lemma 3.6].

Lemma 18: *The following identities are valid:*

$$\begin{aligned} \mathcal{S}_D P_{FETI-1} &= P_{BDD} \mathcal{S}_D, & \mathcal{S}_D &= ES_H^+ B^T, \\ \mathcal{S}_P P_{BDD} &= P_{FETI-1} \mathcal{S}_P, & \mathcal{S}_P &= P_{FETI-1} B_D S R. \end{aligned}$$

Proof. Using the transpose of (4.19) and (4.18), we derive the first identity

$$\begin{aligned} \mathcal{S}_D P_{FETI-1} &= ES_H^+ B^T B_D S B_D^T B S_H^+ B^T \\ &= ES_H^+ (I - E^T R^T) S (I - RE) S_H^+ B^T \\ &= ES_H^+ S (I - RE) S_H^+ B^T - ES_H^+ E^T R^T S S_H^+ B^T \\ &\quad + ES_H^+ E^T R^T S R E S_H^+ B^T \\ &= ES_H^+ S B_D^T B S_H^+ B^T - ES_H^+ E^T R^T S S_H^+ B^T + \\ &\quad + (ES_H^+ E^T) (R^T S R) \mathcal{S}_D \\ &= P_{BDD} \mathcal{S}_D. \end{aligned}$$

Similarly, using (4.19) and (4.18), we derive the second identity as

$$\begin{aligned} \mathcal{S}_P P_{BDD} &= P_{FETI-1} B_D S R E S_H^+ E^T R^T S R \\ &= P_{FETI-1} B_D S (I - B_D^T B) S_H^+ (I - B^T B_D) S R \\ &= P_{FETI-1} B_D S S_H^+ (I - B^T B_D) S R \\ &\quad - P_{FETI-1} B_D S B_D^T B S_H^+ S R \\ &\quad + P_{FETI-1} B_D S B_D^T B S_H^+ B^T B_D S R \\ &= M_{FETI-1} B S_H^+ B^T B_D S S_H^+ E^T R^T S R \\ &\quad - P_{FETI-1} B_D S B_D^T B S_H^+ S R \\ &\quad + P_{FETI-1} (B_D S B_D^T) (B S_H^+ B^T) B_D S R \\ &= P_{FETI-1} (P_{FETI-1} B_D S R). \\ &= P_{FETI-1} \mathcal{S}_P. \quad \blacksquare \end{aligned}$$

Theorem 19: *The spectra of the preconditioned operators P_{BDD} and P_{FETI-1} are the same except possibly for eigenvalues equal to zero and one. Moreover, the multiplicity of any common eigenvalue $\lambda \neq 0, 1$ is identical for the two preconditioned operators.*

Proof. Let u_D be a (nonzero) eigenvector of the preconditioned FETI-1 operator corresponding to the eigenvalue λ_D . Then, by Lemma 18, it holds that $\mathcal{S}_D u_D$ is an eigenvector of the preconditioned BDD operator corresponding to the eigenvalue λ_D , provided that $\mathcal{S}_D u_D \neq 0$. So, assume that $\mathcal{S}_D u_D = 0$. But then it also must be true that

$$\begin{aligned} 0 &= B_D S R (\mathcal{S}_D u_D) = B_D S R E S_H^+ B^T u_D \\ &= B_D S (I - B_D^T B) S_H^+ B^T u_D = B_D S S_H^+ B^T u_D - B_D S B_D^T B S_H^+ B^T u_D \\ &= B_D S S_H^+ B^T u_D - P_{FETI-1} u_D = B_D S S_H^+ B^T u_D - \lambda_D u_D, \end{aligned}$$

and, we get

$$B_D S S_H^+ B^T u_D = \lambda_D u_D.$$

Note that, by (4.16) and (2.10),

$$\begin{aligned}
(B_D S S_H^+ B^T)^2 &= B_D S S_H^+ B^T B_D S S_H^+ B^T \\
&= B_D S S_H^+ (I - E^T R^T) S S_H^+ B^T \\
&= B_D S S_H^+ S S_H^+ B^T - B_D S S_H^+ E^T R^T S S_H^+ B^T \\
&= B_D S S_H^+ B^T - B_D S S_H^+ E^T R^T B^T \\
&= B_D S S_H^+ B^T,
\end{aligned}$$

so $B_D S S_H^+ B^T$ is a projection and therefore λ_D can be equal only to 0 or 1.

Next, let u_P be a (nonzero) eigenvector of the preconditioned BDD operator corresponding to the eigenvalue λ_P . Then, by Lemma 18, it holds that $\mathcal{S}_P u_P$ is an eigenvector of the preconditioned FETI-1 operator corresponding to the eigenvalue λ_P , provided that $\mathcal{S}_P u_P \neq 0$. So, assume that $\mathcal{S}_P u_P = 0$. Then it also must be true that $\mathcal{S}_D \mathcal{S}_P u_P = 0$. Using (4.16) and (2.9), we get

$$\begin{aligned}
0 &= \mathcal{S}_D \mathcal{S}_P u_P = \mathcal{S}_D P_{FETI-1} B_D S R u_P \\
&= P_{BDD} \mathcal{S}_D B_D S R u_P = P_{BDD} E S_H^+ B^T B_D S R u_P \\
&= P_{BDD} E S_H^+ (I - E^T R^T) S R u_P \\
&= P_{BDD} E S_H^+ S R u_P - P_{BDD} E S_H^+ E^T R^T S R u_P \\
&= P_{BDD} u_P - P_{BDD} E S_H^+ E^T R^T S R u_P \\
&= P_{BDD} u_P - P_{BDD}^2 u_P,
\end{aligned}$$

which is the same as

$$\lambda_P u_P - \lambda_P^2 u_P = \lambda_P (1 - \lambda_P) u_P = 0,$$

and therefore λ_P can be equal only to 0 or 1.

Finally, let $\lambda \neq 0, 1$ be an eigenvalue of the operator P_{BDD} with the multiplicity m . From the previous arguments, the eigenspace corresponding to λ is mapped by the operator \mathcal{S}_P into an eigenspace of P_{FETI-1} and since this mapping is one-to-one, the multiplicity of λ corresponding to P_{FETI-1} is $n \geq m$. By the same argument, we can prove the opposite inequality and the conclusion follows. ■

5. ADAPTIVE FETI-DP AND BDDC PRECONDITIONERS

The action of the FETI-DP and BDDC preconditioners is defined on the space \widetilde{W} , which has been specified in Chapter 2 only by the condition (2.7). We note that this condition ensures only that the preconditioners are well defined, but it does not guarantee any of their approximation properties. So, if we would like to improve convergence of both of these methods, the construction of some subspace of \widetilde{W} needs to be studied. The detailed discussion of this space, respective a construction of a restriction operator to a certain subspace, will be the main topic of this chapter. It is based on our previous work [46, 47], but the algorithm presented here is substantially simpler. Also, the formulation of the BDDC preconditioner in Sections 5.1-5.3 is new, and it is a result of a joint research with Jakub Šístek. An efficient parallel implementation will be studied elsewhere.

As we wrote already in Sec. 2.3, the space \widetilde{W} is constructed using *coarse degrees of freedom* that can be, e.g., values at corners, or averages over edges/faces. The space is then given by the requirement that the coarse degrees of freedom on adjacent substructures coincide; for this reason, the terms coarse degree of freedom and *constraint* may be used interchangeably. From now on, we will preferably use the term constraint. Although the formulation of the adaptive algorithm appears to be new and includes also an extension of the adaptive algorithm into three spatial dimension, the basic idea remained the same as in [46, 47]: we build on the algebraic bound from Theorem 9 and as in our previous work, we make use of the fact that this bound can be computed as the solution of a generalized eigenvalue problem. By restricting the eigenproblem onto pairs of *adjacent* substructures, we obtain a *heuristic condition number indicator*. Next, we show how to use the eigenvectors obtained from the solution of the localized generalized eigenvalue problems, which are supported on the interface shared by such pairs, to construct coarse degrees of freedom as constraints in the definition of the space \widetilde{W} . Such procedure results in an optimal decrease of the heuristic indicator. Finally, we illustrate on several numerical examples in two and also three spatial dimensions that this indicator is quite close to the actual condition number and that such approach can result in the identification of troublesome parts of the problem and concentration of the computational work, which leads to an improved convergence at a small additional cost.

This chapter differs from the previous in one aspect: we will need to make substantially more references to substructuring (Sec. 2.3). Nevertheless, we would like to emphasize that our adaptive algorithm is algebraic and it does not rely on any specific properties of the problem.

The adaptive algorithm takes advantage of pairs of adjacent substructures:

Definition 20: *A pair of substructures will be call adjacent if they share either: (a) an edge in 2D, or (b) a face in 3D. The set of all adjacent substructures $\{ij\}$ is denoted by \mathcal{A} and every pair $\{ij\} \in \mathcal{A}$ is represented only once.*

5.1 The preconditioners on a subspace

In this section, which does not contain any adaptivity yet, we will revisit the formulation of the abstract preconditioners, FETI-DP from Sec. 3.1.3 and BDDC from Algorithm 4. First, let us rewrite the hierarchy of spaces, cf. (2.6), as

$$\widehat{W} \subset \widetilde{W}^{avg} \subset \widetilde{W}^c \subset W, \quad (5.1)$$

where \widetilde{W}^c is the space already satisfying some initial constraints. This space is actually considered from now on to replace \widehat{W} in the hierarchy of spaces (2.6). The first natural choice for \widetilde{W}^c , used also in our implementation, is the space constructed using a sufficient number of corner coarse degrees freedom. The operators on \widetilde{W}^c are then obtained by a subassembly of subdomain stiffness matrices, cf. Sec. 2.3, in essentially the same way as by Li and Widlund [41]. Because of implementation related reasons that are discussed in detail later, we assemble only the corner degrees of freedom (unlike [41]).

