

AN ADAPTIVE CHOICE OF PRIMAL CONSTRAINTS FOR BDDC DOMAIN DECOMPOSITION ALGORITHMS*

JUAN G. CALVO[†] AND OLOF B. WIDLUND[‡]

Abstract. An adaptive choice for primal spaces based on parallel sums is developed for BDDC deluxe methods and elliptic problems in three dimensions. The primal space, which forms the global, coarse part of the domain decomposition algorithm and which is always required for any competitive algorithm, is defined in terms of generalized eigenvalue problems related to subdomain edges and faces; selected eigenvectors associated to the smallest eigenvalues are used to enhance the primal spaces. This selection can be made automatic by using tolerance parameters specified for the subdomain faces and edges. Numerical results verify the results and provide a comparison with primal spaces commonly used. They include results for cubic subdomains as well as subdomains obtained by a mesh partitioner. Different distributions for the coefficients are also considered with constant coefficients, highly random values, and channel distributions.

Key words. elliptic problems, domain decomposition, BDDC deluxe preconditioners, adaptive primal constraints

AMS subject classifications. 65F08, 65N30, 65N35, 65N55

1. Introduction. There has recently been a considerable amount of activity in developing adaptive methods for the selection of primal constraints for BDDC algorithms and, in particular, for BDDC deluxe variants. The primal constraints of a BDDC or FETI–DP algorithm provide the global, coarse part of such a preconditioner, and they are of crucial importance for obtaining rapid convergence of these preconditioned conjugate gradient methods for the case of many subdomains. When the primal constraints are chosen adaptively, we aim at selecting a primal space which for a certain dimension of the coarse space provides the fastest rate of the convergence for the iterative method. In the alternative, we can try to develop criteria which will guarantee that the condition number of the iteration stays below a given tolerance. We note that a fair comparison between different algorithms must also take into account the cost of the set-up phase and the iterations to follow. So far a comparative study of these issues for three dimensional problems, similar to the recent study [14] for problems in two dimensions, appears to be missing.

A particular inspiration for our own work has been a talk (see [7]) by Clark Dohrmann at DD21, the twenty-first international conference on domain decomposition methods held in Rennes in June 2012. Dohrmann had then started a joint work with Clemens Pechstein; see also [23]. Their work has recently resulted in a significant contribution to the theory; see [24]. This rich paper also provides a historical context and many references to the literature.

Much of the earlier work for adaptive BDDC and FETI-DP iterative substructuring algorithms, which has been supported by theory, has been confined to developing primal constraints for equivalence classes related to two subdomain boundaries such as those for the subdomain edges for problems defined on domains in the plane; see, in particular, the paper by Klawonn, Radtke, and Rheinbach [14]. In our context, the equivalence classes are sets of finite element nodes which belong to the boundaries of more than one subdomain with the equivalence relation defined by the sets of subdomain boundaries to which the nodes belong. In other words, two nodes on the interface Γ between the subdomains belong to the same

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equivalence class if they belong to the same set of subdomain boundaries $\partial\Omega_i$. While it is important to further study the best way of handling all cases, the basic issues appear to be well settled when the equivalence classes all are defined by just two subdomain boundaries.

We note that this work is relevant for problems posed in $H(\text{div})$ even in three dimensions (3D) since the degrees of freedom on the interface between subdomains for Raviart-Thomas and Brezzi-Douglas-Marini elements are associated only with faces of the elements; see [22, 29]. But for other elliptic problems in 3D, there is, except for quite special subdomain configurations, a need to develop algorithms and results for equivalence classes with three or more subdomain boundaries.

There is early work by Mandel, Šístek, and Sousedík, who developed condition number indicators; cf. [19, 20]. A firm theoretical foundation for these algorithms has now been developed for problems in two dimensions and more recently for an enhanced variant and three dimensions; see [14] and [13], respectively. Talks by Clark Dohrmann and Axel Klawonn at DD23, the twenty-third international conference on domain decomposition methods held in July 2015 on Jeju Island, Korea, have reported on recent progress. A talk by Hyea Hyun Kim in the same session on joint work with Eric Chung and Junxian Wang also has reported considerable progress for a different kind of algorithm. Their main new algorithm for problems in three dimensions is similar but not the same as ours; see further [12] and (3.6). The main result of this paper, which had been developed independently, has been reported on by the second author at the same DD23 mini-symposium.

This paper will focus on using parallel sums for general equivalence classes. The use of parallel sums for equivalence classes with two subdomain boundaries has proven very successful in simplifying the formulas and arguments; see in particular Pechstein [23, 24] and also Section 2.1. We note that algorithms using parallel sums for equivalence classes with more than two subdomain boundaries have been quite successful in numerical experiments by Simone Scacchi and Stefano Zampini, reported in [5], for problems arising in isogeometric analysis and also by Zampini [28] in a study of problems formulated in $H(\text{curl})$ based in part on [9].