Both preconditioners are typically, especially in 3D, characterized by a restriction into some subspace of \widetilde{W}^c satisfying additional constraints on functions: such as equality of their average values across edges or faces. The purpose of this choice is to obtain the scalability with subdomain size. Ideally, one can prove the polylogarithmic condition number bound

$$\kappa \leq \text{const.} \left(1 + \log \frac{H}{h} \right)^2, \quad (5.2)$$

where H is the subdomain size and h is the finite element size. We note that the explanation of (5.2) is outside of the scope of this thesis, and we refer to the detailed discussion, e.g., in the monograph [60]. Here we only note, that the initial selection of constraints in the proposed adaptive approach (as well as in our numerical experiments) has been done such that (5.2) is satisfied.

For the BDDC method, we will define this subspace as

$$\widetilde{W}^{avg} = \left\{ w \in \widetilde{W}^c : D^T w = 0 \right\}. \quad (5.3)$$

Each row of D^T represents one constraint, the constraints are linearly independent, so that D has full rank. The details of the construction of D will be the main topic of this chapter, and the adaptive algorithm from [47] will be greatly simplified – all additional constraints are added as new columns in the matrix D , and as we will see, in a very simple way. In order to relate the preconditioners, let us recall the definition of such subspace in the case of the FETI-DP method, which we have used in our previous work on adaptivity, cf. [47, eq. (17)], as

$$\widetilde{W}^{avg} = \left\{ w \in \widetilde{W}^c : Q_D^T B w = 0 \right\}. \quad (5.4)$$

Here, Q_D is a dual weight matrix, and B is the standard FETI operator enforcing continuity across substructure interfaces. Comparing the two definitions (5.4) and (5.3), we see that the matrices D and Q_D are closely related. And because B is known, the entries of Q_D can be determined from the entries in D . In Sec. 5.6 we will see that this is also true for the additional (adaptive) entries in D , and so the forthcoming adaptive theory and algorithms can be easily transferred in the standard case of the FETI-DP method.

Let us now look more closely at the relation of the operators Q_D and D . Assuming the block diagonal structure of operators as in (2.19), suppose we are given a linear operator in a block-diagonal form as

$$\begin{bmatrix} Q_1 & & \\ & \ddots & \\ & & Q_N \end{bmatrix},$$

such that each block Q_i defines constraints localized to a substructure i and each row k of Q_i defines a constraint $Q_{k,i}$. We note that typically we constrain just one glob at a time, but in general we can constrain the same glob several times; the only requirement is that the constraints must be linearly independent. If we want to prescribe (average) value of a function $w \in \widetilde{W}^c$ on a glob shared by neighboring substructures i and j , we need to satisfy

$$Q_{k,i}w_i = Q_{l,j}w_j, \quad (5.5)$$

where $w_i = w|_{\Omega_i}$, $w_j = w|_{\Omega_j}$ and k, l denote the rows of Q_i, Q_j , respectively, with entries containing the weights of the constrained equation (5.5), which defines the shared constraint. Since $Q_{k,i}$ and $Q_{l,j}$ correspond to the shared constraint on the shared glob, they have the same entries and hence, we can identify the rows k and l . Next, because the operator B in (5.4) has entries $+1, 0, -1$ and it constrains a pair of interface degrees of freedom at a time, we introduce the operators Q_D and D by rewriting (5.5) as

$$Q_{k,i}w|_{\Omega_i} - Q_{l,j}w|_{\Omega_j} = 0 \Rightarrow Q_D^T B w = D^T w = 0,$$

which relates the two definitions of the space \widetilde{W}^{avg} in (5.3) and (5.4). We remark that each additional row of D^T represents one additional constraint.

Construction of the operator D is illustrated by a simple example, shown on Figure 5.1. Consider a domain Ω partitioned into two subdomains Ω_i , $i = 1, 2$,

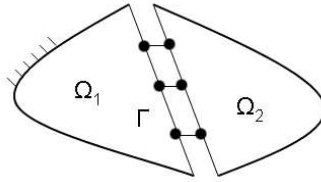


Fig. 5.1: Partition of the domain Ω into two subdomains, sharing an edge Γ .

sharing three nodes on an edge Γ . For simplicity we do not consider corners. The subdomain Ω_2 is floating and in the scalar case we need to enforce at least one average over the shared edge. Such constraint would appear in as a single row in the matrix D^T given in this case as $D^T = [1 \ 1 \ 1 \ -1 \ -1 \ -1]$. We note that, e.g., for elasticity in 2D it is natural to split D^T into two independent rows, each corresponding to displacements in the direction of principal axes. Also, we need to be careful in coupling edge averages in 3D that belong to more than just two substructures and use nonredundant constraint in the same sense as, e.g., [60, Section 6.3.1], so that D^T has a full (row) rank. The necessity of this property of the matrix D will become obvious in the following section.

5.2 Projected BDDC preconditioner

Because the description of the FETI-DP on the subspace defined by (5.4) would now proceed in a much similar way as in [45], we will rather focus on the formulation of the BDDC preconditioner on the subspace defined by (5.3), which appears to be new. In particular, we will restrict the preconditioner in the subspace \widetilde{W}^{avg} using a projection on the nullspace of D^T . We begin by restating the abstract BDDC preconditioner from Algorithm 4 as follows:

Algorithm 21: *The abstract BDDC preconditioner M_{BDDC} from Algorithm 4 restricted to the space \widetilde{W}^{avg} is defined by*

$$M_{BDDC} : r \mapsto u = Ew, \quad w \in \widetilde{W}^{avg} : \quad a(w, z) = \langle r, Ez \rangle, \quad \forall z \in \widetilde{W}^{avg}.$$

The action of the abstract BDDC preconditioner (3.33), respective (3.34), restricted in the space \widetilde{W}^{avg} consists of two steps: solving the system

$$w \in \widetilde{W}^c : \widetilde{S}w = E^T r, \quad \text{subject to } D^T w = 0, \quad (5.6)$$

followed by computation of the approximate solution $u \in \widehat{W}$ as $u = Ew$.

One way of restricting the action of the preconditioner in the space \widetilde{W}^{avg} is to introduce the orthogonal projection P onto the nullspace of D^T as

$$P = I - D (D^T D)^{-1} D^T. \quad (5.7)$$

The system (5.6) can now be written as

$$P\widetilde{S}Pw = PE^T r. \quad (5.8)$$

The two main steps in the construction of the projection P defined by (5.7) are: (1) inverting the system $D^T D$ with the size determined by the number of constraints, and (2) scattering the inverse by action of D . Due to a block structure of D , where each block corresponds to a different glob and because by definition each degree of freedom belongs to at most one glob, the construction of P can be performed in parallel. At this stage of our approach we keep the original degrees of freedom, which gives rise to dense off-diagonal blocks in the projection P and also in the projected operator $P\widetilde{S}P$ (for ‘‘communication’’ between the degrees of freedom that belong to the same glob). The structure of both operators is illustrated in Fig. 5.2. This issue will be resolved in the next section by a generalized change of variables.

Because $P\widetilde{S}P$ can be singular for nontrivial D (then $\text{null } D^T$ is a proper subspace of \widetilde{W}^c), we suggest to solve instead of (5.8) a modified system

$$\left[P\widetilde{S}P + t(I - P) \right] w = PE^T r, \quad (5.9)$$

where $t > 0$ is some scaling constant. Now, the operator $P\widetilde{S}P + t(I - P)$ is regular, while the solutions of the systems (5.6) and (5.9) are the same.

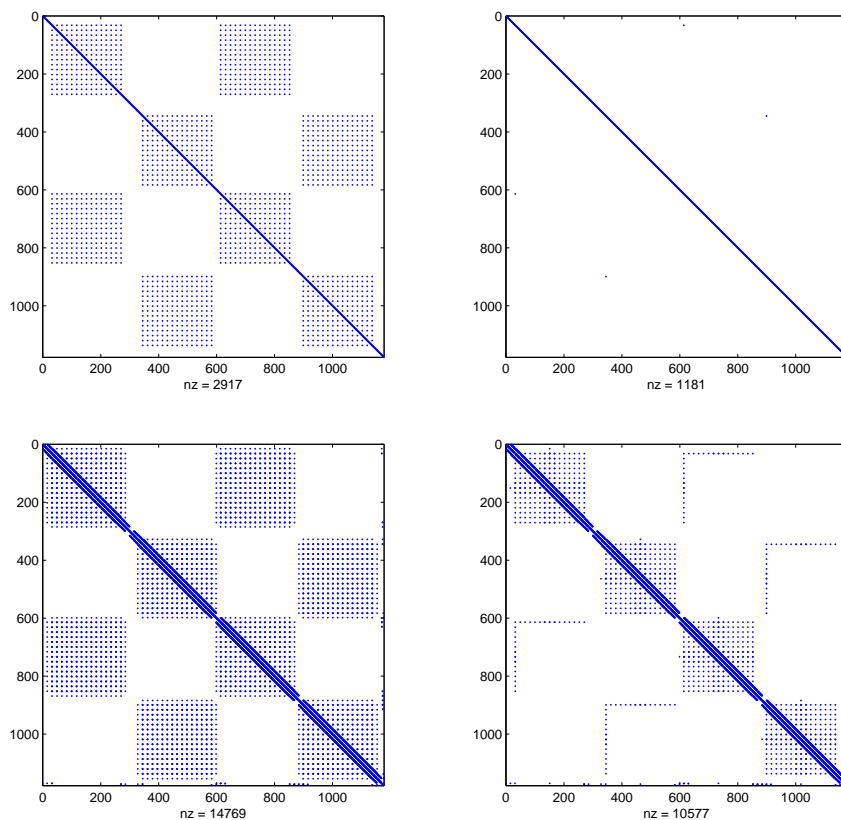


Fig. 5.2: The projections P (top) and the projected operators $P\tilde{S}P+t(I-P)$ (bottom) for Laplace equation in 2D and four substructures: two pairs of substructures are coupled by one edge average. The left side corresponds to the representation by the original degrees of freedom and the operators on the right side were constructed using the change of variables.

5.3 Generalized change of variables

We have seen that the operator $P\tilde{S}P+t(I-P)$ suffers from a loss of sparsity. For this reason, we generalize the change of variables by Li and Widlund [41], so that we could prescribe as constraints quite general edge or face averages and also preserve a more favorable fill-in of the projected operator. We note that any change of variables causes in general some fill-in, but the main idea here is to allow this only in the diagonal blocks and minimize the creation of (dense) off-diagonal blocks. In this section, we will show how to transform the operator \tilde{S} associated with the bilinear form a on the space \tilde{W}^c into a different basis, in which all averages would be represented by explicit degrees of freedom. The dual coupling by the matrix \bar{D} is then done between these individual degrees of freedom, resulting in much smaller (and thus more desirable) fill-in of the projected system operator $P\tilde{S}P+t(I-P)$ as illustrated by Fig. 5.2.

Remark 22: We could treat the degrees of freedom corresponding to averages after the change of variables as corners and assemble them, as advocated in [41]. This would give us no additional fill-in beyond the one caused by the change of variables. We do not adopt such approach here, mainly because of implementation related reasons: different dimensioning of arrays and matrices which is in fact a-priori unknown due to our adaptive construction of constraints.

The new variables are introduced via the transformation $\bar{w} = \mathcal{B}w$, where \mathcal{B} is some regular matrix containing the weights of averages over globs we intend to prescribe; the construction of \mathcal{B} is discussed in detail later in this section. We will denote $\mathcal{B}^{-1} = \mathcal{T}$, so then $w = \mathcal{T}\bar{w}$. Now, using the change of basis we can further modify Algorithm 21 as follows:

Algorithm 23: The BDDC preconditioner $\bar{M}_{BDDC} : \widehat{W}' \rightarrow \widehat{W}$ is defined as $\bar{M}_{BDDC} : r \mapsto u = E\mathcal{T}\bar{w}$, $\bar{w} \in \widetilde{W}^{avg} : a(\mathcal{T}\bar{w}, \mathcal{T}z) = \langle r, E\mathcal{T}z \rangle, \forall z \in \widetilde{W}^{avg}$.

We remark that in the action of the preconditioner, defined by the previous algorithm, we in fact do not use the matrix \mathcal{B} , but only its inverse $\mathcal{B}^{-1} = \mathcal{T}$. The Algorithm 23 consists of two steps: solving the system

$$\mathcal{T}^T \tilde{S} \mathcal{T} \bar{w} = \mathcal{T}^T E^T r, \quad \text{subject to } \bar{D}^T \bar{w} = 0, \quad (5.10)$$

followed by computation of the approximate solution $u \in \widehat{W}$ as $u = E\mathcal{T}\bar{w}$. We would like to emphasize that the operator D used in (5.6) is different from the operator \bar{D} in (5.10); they are related as $\bar{D}^T = D^T \mathcal{T}$ and \bar{D} is much sparser because it couples only the selected pairs of interface degrees of freedom. In fact, the construction of \bar{D} is similar to the construction of the operator B used in the FETI methods. In computations, it can be constructed directly without using either D or \mathcal{T} , knowing only which pairs of the interface degrees of freedom have to be coupled after the change of basis.

We will now describe the construction of the operators \mathcal{B} and \mathcal{T} . So, to use Algorithm 23, we need to transform \tilde{S} into the system given by (5.10). The vector \bar{w} represents the “new” degrees of freedom, such that some of them explicitly represent the weighted average(s) of the original degrees of freedom over globs, and the matrix \mathcal{B} contains in some of its rows the coefficients of the averages assigned to the original degrees of freedom over individual globs.

To illustrate this, let us return to our simple example from Fig. 5.1. Let us say that we would like to prescribe an arithmetic average in the first degree of freedom on the edge Γ . The matrices \mathcal{B} , \mathcal{T} and \bar{D} are in this case given as

$$\mathcal{B} = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \mathcal{T} = \mathcal{B}^{-1} = \begin{bmatrix} 1 & -1 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (5.11)$$

$$\bar{D}^T = [1 \ 0 \ 0 \ -1 \ 0 \ 0].$$

The matrix \mathcal{B} consists of the following submatrices: the top row(s) prescribing average(s), zero block and an identity block of an appropriate size. The matrix \bar{D} couples then the first degree of freedom in the two substructures sharing this glob. Clearly, we could select any other degree(s) of freedom on a glob to prescribe average(s) in, but for construction of \mathcal{B} as above we will be able to find its inverse in a particularly efficient way even for quite general weights.

Remark 24: *The matrix \mathcal{T} in (5.11) is a particular case of the matrix T_E considered in [41, Section 3.3] for the case of arithmetic averages over globs.*

The global operator \mathcal{B} for the transformation of the system operator \tilde{S} has a block structure, where each block corresponds to a different glob. Because, by definition, each degree of freedom belongs to at most one glob, the construction of \mathcal{B} respective finding its inverse \mathcal{T} can be carried out glob by glob cf. [41], in parallel. For this reason and for simplicity, we will describe the generalized change of variables on a block of the global transformation matrix corresponding to only one glob and one substructure. We have already mentioned that the averages can be quite general: their number is limited by the number of degrees of freedom on this glob and also we require their linear independence. More precisely, we would like to guarantee the matrix \mathcal{B} to have a stable inverse \mathcal{T} . Let us denote by \mathcal{B}_{AVG} a block, corresponding to one glob and one substructure, that prescribes the averages, i.e.,

$$\mathcal{B}_{AVG} = \begin{bmatrix} v_1^T \\ \vdots \\ v_n^T \end{bmatrix},$$

where v_1, \dots, v_n are constraint vectors that will be specified in later sections. Now, let us just assume that the vectors v_1, \dots, v_n are linearly independent. Then, we can write

$$\mathcal{B} = \begin{bmatrix} \mathcal{B}_{AVG} & \\ 0 & I \end{bmatrix} = \begin{bmatrix} \mathcal{U} & \mathcal{V} \\ 0 & I \end{bmatrix}. \quad (5.12)$$

Above, we have schematically split the block $\mathcal{B}_{AVG} = [\mathcal{U} \ \mathcal{V}]$ for the only reason: the inverse $\mathcal{B}^{-1} = \mathcal{T}$ can be found more effectively by inverting only the much smaller block \mathcal{U} , with the size given by the number of averages, as

$$\mathcal{T} = \begin{bmatrix} \mathcal{U}^{-1} & -\mathcal{U}^{-1}\mathcal{V} \\ 0 & I \end{bmatrix}, \quad (5.13)$$

However, the invertibility of \mathcal{U} is far from obvious and it might not be possible.

In fact, to be complete at this point, we need to mention another issue, that will become clear in the adaptive context once the reader finishes reading the remaining sections. Let us consider, for simplicity, a group of vectors in \mathbb{R}^n that are linearly independent or possibly even orthogonal. Considering these vectors to be nonzero only at the a-priori selected set of slots clearly destroys the orthogonality, but unfortunately it can destroy also the linear independence of the nonzero pieces of vectors - as we will see later, this is the case of eigenvectors restricted to individual globs.

In our context, we would like to guarantee: (1) the linear independence of the rows in \mathcal{B}_{AVG} and (2) the existence of a stable inverse of some square submatrix of \mathcal{B}_{AVG} . Because we need at least to closely approximate the range \mathcal{B}_{AVG}^T , we can look equivalently for the basis of null \mathcal{B}_{AVG} . In our implementation, we have successfully used the full QR algorithm with column pivoting. This algorithm in `Matlab 7.5` uses LAPACK routine `DGEQP3`. It allows us to factor $\mathcal{B}_{AVG} = QR$ with a column permutation P_E so that the absolute values on the diagonal of R are decreasing. Eventually, we can drop the rows of R where the diagonal entry is less than some threshold value. Then null \mathcal{B}_{AVG} is (at least

closely approximated by) null R , the existence of linearly independent rows of R implies the existence of the same number of linearly independent columns of R , and the permutation P_E helps us to find a reasonable set of such columns. Using this approach, the matrix \mathcal{B}_{AVG} in (5.12) is replaced by the matrix R and the block \mathcal{U} is then given as the left triangular block of the matrix R . We compute the inverse as in (5.13) followed by a multiplication by P_E from the left to obtain the final transformation matrix. Denoting $R = [R_{\mathcal{U}} \ R_{\mathcal{V}}]$, this can be done as

$$\mathcal{T} = P_E \left(I + \begin{bmatrix} R_{\mathcal{U}}^{-1} - I & -R_{\mathcal{U}}^{-1} R_{\mathcal{V}} \\ 0 & 0 \end{bmatrix} \right).$$

Let us now relate the general matrix \mathcal{B} from (5.12) with the one used for one arithmetic average, as in (5.11), for a glob of general size given as \mathcal{B} in (5.14). The general block \mathcal{B}_{AVG} is in such case reduced into the first row of the matrix \mathcal{B} in (5.14), and the block \mathcal{U} from (5.12) is reduced just to the diagonal entry of 1. It is also remarkable that in this case, the inverse of transformation matrix for glob of any size is explicitly known. It is given as

$$\mathcal{B} = \begin{bmatrix} 1 & 1 & \dots & 1 \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}, \quad \mathcal{T} = \mathcal{B}^{-1} = \begin{bmatrix} 1 & -1 & \dots & -1 \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}. \quad (5.14)$$

Let us return for the last time to the formulation of the BDDC preconditioner on the space \widetilde{W}^{avg} , this time including the generalized change of variables. As explained in Section 5.2, one way of enforcing the constraint $\overline{D}^T \overline{w} = 0$ is to introduce the orthogonal projection \overline{P} onto the nullspace of \overline{D}^T as

$$\overline{P} = I - \overline{D} \left(\overline{D}^T \overline{D} \right)^{-1} \overline{D}^T.$$

The projected system (5.10) has the form

$$\overline{P} \mathcal{T}^T \widetilde{\mathcal{S}} \mathcal{T} \overline{P} \overline{w} = \overline{P} \mathcal{T}^T E^T r. \quad (5.15)$$

Again, the operator $\overline{P} \mathcal{T}^T \widetilde{\mathcal{S}} \mathcal{T} \overline{P}$ is singular for nontrivial \overline{D} (then null \overline{D}^T is a proper subspace of \widetilde{W}^c), and so we suggest to solve instead of (5.15) a system

$$\left[\overline{P} \mathcal{T}^T \widetilde{\mathcal{S}} \mathcal{T} \overline{P} + \bar{t}(I - \overline{P}) \right] \overline{w} = \overline{P} \mathcal{T}^T E^T r, \quad (5.16)$$

where $\bar{t} > 0$ is some scaling constant. Now, the operator $\overline{P} \mathcal{T}^T \widetilde{\mathcal{S}} \mathcal{T} \overline{P} + \bar{t}(I - \overline{P})$ is regular and also, the solutions of the systems (5.10) and (5.16) are the same.