We also note that we previously have attempted to design adaptive algorithms, which resulted in quite complicated formulas and limited success. Among other complications, in one of these approaches, the primal constraints then had to be extracted by using a QR factorization of a matrix generated from several bases for spaces of prospective primal constraint vectors related to pairs of Schur complements. We note that an alternative would be to carry out several changes of variables, thus enhancing the primal space in several steps, as is done in [11]. See also a discussion in [24].

In this paper, we will focus on low-order, nodal finite element approximations for scalar elliptic problems in three dimensions

$$(1.1) \quad -\nabla \cdot (\rho(x)\nabla u) = f(x), \quad x \in \Omega, \quad \rho(x) > 0,$$

resulting in a linear system of equations to be solved using BDDC domain decomposition algorithms, in particular, its deluxe variant. We will always assume that the choice of boundary conditions results in a positive definite, symmetric stiffness matrix. Future work is planned on what is known as the economic variant of the BDDC deluxe algorithm, (e-deluxe), cf. [9], and on linear elasticity including the almost incompressible case.

The outline of this paper is as follows: in Section 2, we briefly introduce the BDDC algorithms. This is followed by a discussion of the case of equivalence classes with two subdomain boundaries and a related generalized eigenvalue problem. The success of the adaptive algorithm in this case can be explained by examining the eigenvalues of a generalized eigenvalue problem which is closely related to a *face lemma*. Such a lemma provides a standard

technical tool in domain decomposition theory; see [26, Subsection 4.6.3]. Several numerical experiments reported in Section 2.2 highlight the fact that a small number of primal constraints often can result in a very favorable bound.

We then, in Section 3, focus on the case of equivalence classes with three subdomain boundaries. This is the main part of our paper and is relevant, in particular, for contributions of subdomain edges to the values of a jump operator P_D acting on the elements in a product space related to the subdomains and the finite element space. We derive an upper bound of the square of a norm based on a Schur complement and note that it has been known for over a decade that such bounds provide an estimate of the condition number of the FETI–DP algorithm; see (2.1) and [16]. Given the close connection of the BDDC and FETI–DP algorithms, the bound for that same jump operator is equally relevant for our work; see [18]. We find that the square of this norm of a subdomain edge contribution to $P_D w$ can be bounded from above in terms of three parallel sums of single Schur complements and sums of two others. We then attempt to find a common upper bound of these expressions in terms of the parallel sum of all the relevant Schur complements. This is not successful, and we instead work directly with the operators obtained in the estimate of the jump operator and formulate a generalized eigenvalue problem for each of the edges of the subdomains. We can then select a few eigenvectors associated with the smallest eigenvalues and generate a primal constraint from each of these eigenvectors. These generalized eigenvalue problems are defined in terms of principal minors of relevant Schur complements and Schur complements of these Schur complements associated with a minimal energy extension, e.g., from a subdomain edge of a three-dimensional finite element problem. We also provide a bound on the condition number in terms of the smallest eigenvalues for the subdomain faces and edges which have been left out when constructing the primal space. We note that Kim et al. [12] have followed a quite similar path although their upper bound for the norm of the jump operator differs from ours.

In a section that follows, we indicate how to extend our preconditioner and bounds to equivalence classes with four subdomain boundaries; no new ideas are required. Section 3 is concluded by the definition of alternative generalized eigenvalue problems which has been used with success in earlier work by Simone Scacchi and Stefano Zampini [5, 29]. So far these algorithms lack a theoretical foundation.

Our paper concludes, in Section 4, by demonstrating the performance of our algorithm in a series of numerical experiments using regular subdomains as well as subdomains generated by a METIS mesh partitioner; see [10]. We demonstrate that we can obtain fast convergence for problems with a quite irregular coefficient inside the subdomains. We also report on experiments with two alternative algorithms based on other generalized eigenvalue problems using parallel sums and sums of the two sets of Schur complements; we have not been able to provide a theoretical justification for these variants.

2. Equivalence classes and BDDC algorithms. This section begins with a short introduction to BDDC algorithms; for more details, see, e.g., [17]. For an introduction to its deluxe variant, see, e.g., [27].

BDDC algorithms are domain decomposition algorithms based on the decomposition of the domain Ω of an elliptic operator into non-overlapping subdomains Ω_i , each often associated with tens of thousands of degrees of freedom. The subdomain interface Γ_i of Ω_i does not cut through any elements and is defined by $\Gamma_i := \partial\Omega_i \setminus \partial\Omega$. Its equivalence classes are associated with the subdomain faces, edges, and vertices of $\Gamma := \bigcup_i \Gamma_i$, the interface of the entire decomposition. Thus, for a problem in three dimensions, a subdomain face is associated with the degrees of freedom of the nodes belonging to the interior of the intersection of two boundaries of two neighboring subdomains Ω_i and Ω_j and does not include any nodes on the boundary of the face. If such a set consists of several disjoint components, then each of them

will be classified as a face. Those of a subdomain edge are typically associated with a set of nodes common to three or more subdomain boundaries, while the endpoints of the subdomain edges are the subdomain vertices which are associated with even more subdomains.