Finally, let us rewrite the Algorithm 23 in an algebraic form as:

Algorithm 25: *The action of the BDDC preconditioner $\overline{M}_{BDDC} : \widehat{W}^t \rightarrow \widehat{W}$ projected in the space \widetilde{W}^{avg} with the generalized change of variables consists of the two steps: solving the system*

$$\left[\overline{P} \mathcal{T}^T \widetilde{\mathcal{S}} \mathcal{T} \overline{P} + \bar{t}(I - \overline{P}) \right] \overline{w} = \overline{P} \mathcal{T}^T E^T r,$$

followed by the computation of the approximate solution $u \in \widehat{W}$ as $u = E \mathcal{T} \overline{w}$.

5.4 Eigenvalue formulation of the condition number bound

From now on we will focus on the method of selecting the constraints used in the adaptive construction of the space \widetilde{W}^{avg} , that is, the construction of the matrix D . We begin by restating of the condition number bound from Theorem 9 as

$$\omega = \sup_{w \in \widetilde{W}^c} \frac{\|B_D^T B w\|_{\widetilde{S}}^2}{\|w\|_{\widetilde{S}}^2} = \sup_{w \in \widetilde{W}^c} \frac{\|(I - RE) w\|_{\widetilde{S}}^2}{\|w\|_{\widetilde{S}}^2}. \quad (5.17)$$

Note that in the present context, Theorem 9 and hence (5.17) should be in fact formulated on the space \widetilde{W}^{avg} , cf. (5.1) and (5.3)-(5.4). Here, the formulation of the condition number bound on \widetilde{W}^c serves only as a point of departure for the adaptive method, our main interest in this chapter. Clearly, the condition number bound (5.17) can be written as a generalized eigenvalue problem on \widetilde{W}^c . The stationary points of the Rayleigh quotient $\|(I - RE) w\|_{\widetilde{S}}^2 / \|w\|_{\widetilde{S}}^2$ are the eigenvectors and the values of the Rayleigh quotient at the stationary points are the eigenvalues of the generalized eigenvalue problem

$$(I - RE)^T \widetilde{S} (I - RE) w = \lambda \widetilde{S} w. \quad (5.18)$$

The maximization problem (5.17) thus becomes the problem to find the maximal eigenvalue of (5.18). The matrix on the left-hand side is symmetric positive semidefinite, the matrix \widetilde{S} is symmetric positive definite, and the eigenvalues λ_k can be ordered, with no loss of generality, as $\lambda_1 \geq \lambda_2 \geq \dots \geq 0$. We note that we do not advocate solving (5.18) numerically in practice; this section serves as a preparation for the development of a local condition number indicator.

Lemma 26 ([47, Lemma 10]): *Let $d(\cdot, \cdot)$ be symmetric positive semidefinite bilinear form on a linear space V of dimension n and $e(\cdot, \cdot)$ symmetric positive definite bilinear form on that space. Then the generalized eigenvalue problem in variational form*

$$u \in V : d(u, v) = \lambda e(u, v), \quad \forall v \in V$$

has n linearly independent eigenvectors u_k and the corresponding eigenvalues $\lambda_k \geq 0$. Order $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n \geq 0$. Then for any subspace $V_k \subset V$ of dimension k ,

$$\max_{u \in V_k, u \neq 0} \frac{d(u, u)}{e(u, u)} \geq \lambda_{k+1},$$

with equality if

$$V_k = \{u \in V : d(u_l, u) = 0, \quad \forall l = 1, \dots, k\}. \quad (5.19)$$

We can use Lemma 26 to show an optimal construction of the space \widetilde{W}^{avg} . Each row of D^T is constructed using the eigenvectors from the solution of (5.18):

Theorem 27: *Let w_i be the eigenvectors and λ_i the eigenvalues from (5.18), without loss of generality ordered as $\lambda_1 \geq \lambda_2 \geq \dots \geq 0$. Take $k \geq 0$ and let us define the operator D by*

$$\begin{aligned} d_i^T &= w_i^T (I - RE)^T \widetilde{S} (I - RE), \quad i = 1, \dots, k \\ D &= [d_1 \quad d_2 \quad \dots \quad d_k]. \end{aligned} \quad (5.20)$$

Then $\omega = \lambda_{k+1}$ and $\omega \geq \lambda_{k+1}$ for other construction of D^T by at most k rows.

Proof. Apply Lemma 26 with $V = \widetilde{W}^c$, $u = w$, and

$$\frac{d(u, u)}{e(u, u)} = \frac{\|(I - RE)w\|_{\widetilde{S}}^2}{\|w\|_{\widetilde{S}}^2} = \frac{w^T (I - RE)^T \widetilde{S} (I - RE) w}{w^T \widetilde{S} w}.$$

The orthogonality conditions in (5.19) become

$$\underbrace{w_i^T (I - RE)^T \widetilde{S} (I - RE) w}_{d_i^T} = 0, \quad i = 1, \dots, k, \quad (5.21)$$

and V_k becomes \widetilde{W}^{avg} . ■

Next, we will formalize an immediate intuitive result that enforcing a constraint “by parts” can only improve the condition number bound (5.17). In particular, we will enforce constraints by parts of the global eigenvector restricted to one glob at a time. We remark that a glob is understood to be relatively open and any two distinct globs are disjoint. We will identify a glob with the set of degrees of freedom associated with it. The set of all globs will be denoted by $\mathcal{K}_{\mathcal{G}}$. For a glob $\mathcal{G} \in \mathcal{K}_{\mathcal{G}}$ we define a glob projection $R_{\mathcal{G}} : w \in \widetilde{W}^c \rightarrow R_{\mathcal{G}}w \in \widetilde{W}^c$, where $R_{\mathcal{G}}w$ is the vector that has the same values as w for all degrees of freedom in \mathcal{G} , and all other degrees of freedom are set to zero. so for $\mathcal{G} = 1, \dots, N^{\mathcal{G}}$, the glob projection can be written as

$$R_{\mathcal{G}} = \begin{bmatrix} R_1 \\ \vdots \\ R_{N^{\mathcal{G}}} \end{bmatrix}, \quad \sum_{\mathcal{G} \in \mathcal{K}_{\mathcal{G}}} R_{\mathcal{G}} = I. \quad (5.22)$$

Now, we can define the matrix $D_{\mathcal{G}}$ as in (5.20) by imposing each constraint restricted to one glob at a time as a new column of $D_{\mathcal{G}}$, i.e.,

$$D_{\mathcal{G}} = [R_{\mathcal{G}}d_1 \quad R_{\mathcal{G}}d_2 \quad \dots \quad R_{\mathcal{G}}d_k]. \quad (5.23)$$

It is easy now to show that constraining each glob separately can only improve the condition number bound (5.17):

Lemma 28: *Let us define the spaces $\widetilde{W}_{\mathcal{G}}^{avg}$ and \widetilde{W}^{avg} as the nullspaces of $D_{\mathcal{G}}^T$ from (5.23) and D^T from (5.20), respectively. Let us also define by (5.17) the respective condition number bounds $\omega_{\mathcal{G}}$ and ω . Then, the bounds satisfy*

$$\omega_{\mathcal{G}} \leq \omega.$$

Proof. Let us define $D_{\mathcal{G}}$ by (5.23) and consider, for simplicity, just one vector of constraints, i.e., let $k = 1$. The extension for $k > 1$ is straightforward. Then, for any $w \in \widetilde{W}_{\mathcal{G}}^{avg}$, we have

$$0 = D_{\mathcal{G}}^T w = (R_{\mathcal{G}}d_1)^T w \Rightarrow \left(\sum_{\mathcal{G} \in \mathcal{K}_{\mathcal{G}}} R_{\mathcal{G}}d_1 \right)^T w = D^T w = 0,$$

so $\widetilde{W}_{\mathcal{G}}^{avg} \subset \widetilde{W}^{avg}$ and the conclusion follows. ■

As we have already mentioned, computation of global eigenvectors is computationally expensive and therefore not convenient for practical implementation. Numerical experiments also indicate that when there are just several troublesome parts in the global problem, it is sufficient to impose the additional constraints only locally.

5.5 Local indicator of the condition number bound

From now on, we need to assume the full substructuring framework from Sec. 2.3. We need to define *local* versions of some spaces and operators from Section 2.2. So, for each pair $\{ij\} \in \mathcal{A}$ of substructures, we define a space $W_{ij} = W_i \times W_j$, similarly as (2.18), by considering only the pair $\{ij\}$. Next, we define \widetilde{W}_{ij}^c as the subspace of all functions from \widetilde{W}_{ij} that satisfy the initial constraints on the interface $\Gamma_{ij} = \partial\Omega_i \cap \partial\Omega_j$ and the system operator \widetilde{S}_{ij} is obtained by subassembly of the system operators corresponding to substructures i and j . Finally, we define \widehat{W}_{ij} as the subspace of all functions from \widetilde{W}_{ij} such that the values of all degrees of freedom on the interface between substructures i and j coincide. We need to define two more operators as analogy to (2.2) and (2.8). The operator E_{ij} is a projection onto \widehat{W}_{ij} ,

$$E_{ij} : W_{ij} \rightarrow \widehat{W}_{ij}, \quad E_{ij}^2 = E_{ij}, \quad \text{range } E_{ij} = \widehat{W}_{ij},$$

and R_{ij} is the natural injection from \widehat{W}_{ij} to W_{ij} ,

$$R_{ij} : \widehat{W}_{ij} \rightarrow W_{ij}, \quad R_{ij} : w_{ij} \in \widehat{W}_{ij} \mapsto w_{ij} \in W_{ij},$$

Clearly, in analogy to (2.9),

$$E_{ij}R_{ij} = I_{\widehat{W}_{ij}}.$$

We will assume, in addition to (2.7), that the selection of corner degrees of freedom as initial constraints has been made in such a way that:

Assumption 29: *Let us assume that the initial constraints (those present before the selection of additional ones) are already sufficient to prevent relative rigid body motions of any pair of adjacent substructures, so*

$$\forall w_{ij} \in \widetilde{W}_{ij}^c : \widetilde{S}_{ij}w_{ij} = 0 \Rightarrow (I - R_{ij}E_{ij})w_{ij} = 0,$$

i.e., the coarse degrees of freedom are sufficient to constrain the rigid body modes of the two substructures into a single set of rigid body modes, which are then continuous across the interface Γ_{ij} .

Finally, let $\mathcal{R}_{ij} : \widetilde{W}^c \rightarrow \widetilde{W}_{ij}^c$ be the 0 – 1 matrix that restrict global vectors of degrees of freedom to the intersection of substructures i and j . The global vector of degrees of freedom w can be obtained from a local w_{ij} as

$$w = \mathcal{R}_{ij}^T w_{ij},$$

where $w \in \widetilde{W}^c$ has zero entries everywhere outside of the subset \mathcal{S}_{ij} , which is defined as the set of entries corresponding to the interface Γ_{ij} .

Remark 30: *It is notable that the local spaces and operators arise naturally in exactly the same way as the analogical global spaces and operators defined in Sec. 2.2-2.3 by considering only one pair of adjacent substructures at a time. This is, in particular, very convenient for practical implementation of adaptive constraints: we can use the same routines to obtain local versions of operators. Moreover, the local problems can be solved completely in parallel.*

We note that the construction of local problems is not a restriction in the usual sense, and in fact

$$\widetilde{W}^c \subsetneq \mathcal{R}_{ij}^T \widetilde{W}_{ij}^c \subsetneq W, \quad \forall \{ij\} \in \mathcal{A},$$

because in general any (initial) constraint can be shared by more substructures than just by a considered pair $\{ij\} \in \mathcal{A}$. Typical examples are corners, and also edges in three dimensions - if they are constrained a-priori.

In analogy to [47], we propose as the indicator of the condition number bound to use the maximum of the bounds ω_{ij} from (5.17) computed for pairs of adjacent substructures. So, we define the *condition number indicator* $\tilde{\omega}$ by

$$\tilde{\omega} = \max_{\{ij\} \in \mathcal{A}} \omega_{ij}, \quad \omega_{ij} = \sup_{w_{ij} \in \widetilde{W}_{ij}^c} \frac{\|(I - R_{ij}E_{ij})w_{ij}\|_{\widetilde{S}_{ij}}^2}{\|w_{ij}\|_{\widetilde{S}_{ij}}^2}. \quad (5.24)$$

Similarly to (5.18), finding $\tilde{\omega}$ is equivalent to finding the largest eigenvalue from the set of local generalized eigenvalue problems

$$(I - R_{ij}E_{ij})^T \widetilde{S}_{ij} (I - R_{ij}E_{ij}) w_{ij} = \lambda_{ij} \widetilde{S}_{ij} w_{ij}. \quad (5.25)$$

To guarantee that each ω_{ij} is finite, we need

$$\forall w_{ij} \in \widetilde{W}_{ij}^c : \widetilde{S}_{ij} w_{ij} = 0 \Rightarrow (I - R_{ij}E_{ij}) w_{ij} = 0,$$

which is satisfied when a pair of adjacent substructures i and j linked by only the coarse degrees of freedom do not form a mechanism. In our settings it holds automatically due to Assumption 29. Still, the matrices on both sides of (5.25) are typically singular regardless of Assumption 29, because of rigid body modes that move adjacent substructures i and j as a whole.

Remark 31: *The operators \widetilde{S}_{ij} are symmetric, but in general only positive semidefinite. Also, the nullspaces of operators in (5.25) are related as*

$$\text{null } \widetilde{S}_{ij} \subset \text{null } (I - R_{ij}E_{ij})^T \widetilde{S}_{ij} (I - R_{ij}E_{ij}). \quad (5.26)$$

In the numerical experiments we have used Matlab function `eig` with Choleski decomposition, and also Matlab version of `lobpcg` developed by Knyazev [31]. Both algorithms worked despite of singular of \widetilde{S}_{ij} due to property (5.26), because in this case they pass to factorspace on which the problem (5.25) is defined with \widetilde{S}_{ij} positive definite. We note, that if `lobpcg` is used with a preconditioner, one must make sure that it is invariant on the $\text{null } \widetilde{S}_{ij}$. Also, unless the component the solution in the direction of the nullspace is small, the errors will accumulate, which may eventually result in instability of the code at the Rayleigh-Ritz step, but only after a large number of steps [32]. In our experience, it was sufficient to use `lobpcg` without preconditioner, and also since we need to compute the eigenvectors only approximately, cf. Sec. 5.7, with only a modest number of iterations. For the sake of generality, we will continue as this was not the case and we would need to compute with \widetilde{S}_{ij} positive definite.

To reduce (5.25) to a problem with the matrix on the right-hand side positive definite, we use matrices Z_i, Z_j that generate a superspace of rigid body modes of the two substructures:

$$\text{null } S_i \subset \text{range } Z_i, \quad \text{null } S_j \subset \text{range } Z_j \quad (5.27)$$

The matrices Z_i and Z_j are often available from finite element software, or, based on the type of the problem, the kernels of local stiffness matrices are known explicitly, cf., e.g., [11, 26]. Let

$$Z_{ij} = \begin{bmatrix} Z_i \\ Z_j \end{bmatrix}.$$

Then

$$\text{null } \tilde{S}_{ij} \subset \text{range } Z_{ij}, \quad (5.28)$$

and because \tilde{S}_{ij} is non-negative, it holds that $Z_{ij}^T \tilde{S}_{ij} Z_{ij} y = 0 \Leftrightarrow Z_{ij} y \subset \text{null } \tilde{S}_{ij}$. So, we can find a basis of $\text{null } \tilde{S}_{ij}$ by computing first the nullspace of a much smaller symmetric positive semidefinite matrix,

$$\text{null} \left(Z_{ij}^T \tilde{S}_{ij} Z_{ij} \right) = \text{range } K_{ij}, \quad (5.29)$$

and applying the QR decomposition

$$Z_{ij} K_{ij} = Q_{ij} R_{ij}, \quad Q_{ij}^T Q_{ij} = I,$$

which gives

$$\text{range } Q_{ij} = \text{null } \tilde{S}_{ij}.$$

Consequently,

$$\Pi_{ij} = I - Q_{ij} Q_{ij}^T \quad (5.30)$$

is the orthogonal projection onto $\text{range } \tilde{S}_{ij}$. We will use the following result:

Lemma 32: *Let S, T, Π be square matrices of the same size, Π an orthogonal projection, $t \neq 0$, and $\lambda \neq 0$ scalars, and u a vector. Then*

1. *It holds that*

$$\Pi T \Pi w = \lambda \Pi S \Pi w \text{ and } w \in \text{range } \Pi \quad (5.31)$$

if and only

$$\Pi T \Pi w = \lambda (\Pi S \Pi + t(I - \Pi)) w. \quad (5.32)$$

2. *If S is symmetric and positive definite on $\text{range } \Pi$ and $t > 0$, then $\Pi S \Pi + t(I - \Pi)$ is symmetric positive definite.*

Proof.

1. Assume that (5.31) holds. Then $(I - \Pi)w = 0$, and (5.32) follows. On the other hand, if (5.32) holds, then $(I - \Pi)w \in \text{range } \Pi$ because $t \neq 0$ and $\lambda \neq 0$, so $(I - \Pi)w = 0$, and, consequently, (5.31) holds.
2. Let S be symmetric and positive definite on $\text{range } \Pi$ and $v = w + z$, $w \in \text{range } \Pi$, $z \in \text{null } \Pi$. Then

$$\begin{aligned} v^T (\Pi S \Pi + t(I - \Pi)) v &= w^T \Pi S \Pi w + tz^T (I - \Pi) z \\ &= w^T S w + tz^T z > 0, \end{aligned}$$

unless $w = z = 0$. ■

Theorem 33: *Let $t > 0$ and let Π_{ij} be defined by (5.30). Then the nonzero eigenvalues and the eigenvectors of (5.25) are same as those of the following generalized eigenvalue problem*

$$(I - R_{ij}E_{ij})^T \tilde{S}_{ij} (I - R_{ij}E_{ij}) w_{ij} = \lambda_{ij} \left(\Pi_{ij} \tilde{S}_{ij} \Pi_{ij} + t(I - \Pi_{ij}) \right) w_{ij}. \quad (5.33)$$

The matrix on the left-hand side of (5.33) is symmetric positive semidefinite and the matrix on the right-hand side is symmetric positive definite. In particular, the upper bound ω_{ij} on the condition number from (5.24) is the maximal eigenvalue of (5.33).

Proof. The equivalence of (5.25) and (5.33) follows from Lemma 32 (1). Positive definiteness of the matrix $\Pi_{ij} \tilde{S}_{ij} \Pi_{ij} + t(I - \Pi_{ij})$ follows from Lemma 32 (2) and the assumption that \tilde{S}_{ij} is positive definite on $\text{range } \Pi_{ij}$. ■

If no boundary conditions were applied to subdomain stiffness matrices, we can adopt more elegant approach. In such case we get equality in equation (5.28), so that $\text{null } \tilde{S}_{ij} = \text{range } Z_{ij}$, and the projections Π_{ij} are simply

$$\Pi_{ij} = I - Z_{ij} Z_{ij}^T.$$

We note that similar idea lies behind the Total FETI by Dostál et. al. [11].