Given the stiffness matrix $A^{(i)}$ of the subdomain Ω_i , we obtain a subdomain Schur complement $S^{(i)}$ by eliminating the interior variables, i.e., all those that do not belong to Γ_i . We will also work with principal minors of these Schur complements associated with faces F and edges E denoting them by $S_{FF}^{(i)}$ and $S_{EE}^{(i)}$, respectively.

The interface space is divided into a *primal* subspace of functions which are continuous across Γ and a complementary, *dual* subspace for which we will allow multiple values across the interface during part of the iteration. In this study, all the subdomain vertex variables will always belong to the primal set.

The BDDC and FETI-DP algorithms can be described in terms of three product spaces of finite element functions/vectors defined by their interface nodal values:

$$\widehat{W}_\Gamma \subset \widetilde{W}_\Gamma \subset W_\Gamma.$$

W_Γ is a product space of the spaces defined on the interfaces Γ_i without any continuity constraints across the interface. Elements of \widetilde{W}_Γ have common values of the primal variables but allow multiple values of the dual variables while the elements of \widehat{W}_Γ are continuous at all nodes on Γ . We will change variables, explicitly introducing the primal variables and a complementary sets of dual variables in order to simplify the presentation; see, e.g., [17]. After eliminating the interior variables, we can then write the subdomain Schur complements as

$$S^{(i)} = \begin{bmatrix} S_{\Delta\Delta}^{(i)} & S_{\Delta\Pi}^{(i)} \\ S_{\Pi\Delta}^{(i)} & S_{\Pi\Pi}^{(i)} \end{bmatrix}.$$

We will partially subassemble the $S^{(i)}$, obtaining \widetilde{S} , enforcing the continuity of the primal variables only. Thus, we then work in \widetilde{W}_Γ . In each step of the iteration, we solve a linear system with the coefficient matrix \widetilde{S} . In the alternative, we could also work with a linear system with a matrix obtained by partially subassembling the subdomain stiffness matrices $A^{(i)}$. We note that solving these linear systems will be considerably much faster than working with the fully assembled system provided that the dimension of the primal space is modest. At the end of each iteration, the approximate solution is made continuous at all nodal points of the interface; continuity is restored by applying a weighted averaging operator E_D , which maps \widetilde{W}_Γ into \widehat{W}_Γ .

In each iteration, we first compute the residual of the fully assembled Schur complement system. We then apply E_D^T to obtain a right-hand side for the partially subassembled linear system, solve this system, and then apply E_D . This last step changes the values on Γ unless the iteration has converged and can result in non-zero residuals at nodes not on Γ . In a final step of each iteration step, we eliminate these residuals by solving a Dirichlet problem on each of the subdomains. We always accelerate the iteration with the preconditioned conjugate gradient algorithm.

2.1. BDDC deluxe. When designing a BDDC algorithm, we have to choose an effective set of primal constraints and also a good recipe for the averaging across the interface. This paper concerns the choice of the primal constraints while we will always use the deluxe recipe in the construction of the averaging operator E_D .

We note that in work on three-dimensional problems formulated in $H(\mathbf{curl})$, it was found that traditional averaging recipes did not always work well; cf. [8, 9]. The same is true for problems in $H(\mathbf{div})$; see [22]. This occasional failure has its roots in the fact that there are two

sets of material parameters in these applications. The deluxe scaling that was then introduced has also proven quite successful for a variety of other applications including isogeometric analysis; cf. [5, 4]. For a survey, see [27].

A face component of the average operator E_D across a subdomain face $F \subset \Gamma$ common to two subdomains Ω_i and Ω_j is defined in terms of the principal minors $S_{FF}^{(k)}$ of the matrix $S^{(k)}$, $k = i, j$. The deluxe averaging operator for F is then defined by

$$\bar{w}_F := (E_D w)_F := \left(S_{FF}^{(i)} + S_{FF}^{(j)} \right)^{-1} \left(S_{FF}^{(i)} w_F^{(i)} + S_{FF}^{(j)} w_F^{(j)} \right).$$

Here, $w_F^{(i)}$ is the restriction of $w^{(i)}$ to the face F , etc.

The action of $(S_{FF}^{(i)} + S_{FF}^{(j)})^{-1}$ can be implemented by solving a Dirichlet problem on $\Omega_i \cup F \cup \Omega_j$, where F is the face between the two subdomains. This can add significantly to the cost. We can also compute the Schur complements, add them, and factor the sum. We note that if we would use the popular numerical factorization package MUMPS [1], we could exploit that these Schur complements are provided when the subdomain matrices are factored. In an economic variant (e-deluxe), we replace this large domain by a thin domain built from one or a few layers of elements next to the face, and this often results in very similar iteration counts; see, e.g., [9]. The advantage of using the e-deluxe variant will depend considerably on the software used in assembling a program; a discussion of these matters can be found in a recent paper on problems posed in $H(\text{div})$; see [22].