Remark 34: *The matrices in the generalized eigenvalue problems (5.29) and (5.33) are dense. If it is more efficient to represent the matrices as dense or to use an eigensolver that requires only matrix-vector multiplications depends on the size of the substructures and the dimension of the problem.*

5.6 Adaptive selection of constraints

We define, in analogy to (5.3), the subspace $\tilde{W}_{ij}^{avg} \subset \tilde{W}_{ij}^c$ as

$$\tilde{W}_{ij}^{avg} = \left\{ w \in \tilde{W}_{ij}^c : D_{ij}^T w_{ij} = 0 \right\}. \quad (5.34)$$

We note that the space \tilde{W}_{ij}^{avg} is defined only for the theoretical purposes in Theorem 35. The definition (5.34) allows us now to guarantee that ω_{ij} does not exceed a given target value τ by adding a minimal number of coarse degrees of freedom. We formulate an analog to Theorem 27 and also to [47, Theorem 11]:

Theorem 35: *Let $w_{ij,k}$ be the eigenvectors and $\lambda_{ij,k}$ the eigenvalues from (5.25), without loss of generality ordered as $\lambda_{ij,1} \geq \lambda_{ij,2} \geq \dots \geq 0$. Take $k_{ij} \geq 0$ and let us define the operator D_{ij} by*

$$d_{ij,\ell}^T = w_{ij\ell}^T (I - R_{ij}E_{ij})^T \tilde{S}_{ij} (I - R_{ij}E_{ij}), \quad \ell = 1, \dots, k_{ij}, \quad (5.35)$$

$$D_{ij} = \begin{bmatrix} d_{ij,1} & d_{ij,2} & \dots & d_{ij,k_{ij}} \end{bmatrix}. \quad (5.36)$$

Then $\omega_{ij} = \lambda_{ij,k_{ij}+1}$, and $\omega_{ij} \geq \lambda_{ij,k_{ij}+1}$ for any other construction of D_{ij}^T by at most k_{ij} rows. In particular, if $\lambda_{ij,k_{ij}+1} \leq \tau$ for all pairs of adjacent substructures $\{ij\} \in \mathcal{A}$, then $\tilde{\omega} = \max_{\{ij\} \in \mathcal{A}} \lambda_{ij,k_{ij}+1} \leq \tau$.

Proof. Apply Lemma 26 with $V = \widetilde{W}_{ij}^c$, $u = w_{ij}$, and

$$\frac{d(u, u)}{e(u, u)} = \frac{\|(I - R_{ij}E_{ij})w_{ij}\|_{\widetilde{S}_{ij}}^2}{\|w_{ij}\|_{\widetilde{S}_{ij}}^2} = \frac{w_{ij}^T (I - R_{ij}E_{ij})^T \widetilde{S}_{ij} (I - R_{ij}E_{ij}) w_{ij}}{w_{ij}^T \widetilde{S}_{ij} w_{ij}}.$$

The orthogonality conditions in (5.19) become

$$\underbrace{w_{ij\ell}^T (I - R_{ij}E_{ij})^T \widetilde{S}_{ij} (I - R_{ij}E_{ij}) w_{ij}}_{d_{ij,\ell}^T} = 0, \quad \ell = 1, \dots, k_{ij},$$

and V_k becomes \widetilde{W}_{ij}^{avg} . \blacksquare

The additional constraints in D are constructed from the columns of D_{ij} in a very simple way: all constraints obtained from the solution of local subproblem corresponding to a pair $\{ij\} \in \mathcal{A}$ are extended by zero outside of the subset of degrees of freedom \mathcal{S}_{ij} corresponding to Γ_{ij} and inserted as new columns in D , i.e., schematically

$$D = [\dots \mathcal{R}_{ij}^T D_{ij,\ell} \dots], \quad \forall \{ij\} \in \mathcal{A}, \quad \ell = 1, \dots, k_{ij}. \quad (5.37)$$

Note that such construction is much simpler compared to our approach in [47].

Now, Theorem 35 allows us to add constraints that decrease the indicator ω_{ij} in an optimal manner, and the proposed adaptive algorithm follows:

Algorithm 36: *To add coarse degrees of freedom to guarantee that $\omega_{ij} \leq \tau$, for a given a target value τ :*

1. *Compute the eigenvalues and eigenvectors of (5.33), starting from the largest eigenvalues, until the first ℓ_{ij} is found such that $\lambda_{ij,\ell_{ij}+1} \leq \tau$.*
2. *Use eigenvectors from above to obtain local constraints $d_{ij,\ell}$ by (5.35).*
3. *Add in the matrix D the additional columns obtained from $d_{ij,\ell}$ by (5.37).*

Remark 37: *We have confirmed that after the new coarse degrees of freedom are added, the values of new indicators ω_{ij} are equal to the eigenvalues $\lambda_{ij,\ell_{ij}+1}$.*

So far, we have described the construction of the operator D used in the definition of the BDDC preconditioner in Section 5.1. As the starting point, we have used the right-hand side of equation (5.17), and exclusively the operators from the definition of the BDDC method. We note that, as a direct consequence of Theorem 9, we could have equivalently used the left-hand side of (5.17) and the operators from the definition of the FETI-DP method, as in our previous work [47]. So, our current work is in a sense “dual” to [47]. To be complete at this point, it remains to construct the augmentation of the dual constraint matrix Q_D from the augmentation of D . In particular, we will show that the additional entries in Q_D can be obtained by “tearing” the matrix D into two parts and using one part, simply as it is, to define the additional columns in Q_D . Comparing the two definitions of the space \widetilde{W}^{avg} by (5.3) and (5.4), we see that

$$D^T = Q_D^T B.$$

The matrix B enforces continuity across substructure interface and contains in each row exactly one $+1$ and one -1 entry; each row of B thus constraints one degree of freedom shared by two substructures at a time. The key observations are: (1) each degree of freedom in the local problem belongs to at most two substructures at a time and (2) each constraint constructed as in (5.35) using a local eigenvector w , can be written (dropping for simplicity all subscripts) as

$$d^T = w^T (I - RE)^T \tilde{S} (I - RE) \Rightarrow d = (I - RE)^T \tilde{S} [w - \bar{w}], \quad (5.38)$$

where $\bar{w} = REw$ is the average of vector w across interface. We immediately see, that the entries in d corresponding to the degrees of freedom present in only one substructure are zero. The entry in d corresponding to a degree of freedom on the interface Γ_{ij} can be computed, for a single degree of freedom x with entries x_i, x_j in vector w , and E being an arithmetic average $\bar{x} = (x_i + x_j)/2$, as

$$x_i - \bar{x} = \frac{x_i - x_j}{2}, \quad x_j - \bar{x} = \frac{-x_i + x_j}{2} = -\frac{x_i - x_j}{2},$$

so the entries in d corresponding to x have the same abs. value but opposite sign.

The implementation of both preconditioners can follow Sections 5.1-5.3. We also remark, that an interesting approach to implementation of the BDDC preconditioner, based on the original formulation of the method [9, 44], capable of handling general averages, has been described by Šístek et al. [61].

5.7 Numerical results

We have successfully tested the proposed adaptive algorithm on several examples of linear elasticity in two and three spatial dimensions. The averaging operator was constructed with weights proportional to the diagonal entries of the substructure matrices before elimination of interiors. The computations were done in `Matlab`. The generalized eigenproblems on pairs of substructures were solved using the function `eig` with Choleski decomposition, and we have also successfully tested `Matlab` version of the `lobpcg` algorithm by Knyazev [31]. Both methods worked despite of singularities of local stiffness matrices, cf. Remark 31, and the technique described in Theorem 33 was in fact not necessary.

5.7.1 Two-dimensional linear elasticity

The method was tested on plane elasticity, discretized by Lagrange bilinear elements on a rectangular mesh decomposed into 16 substructures, with one edge between the substructures jagged (Fig. 5.3). The initial set of coarse degrees of freedom consisted of all corner degrees of freedom. The set \mathcal{A} of all pairs of adjacent substructures to compute the condition number indicator $\tilde{\omega}$ by (5.24) was chosen as the set of all pairs of substructures with a common edge. The subsets \mathcal{S}_{ij} to define new coarse degrees of freedom were taken as edges (excluding corners).

In Table 5.1, we show that the eigenvalues $\lambda_{ij,k}$ associated with edges between substructures clearly distinguish between the problematic edge and the others. Table 5.2 demonstrates that the addition of the coarse degrees of freedom created from the associated eigenvectors according to Theorem 35 decreases

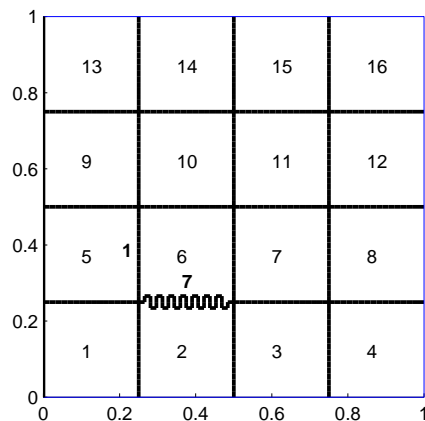


Fig. 5.3: Mesh with $H/h = 16$, 4×4 substructures, and one jagged edge between substructures 2 and 6. Zero displacement is imposed on the left edge. For compressible elasticity (Tables 5.1 and 5.2) and tolerance $\tau = 10$, 7 coarse degrees of freedom at the jagged edge and 1 coarse degree of freedom at an adjacent edge are added automatically.

i	j	$\lambda_{ij,1}$	$\lambda_{ij,2}$	$\lambda_{ij,3}$	$\lambda_{ij,4}$	$\lambda_{ij,5}$	$\lambda_{ij,6}$	$\lambda_{ij,7}$	$\lambda_{ij,8}$
1	2	3.7	2.3	1.4	1.3	1.1	1.1	1.1	1.1
1	5	5.8	3.2	2.3	1.4	1.2	1.1	1.1	1.1
2	3	6.0	2.5	1.7	1.3	1.2	1.1	1.	1.1
2	6	21.7	19.5	17.8	14.9	14.5	11.7	11.2	9.7
3	4	3.3	2.3	1.4	1.3	1.1	1.1	1.1	1.1
3	7	7.1	5.1	3.2	1.8	1.4	1.3	1.2	1.1
4	8	5.9	3.4	2.6	1.4	1.2	1.1	1.1	1.1
5	6	12.0	4.9	4.4	1.8	1.6	1.3	1.3	1.2
5	9	5.9	3.4	2.6	1.4	1.3	1.3	1.1	1.1
6	7	8.7	4.9	3.9	1.8	1.5	1.3	1.2	1.1
6	10	7.3	4.8	3.4	1.8	1.4	1.3	1.2	1.1

Tab. 5.1: Several largest eigenvalues $\lambda_{ij,k}$ for several edges for the elasticity problem from Fig. 5.3 with $H/h = 16$. $(i, j) = (2, 6)$ is the jagged edge.