Deluxe averaging operators are also developed for subdomain edges and any other equivalence classes of interface variables, and the operator E_D is assembled from all these components; see further Section 3. Our bound for this operator will be obtained from bounds for the individual equivalence sets and will include factors that depend on the number of equivalence classes associated with the faces and edges of the individual subdomains; see Theorems 3.2 and 3.4.

The core of any estimate for a BDDC algorithm is the norm of the averaging operator E_D . By an algebraic argument known for FETI-DP since 2002, we know that

$$(2.1) \quad \kappa \left(M_{BDDC}^{-1} \hat{S} \right) \leq \|E_D\|_{\tilde{S}};$$

see [16]. Here, κ is the condition number of the iteration matrix, M_{BDDC}^{-1} denotes the BDDC preconditioner, and \hat{S} the fully assembled Schur complement of the problem.

The analysis of any BDDC deluxe algorithm can be reduced to establishing bounds for the individual subdomains. The analysis of traditional BDDC algorithms requires the use of an extension theorem, cf. [15]; the deluxe version does not.

Instead of developing an estimate for E_D , we will work with $P_D := I - E_D$. Instead of estimating the norm of E_D , we will bound that of P_D ; we note that as proven in [24, Appendix A], the norm of these operators are the same. Thus, instead of estimating $(R_F^T \bar{w}_F)^T S^{(i)} R_F^T \bar{w}_F$, we will work with the $S^{(i)}$ -norm of $R_F^T (w_F^{(i)} - \bar{w}_F)$. Here, R_F denotes the restriction to the face F . By elementary algebra, we find that

$$w_F^{(i)} - \bar{w}_F = \left(S_{FF}^{(i)} + S_{FF}^{(j)} \right)^{-1} S_{FF}^{(j)} (w_F^{(i)} - w_F^{(j)}).$$

More algebra gives, by using that $S_{FF}^{(i)} := R_F S^{(i)} R_F^T$,

$$\begin{aligned} & \left(R_F^T (w_F^{(i)} - \bar{w}_F) \right)^T S^{(i)} \left(R_F^T (w_F^{(i)} - \bar{w}_F) \right) \\ &= (w_F^{(i)} - w_F^{(j)})^T S_{FF}^{(j)} \left(S_{FF}^{(i)} + S_{FF}^{(j)} \right)^{-1} S_{FF}^{(i)} \left(S_{FF}^{(i)} + S_{FF}^{(j)} \right)^{-1} S_{FF}^{(j)} (w_F^{(i)} - w_F^{(j)}). \end{aligned}$$

Adding a similar contribution from Ω_j , we obtain, following Clemens Pechstein, that the relevant expression of the energy is

$$\begin{aligned} & (w_F^{(i)} - w_F^{(j)})^T S_{FF}^{(i)} \left(S_{FF}^{(i)} + S_{FF}^{(j)} \right)^{-1} S_{FF}^{(j)} (w_F^{(i)} - w_F^{(j)}) \\ & = (w_F^{(i)} - w_F^{(j)})^T S_{FF}^{(i)} : S_{FF}^{(j)} (w_F^{(i)} - w_F^{(j)}). \end{aligned}$$

The matrix of this positive definite, symmetric quadratic form is a *parallel sum*; we will use the notation

$$A : B := A(A + B)^{-1}B;$$

cf. [2]. We note that if A and B are positive definite, then $A : B = (A^{-1} + B^{-1})^{-1}$. If $A + B$ is only positive semi-definite, then we can replace $(A + B)^{-1}$ by $(A + B)^\dagger$, a generalized inverse, without any complications. However, see [25] and Section 3 for a discussion of the case of parallel sums of more than two positive semi-definite operators. We can also work with shifted, positive definite operators obtained by adding a small positive multiple of the identity operator to the operators that are singular. This idea has worked well in our experiments; using generalized inverses have produced results of quite similar quality.

In standard BDDC theory, the required estimate can then be obtained by using a *face lemma*, cf. [26, subsection 4.6.3], where such a result is established for constant coefficients in each subdomain and for polyhedral subdomains. For an adaptive algorithm, this result is replaced by the use of a generalized eigenvalue problem. Thus, we first solve the generalized eigenvalue problem

$$(2.2) \quad \check{S}_{FF}^{(i)} : \check{S}_{FF}^{(j)} \phi = \lambda S_{FF}^{(i)} : S_{FF}^{(j)} \phi.$$

Here,

$$\check{S}_{FF}^{(i)} := S_{FF}^{(i)} - S_{F'F}^{(i)T} S_{F'F'}^{(i)-1} S_{F'F}^{(i)},$$

with $S_{F'F'}^{(i)}$ the principal minor of $S^{(i)}$ with respect to $\Gamma_i \setminus F$ and $S_{F'F}^{(i)}$ an off-diagonal block of $S^{(i)}$. This Schur complement of a Schur complement represents the minimum norm extension of any finite element function defined on F and will therefore provide a uniform bound for any extension of the values on F to the rest of Γ_i . In other words, $w_F^{(i)T} \check{S}_{FF}^{(i)} w_F^{(i)} \leq a_i(w, w)$ for any w that equals $w_F^{(i)}$ on the face F . We note that the choice of $\check{S}_{FF}^{(i)} : \check{S}_{FF}^{(j)}$ as one of the matrices of the generalized eigenvalue problem is fully motivated in the proof of [24, Lemma 5.24].