H/h	$Ndof$	τ	Nc	$\tilde{\omega}$	κ	it
4	578		42	10.3	5.6	19
		10	43	5.2	4.0	18
		3	44	3.0	4.0	18
16	8450	2	58	2.0	2.8	15
			42	22	20	37
		10	50	8.7	9.9	29
		3	77	3.0	4.6	22
64	132098	2	112	2.0	2.6	15
			42	87	40	55
		10	89	9.8	9.9	36
		3	151	3.0	4.7	22
		2	174	2.0	2.9	17

Tab. 5.2: BDDC results for plane elasticity on a square with one jagged edge. The Lamé coefficients are $\lambda = 1$ and $\mu = 2$. H/h is the number of elements per substructure in one direction, $Ndof$ the number of degrees of freedom in the problem, τ the condition number tolerance as in Theorem 35, Nc the number of coarse degrees of freedom, $\tilde{\omega}$ the a-priori condition number indicator from (5.24), κ the approximate condition number computed from the Lanczos sequence in conjugate gradients, and it the number of BDDC iterations for relative residual tolerance 10^{-8} .

H/h	$Ndof$	τ	Nc	$\tilde{\omega}$	κ	it
4	578		42	284.7	208.4	65
		10	68	8.2	8.6	28
		5	89	5.0	4.6	22
		3	114	2.9	2.6	16
16	8450		42	1012.0	1010.0	157
		10	87	9.9	9.6	29
		5	94	4.9	4.4	22
		3	126	3.0	2.9	19
64	132098		42	6909.8	1470.9	15
		10	183	9.8	9.7	37
		5	213	5.0	4.9	26
		3	274	3.0	3.0	20

Tab. 5.3: BDDC results for almost incompressible plane elasticity on a square with one jagged edge. The Lamé coefficients are $\lambda = 1000$ and $\mu = 2$. The headings are same as in Table 5.2.

the condition number of the preconditioned system to approximately the prescribed value τ . Tables 5.3 and 5.4 contain the results of the same test for almost incompressible elasticity; here the iterations converge poorly or not at all without the additional coarse degrees of freedom, but adding the coarse degrees of freedom again decreases the condition number of the preconditioned system to approximately the prescribed value τ , and, in particular, the convergence of the iterations is recovered. This incompressible elasticity problem is particularly hard for an iterative method because standard bilinear elements were used instead of stable elements or reduced integration. The number of the added coarse degrees of freedom grows as the material approaches incompressibility. Nevertheless, we do not advocate the present method or the elements used for the solution of almost incompressible problems. The purpose of this test was to show that the method can identify the problematic part of the problem and deal with it. The study of the adaptive FETI-DP and BDDC preconditioners for nearly incompressible elasticity [10], or Stokes problem [39, 40], would be of independent interest.

We have also simulated the effect of approximate eigensolvers. The eigenvector w_{ij} from (5.33) was replaced by $\tilde{w}_{ij} = w_{ij} + \varepsilon r$, where r is a random vector with independent normally distributed entries, and ε was determined from the condition $|Y_{ij}\varepsilon r| = 0.5 |Y_{ij}w_{ij}|$, where $|\cdot|$ is the Euclidean norm. The eigenvalues λ_{ij} were replaced by the Rayleigh-Ritz values $\tilde{w}_{ij}^T X_{ij} \tilde{w}_{ij} / \tilde{w}_{ij}^T Y_{ij} \tilde{w}_{ij}$. The approximate eigenvectors and eigenvalues were then used in all computations instead of the exact ones. The results were essentially identical within display accuracy to those in Table 5.3.

5.7.2 Three-dimensional linear elasticity

The method was also tested on a realistic three-dimensional problem of linear elasticity, a nozzle box of a ŠKODA steam turbine 28 MW for the electric power plant Nováky, Slovakia, loaded by steam pressure*. The body of the nozzle box was discretized using isoparametric quadratic finite elements with 40 254 degrees of freedom and decomposed into 16 substructures, see Figs. 5.4-5.5. The initial set of coarse degrees of freedom consisted of all corner degrees of freedom and three arithmetic averages over each edge (one for each spatial dimension). The set \mathcal{A} of all pairs of adjacent substructures to compute the condition number indicator $\tilde{\omega}$ by (5.24) was chosen as the set of all pairs of substructures with a common face. The subsets \mathcal{S}_{ij} to define new coarse degrees of freedom were taken as faces (i.e., open sets excluding edges and corners). We note, that in fact the eigenvectors were computed over the whole set of degrees of freedom shared by the pairs of adjacent substructures, i.e., over faces and shared edges, and restricted on the faces. We have used this approach for the following reasons: (1) initial set of constraints is sufficient to guarantee the polylogarithmic condition number bound (5.2) cf., e.g., [60, Section 6.4], (2) corners and faces alone are not suitable for elasticity in 3D, cf. [44, Remark 4], (3) if we use the generalized change of variables, because edges are typically shared by more than one pair of adjacent substructures, there might not be in general enough degrees of freedom on the edges to prescribe the averages in. We note, that the

* Courtesy of Jaroslav Novotný, Institute of Thermomechanics, Czech Academy of Sciences, and Jakub Sístek, Faculty of Mechanical Engineering, Czech Technical University in Prague.

restriction of eigenvectors on the faces might violate the requirement of linear independence of constraints, discussed in Section 5.3. The generalized change of variables using QR with column pivoting should be able to resolve such situations. Moreover, the proposed adaptive algorithm seems to be robust, and in our examples we have observed essentially the same performance (number of iterations and condition number estimate) of the two implementations of the BDDC preconditioner: with and without the change of variables.

Table 5.5 shows the convergence of the BDDC algorithm using standard arithmetic averages over edges and faces. Note, that the number of corner coarse degrees of freedom was not sufficient to guarantee the convergence. Comparing Tables 5.5 and 5.6, we actually see that when we add additional constraints the improvement in number of iterations and condition number is relatively small. This indicates that for this problem three arithmetic averages per face already work well enough as there are no interfaces that would require extra work - the quality of the decomposition is uniform, as also seen in Figs. 5.4-5.5. However, we can still improve the condition number as well as the number by iterations. First, we have tried to add three eigenvectors on each face instead of simple arithmetic averages - comparing first row in Table 5.6 with the last row in Table 5.5 we see, that the eigenvectors obtained from the local eigenproblems work better than just arithmetic averages. Our explanation is that such constraints might approximate better the direction of global eigenvectors corresponding to the extreme eigenvalues. The remaining rows in the Table 5.6 correspond to the different thresholds τ so that all eigenvectors of the local problems corresponding to eigenvalues greater or equal to τ are added as a new constraints restricted to corresponding faces. We see that such method leads to a redistribution of number of prescribed averages on different faces and that, e.g., with $\tau = 20$ the total number of prescribed constraints is still lower compared to arithmetic averages, but the number of iterations is improved by almost 25% and the condition number estimate κ is improved by more than 50%. This results, also with regard to the results of the numerical experiments in the two spatial dimensions, lead to a conjecture that we would be able to demonstrate robustness of the presented algorithm in the three spatial dimensions also on problems where properties of the mesh decomposition would be much more unfavorable.

H/h	$Ndof$	τ	Nc	$\tilde{\omega}$	κ	it
4	578		42	2743.9	1875.04	158
		10	118	4.6	3.5	17
		5	118	4.6	3.5	17
		3	120	2.9	2.7	16
16	8450		42	9483.5	9389.9	113
		10	97	9.6	10.1	33
		5	120	5.0	5.0	24
		3	280	3.0	2.9	18
64	132098		42	29680.6	NA	∞
		10	218	9.8	9.6	40
		5	269	4.9	4.2	25
		3	313	3.0	2.9	18

Tab. 5.4: BDDC results for almost incompressible plane elasticity on a square with one jagged edge. The Lamé coefficients are $\lambda = 10000$ and $\mu = 2$. The headings are same as in Table 5.2.

constraints	$nglobs$	Nc	it	κ
corners	37	111	NA	NA
corners+edges	56	168	106	1021.9
corners+faces	69	207	53	49.8
corners+edges+faces	88	264	47	40.3

Tab. 5.5: BDDC results for the turbine nozzle box problem, nonadaptive approach with corner constraints and arithmetic averages over edges/faces, $nglob$ is the number of such constrained entities and each one of them generates three constraints (one for each spatial dimension), Nc is the total number of coarse degrees of freedom, it is the number of BDDC iterations for relative residual tolerance 10^{-8} and κ is the approximate condition number computed from the Lanczos sequence in conjugate gradients.

τ	$\tilde{\omega}$	Nc	it	κ
-	69.5	264	40	26.6
50	48.9	209	50	44.9
40	39.0	216	45	29.6
20	19.6	247	36	17.3
10	10.0	311	28	12.7
5	5.0	434	22	9.2

Tab. 5.6: BDDC results for the turbine nozzle box problem using the adaptive approach. First row corresponds to the case when three eigenvectors are added on each face. Remaining rows correspond to varying τ as the condition number tolerance as in Theorem 35, $\tilde{\omega}$ the a-priori condition number indicator from (5.24), The remaining headings are same as in Table 5.5.