We note that the eigenvalue problem (2.2) can be replaced by an eigenvalue problem which uses the inverses of the operators and that, following Zampini, we can extract the inverses of all the matrices $\check{S}_{FF}^{(i)}$ from the inverse of $S^{(i)}$; the inverse of $\check{S}_{FF}^{(i)}$ appears as a principal minor of the inverse of $S^{(i)}$. The same trick can also be used to obtain all the matrices required for eigenvalue problems related to the subdomain edges which are developed in Section 3. The inverses of $S_{FF}^{(i)}$, etc., are computed via Cholesky factorizations. There are of course also costs in the set-up phase of the algorithm to solve a generalized eigenvalue problem for each subdomain face and each subdomain edge. We note that all these computations are local and can be carried out in parallel. Detailed information on the relative cost of the set-up phase and the iteration are provided for some large-scale parallel computations in [22].

Primal constraints are then generated by using the eigenvectors of a few of the smallest eigenvalues of (2.2) and making $(\check{S}_{FF}^{(i)} : \check{S}_{FF}^{(j)})(w_F^{(i)} - w_F^{(j)})$ orthogonal to these eigenvectors.

This orthogonality condition allows us to conclude that

$$w_{F\Delta}^T (S_{FF}^{(i)} : S_{FF}^{(j)}) w_{F\Delta} \leq \frac{1}{\lambda_{tol}^F} w_{F\Delta}^T (\check{S}_{FF}^{(i)} : \check{S}_{FF}^{(j)}) w_{F\Delta}$$

for any element $w_{F\Delta} \in W_\Delta$, where λ_{tol}^F is the smallest eigenvalue of the eigenvectors that have not been chosen when we select the primal constraints. By using all the eigenvectors as a new basis for the subspace associated with an individual subdomain face, we can easily separate primal and dual subspaces.

We note that the subdomain matrices $A^{(i)}$ are singular for interior subdomains and so are the Schur complements $\check{S}_{FF}^{(i)}$. As it was previously pointed out, we can replace the inverses in the definition of the parallel sum, etc., by generalized inverses without any further complications.

We now note that $w_F^{(i)} - w_F^{(j)}$ belongs to the dual space and that therefore

$$\begin{aligned} (w_F^{(i)} - w_F^{(j)})^T S_{FF}^{(i)} : S_{FF}^{(j)} (w_F^{(i)} - w_F^{(j)}) \\ \leq \frac{1}{\lambda_{tol}^F} (w_F^{(i)} - w_F^{(j)})^T \check{S}_{FF}^{(i)} : \check{S}_{FF}^{(j)} (w_F^{(i)} - w_F^{(j)}). \end{aligned}$$

What remains is to estimate the expression on the right hand side by the energy attributed to the two subdomains Ω_i and Ω_j . To do so, we will use a formula for the parallel sum of two operators; cf. [3, Theorem 9], see also [24, Corollary 5.11].

LEMMA 2.1. *Let A and B be two symmetric, positive semi-definite matrices of the same order. Then, $z^T A : Bz = \inf_{z=x+y} (x^T Ax + y^T By)$.*

Choosing $x = w_F^{(i)}$ and $y = -w_F^{(j)}$, we find that we have established the following result.

LEMMA 2.2. *Let λ_{tol}^F be the smallest eigenvalue of (2.2) not chosen when selecting the primal constraints for a subdomain face F . We then have*

$$(2.3) \quad \|(P_D w)|_F\|_S^2 \leq \frac{1}{\lambda_{tol}^F} (a_i(w, w) + a_j(w, w)),$$

where $a_i(\cdot, \cdot)$ is the bilinear form associated with (1.1) obtained by restricting the integration to Ω_i , etc.

We note that a less precise version of formula (2.3) has previously been developed with the factor $\frac{2}{\lambda_{tol}^F}$; see, e.g., [14] as well as in the original version of this paper.

2.2. Convergence of eigenvalues. The success of this kind of algorithm is closely related to the rapid convergence of the eigenvalues of (2.2) to 1. Numerical experiments reported in four plots illustrate a rapid decay of the eigenvalues of $S_{FF}^{(i)-1} (S_{FF}^{(i)} - \check{S}_{FF}^{(i)})$ even for problems with highly oscillatory coefficients; see Figure 2.1. The same can be said for subdomains generated by the METIS mesh partitioner software; see Figure 2.2. This shows that the eigenvalues of $S_{FF}^{(i)-1} \check{S}_{FF}^{(i)}$ approach 1 quite rapidly and that, except on a very small subspace, the action of $S_{FF}^{(i)}$ and $\check{S}_{FF}^{(i)}$ are virtually the same. Therefore the same can be said of $S_{FF}^{(i)} : S_{FF}^{(j)}$ and $\check{S}_{FF}^{(i)} : \check{S}_{FF}^{(j)}$. This fact is illustrated in four additional plots; see Figures 2.3 and 2.4.