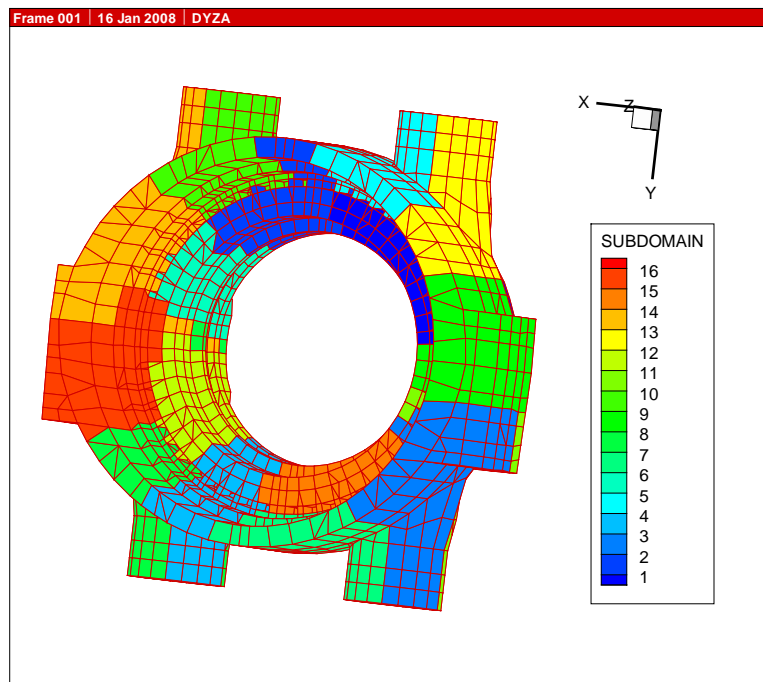
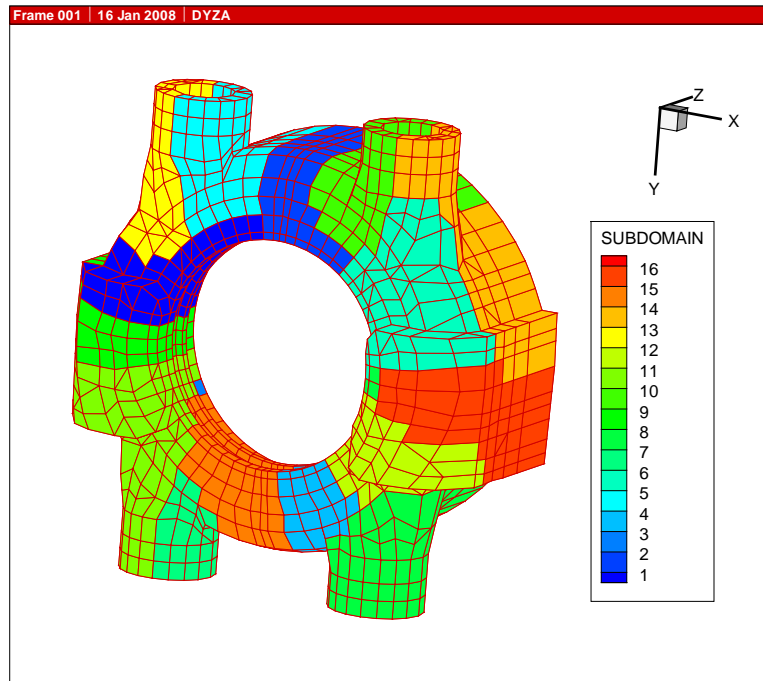


Fig. 5.4: Domain decomposition for the turbine nozzle box problem.

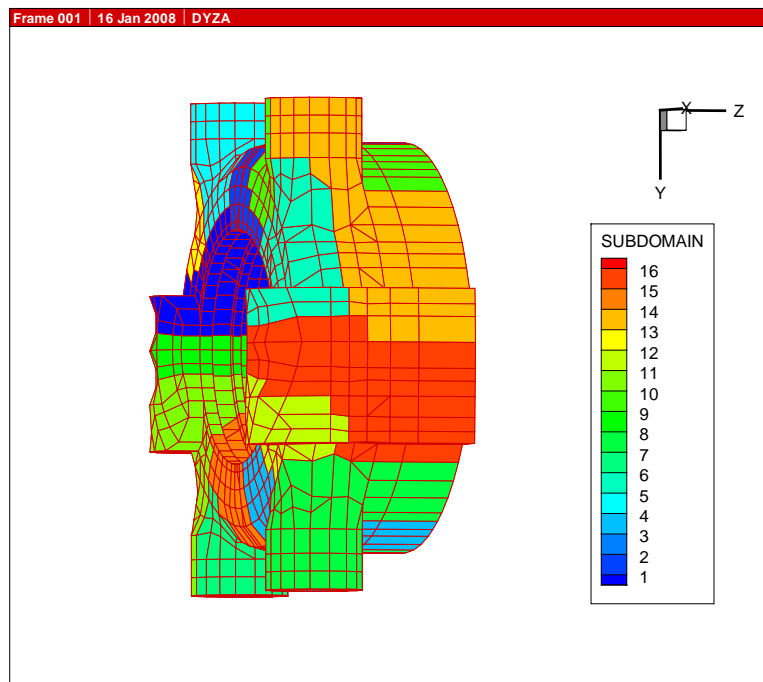
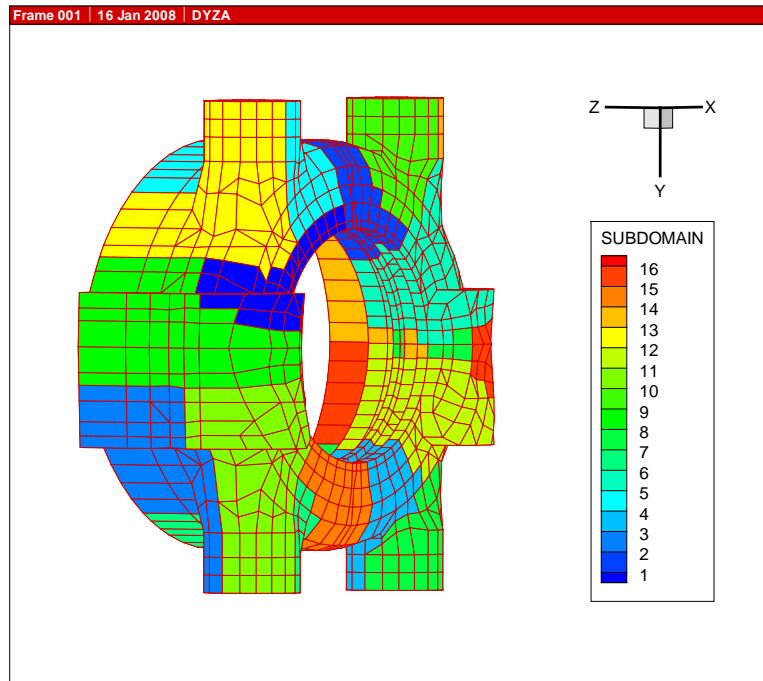


Fig. 5.5: Domain decomposition for the turbine nozzle box problem.

6. CONCLUSION

Theoretical analysis of the preconditioners used in iterative substructuring is very important. It helps us with better understanding of these methods, to find possible simplifications of their formulations, to establish connections between different versions of algorithms or with tools improving their performance, esp. in presence of adverse circumstances. We have addressed all of these aspects. Most results have been already published in journal articles [47, 48], conference proceedings [46], and a technical report [58] (submitted for publication). The main results of this thesis can be summarized as follows:

- Identification of a minimalist set of assumptions necessary to formulate the most popular methods from FETI and BDD families in Section 2.2, based on our recent work on BDDC and FETI-DP under such assumptions [48].
- Derivation of the following methods: FETI-1, FETI-DP, their primal variants denoted respectively as P-FETI-1 and P-FETI-DP (derivation has been omitted by Fragakis and Papadrakakis in [21]) in Section 3.1, and of BDD and BDDC in Section 3.2 – all under minimalist assumptions [48, 58].
- A proof that the P-FETI-DP and BDDC preconditioners are the same, and also that the preconditioner by Cros [8] can be interpreted as either of them [48, 58], formulated here in Section 3.2.2 as Theorems 5 and 6.
- Derivation of the condition number bound for BDDC and FETI-DP, and a proof showing that the spectra (except possibly of eigenvalues equal to one) of these two preconditioned operators are the same [48], formulated here in Section 4.1 as Theorems 9 and 12, respectively.
- Translation of the ideas of Fragakis and Papadrakakis [20, 21] into the framework usual in the domain decomposition community and, in particular, showing in Section 4.2 by Theorem 15 that a particular version of P-FETI-1 gives the same algorithm as BDD, and by Theorem 19 that the spectra (except eigenvalues equal to zero and one) of the preconditioned operators of BDD and this version of FETI-1 are the same [58].
- Formulation of the BDDC preconditioner using a projection on a subspace, and a generalization of the change of variables by Li and Widlund [41]. This work appears here for the first time in Sections 5.1-5.3. It is based on a joint research with Jakub Šístek from the Faculty of Mechanical Engineering, Czech Technical University in Prague.
- An adaptive algorithm that aims heuristically to achieve a predetermined convergence rate of FETI-DP and BDDC by adding constraints using the solutions of eigenproblems associated with pairs of adjacent substructures.

The method is based on our previous work in two dimensions [46, 47], however the formulation presented here in Chapter 5 and, in particular, in Sections 5.4-5.6 appears to be new. It uses the formulation of the preconditioners on a subspace and the generalized change of variables.

- The adaptive algorithm has been here for the first time extended into three spatial dimensions. The description of the 3D adaptive algorithm is given in Section 5.7.2. Also, for the solution of the generalized eigenvalue problems that the adaptive algorithm needs to solve, we have successfully tested the `lobpcg` algorithm developed by Knyazev [31], which is incorporated in the `HYPRE` and also available as an external block to the `PETSc`. The use of `lobpcg` allows to increase substantially the efficiency of the method, because the eigenvalue problems need to be solved only approximately, and the fact that they are singular is not an issue any more. We have used only function `eig` built in `Matlab` in our previous work [46, 47].
- Numerical examples in Section 5.7 illustrate the effectiveness of the proposed adaptive method and, in particular, that the algorithm successfully achieves a predetermined convergence rate of the FETI-DP and BDDC methods by adding constraints using the solutions of eigenproblems associated with pairs of adjacent substructures. The results in two spatial dimensions (Section 5.7.1) are the same as the results published in [47], and the results in three spatial dimensions (Section 5.7.2) are new.

Future developments include an efficient parallel implementation of the adaptive method, and further tests on industrial problems. An extensions of the adaptive approach to the case of Multilevel BDDC [49] would be also important to make possible the solution of problems that are both very large and numerically difficult.

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