In the case of a random coefficient $\rho(x)$, we use a uniform distribution to pick a number r in the interval $[-3, 3]$ and then assign the value 10^r to ρ in individual elements.

As a consequence of these findings, the eigenvalues of (2.2) converge to 1 quite rapidly even for problems with large changes in the coefficients inside the subdomains. Therefore, we do not need to expand the primal space very much.

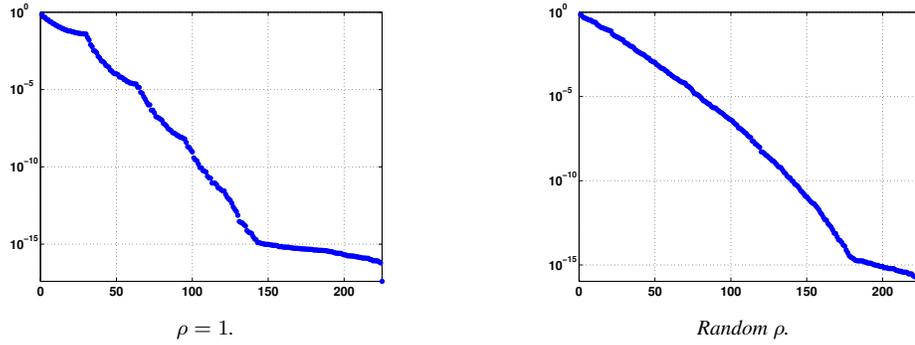


FIG. 2.1. Eigenvalues of $S_{FF}^{(i)-1}(S_{FF}^{(i)} - \check{S}_{FF}^{(i)})$ for a face with 225 nodes of 3D problems with cubic subdomains.

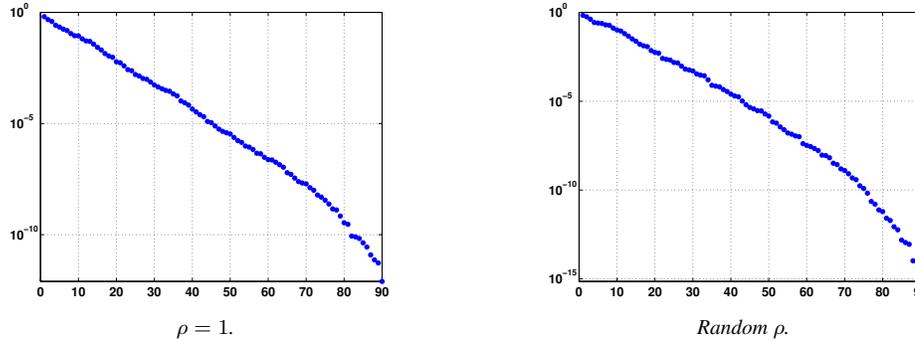


FIG. 2.2. Eigenvalues of $S_{FF}^{(i)-1}(S_{FF}^{(i)} - \check{S}_{FF}^{(i)})$ for a face with 90 nodes of 3D problems with METIS subdomains.

Figures 2.1 and 2.2 suggest that the operator $S_{FF}^{(i)-1}(S_{FF}^{(i)} - \check{S}_{FF}^{(i)})$ is associated with a compact operator. We can offer an explanation at least for the case with constant coefficients. We first recall that the trace class of $H^1(\Omega_i)$ is $H^{1/2}(\partial\Omega_i)$. For a face $F \subset \partial\Omega_i$, the trace semi-norm is defined by

$$(2.4) \quad |u|_{H^{1/2}(F)}^2 := \int_F \int_F \frac{|u(x) - u(y)|^2}{|x - y|^3} dS_x dS_y.$$

We obtain the $H^{1/2}(F)$ -norm by adding $1/H_F \|u\|_{L^2(F)}^2$, where H_F is the diameter of F . We find that the $S_{FF}^{(i)}$ -norm is equivalent to the norm obtained by restricting (2.4) to the finite element space; cf. [26, Lemma 4.6].

It is also known that the $H^{1/2}(\Gamma_i)$ -norm of the minimal norm extension of any element $u \in H^{1/2}(F)$ is bounded uniformly by $\|u\|_{H^{1/2}(F)}$. But it is also known that an extension by zero even for $H_0^{1/2}(F)$, the closure of $C_0^\infty(F)$ in this norm, fails to be uniformly bounded. The subspace for which the extension by zero is bounded is known as $H_0^{1/2}(F)$. A norm for this subspace is given by

$$(2.5) \quad \|u\|_{H_0^{1/2}(F)}^2 := |u|_{H^{1/2}(F)}^2 + \int_F \frac{|u(x)|^2}{d(x)} dS_x,$$

where $d(x)$ is the distance from x to ∂F . The formula (2.5) can be derived for any Lipschitz

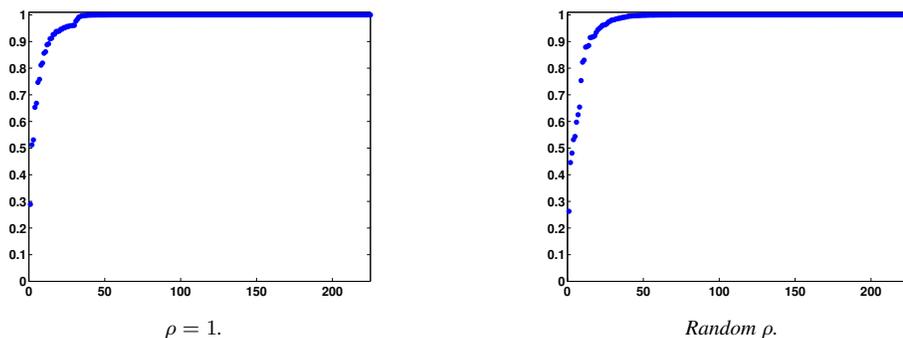


FIG. 2.3. Eigenvalues of $\check{S}_{FF}^{(i)} : \check{S}_{FF}^{(j)}\phi = \lambda S_{FF}^{(i)} : S_{FF}^{(j)}\phi$ for a face with 225 nodes of 3D problems with cubic subdomains.

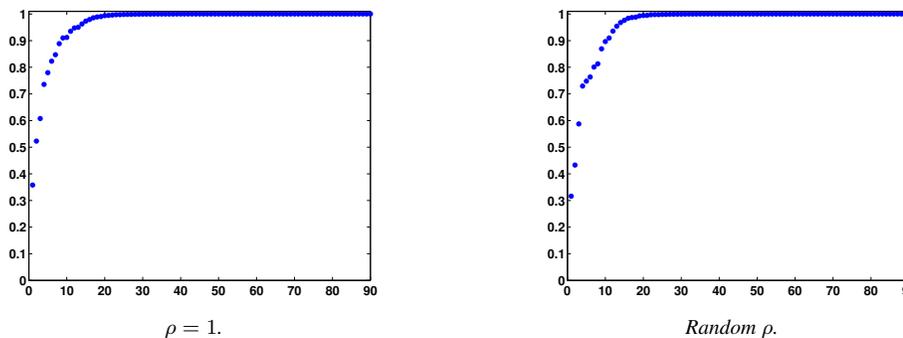


FIG. 2.4. Eigenvalues of $\check{S}_{FF}^{(i)} : \check{S}_{FF}^{(j)}\phi = \lambda S_{FF}^{(i)} : S_{FF}^{(j)}\phi$ for a face with 90 nodes of 3D problems with METIS subdomains.

region by considering the square of the $H^{1/2}(\Gamma_i)$ -norm of the extension of $u(x)$ by zero onto $F' := \Gamma_i \setminus F$; see, e.g., [21].

A reflection of the fact that $H_{00}^{1/2}$ is a true subspace of $H_0^{1/2}(F)$ is the well-known bound for finite element spaces

$$\|u_h\|_{H_0^{1/2}(F)}^2 \leq C (1 + \log(H_i/h_i))^2 \|u_h\|_{H^{1/2}(F)}^2,$$

which is known to be sharp; see [6, Lemma 4.2 and Remark 4.3] and also [26, Lemma 4.24]. It is interesting to note that this estimate gives us an estimate of the smallest non-zero eigenvalue of (2.2); we can establish that in the special case considered, this eigenvalue is proportional to $1/(1 + \log(H/h))^2$; see also [26, Subsubsection 4.6.3].

The restriction of the new term $\int_F \frac{|u(x)|^2}{d(x)} dx$ to the finite element space gives a weighted mass matrix which is spectrally equivalent to a diagonal matrix with elements varying in proportion to $1/d(x)$. This matrix is easily seen to be well approximated by a matrix of low rank since the weight function $1/d(x)$ varies between values of $2/H_i$ and of $1/h_i$. It then follows that the matrix $S_{FF}^{(i)-1}(S_{FF}^{(i)} - \check{S}_{FF}^{(i)})$ can be approximated well by a matrix of low rank.

3. Equivalence classes with three subdomain boundaries. We begin this section by considering parallel sums of more than two operators. We will work with symmetric matrices which all are at least positive semi-definite. We recall that for a pair of symmetric, positive

definite matrices A and B , their parallel sum is given by $A : B := A(A + B)^{-1}B$ or $(A^{-1} + B^{-1})^{-1}$. If $A + B$ is singular, we can work with a generalized inverse.

For three positive definite matrices, we can define their parallel sum by

$$A : B : C := (A^{-1} + B^{-1} + C^{-1})^{-1},$$

with similar formulas for four or more matrices. A quite complicated formula for $A : B : C$ is given in [25] for the general case when some or all of the matrices might be only positive semi-definite. It is also shown in [25, Theorem 3] that $A : B : C = (A^\dagger + B^\dagger + C^\dagger)^\dagger$ if and only if the three operators A, B , and C have the same range. In our context, this is not always the case since the matrix $\check{S}_{EE}^{(i)}$ defined below will be singular if Ω_i is an interior subdomain while it will be non-singular if $\partial\Omega_i$ intersects a part of $\partial\Omega$ where a Dirichlet condition is imposed. This issue can be avoided by making all operators non-singular by adding a small positive multiple of the identity to the singular operators.

As we previously have pointed out, our interest in working with parallel sums with more than two operators is inspired by Scacchi's and Zampini's success in using parallel sums of more than two operators.

We will first focus on a case of an equivalence class common to three subdomain boundaries as it arises for most subdomain edges in a three-dimensional finite element context if the subdomains are generated using a mesh partitioner. We will use the notation $S_{EE}^{(i)}$, $S_{EE}^{(j)}$, and $S_{EE}^{(k)}$ for the principal minors, of the degrees of freedom of an edge E , of the subdomain Schur complements of the three subdomains that have this subdomain edge in common. The Schur complements of the Schur complements representing the minimal energy extensions to individual subdomains of given values on the subdomain edge E will be denoted by $\check{S}_{EE}^{(i)}$, $\check{S}_{EE}^{(j)}$, etc., and are defined by

$$(3.1) \quad \check{S}_{EE}^{(i)} := S_{EE}^{(i)} - S_{E'E}^{(i)T} S_{E'E'}^{(i)-1} S_{E'E}^{(i)}, \quad \text{etc.}$$

Here $S_{E'E'}^{(i)}$ is the principal minor of $S^{(i)}$ of $\Gamma_i \setminus E$, and $S_{E'E}^{(i)}$ is an off-diagonal block.

We can now introduce the deluxe average over the edge E by

$$(3.2) \quad \bar{w}_E := \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} \left(S_{EE}^{(i)} w_E^{(i)} + S_{EE}^{(j)} w_E^{(j)} + S_{EE}^{(k)} w_E^{(k)} \right).$$

We then establish that the contribution of the subdomain Ω_i to the square of the norm of the contribution of the edge to $P_D w = w - E_D w$ is the square of the $S_{EE}^{(i)}$ -norm of

$$\left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} \left(\left(S_{EE}^{(j)} + S_{EE}^{(k)} \right) w_E^{(i)} - S_{EE}^{(j)} w_E^{(j)} - S_{EE}^{(k)} w_E^{(k)} \right),$$

which can be estimated by the sum of

$$\begin{aligned} & 3w_E^{(i)T} \left(S_{EE}^{(j)} + S_{EE}^{(k)} \right) \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} S_{EE}^{(i)} \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} \left(S_{EE}^{(j)} + S_{EE}^{(k)} \right) w_E^{(i)}, \\ & 3w_E^{(j)T} S_{EE}^{(j)} \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} S_{EE}^{(i)} \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} S_{EE}^{(j)} w_E^{(j)}, \end{aligned}$$

and

$$3w_E^{(k)T} S_{EE}^{(k)} \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} S_{EE}^{(i)} \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} S_{EE}^{(k)} w_E^{(k)}.$$

Here, we can replace $w_E^{(i)}$ by the difference $w_{E\Delta}^{(i)}$ between the original $w_E^{(i)}$ and an appropriate element in the primal space. The same shift is used to construct $w_{E\Delta}^{(j)}$ and $w_{E\Delta}^{(k)}$.

The other two subdomains also contribute terms which can be obtained from the formulas above by changing superscripts appropriately. The three terms that involve $w_{E\Delta}^{(i)}$ are

$$\begin{aligned} & 3w_{E\Delta}^{(i)T} \left(S_{EE}^{(j)} + S_{EE}^{(k)} \right) \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} S_{EE}^{(i)} \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} \left(S_{EE}^{(j)} + S_{EE}^{(k)} \right) w_{E\Delta}^{(i)}, \\ & 3w_{E\Delta}^{(i)T} S_{EE}^{(i)} \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} S_{EE}^{(j)} \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} S_{EE}^{(i)} w_{E\Delta}^{(i)}, \end{aligned}$$

and

$$3w_{E\Delta}^{(i)T} S_{EE}^{(i)} \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} S_{EE}^{(k)} \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} S_{EE}^{(i)} w_{E\Delta}^{(i)}.$$

By first adding the second and third terms and then using $A(A+B)^{-1}B = B(A+B)^{-1}A$, we find that we can write the sum of these three terms as

$$3w_{E\Delta}^{(i)T} S_{EE}^{(i)} : \left(S_{EE}^{(j)} + S_{EE}^{(k)} \right) w_{E\Delta}^{(i)}.$$

There are also two additional terms representing the squares of certain norms of $w_{E\Delta}^{(j)}$ and $w_{E\Delta}^{(k)}$. They are obtained by appropriately permuting the superscripts.

This formula represents a simplification of what was worked out in a joint paper with Beirão da Veiga et al. [4] and also in the development of the theory in a more recent paper with Dohrmann on three-dimensional problems in $H(\mathbf{curl})$; see [9]. We can now immediately obtain a bound of the square of the norm of this edge-component of $P_D w$ by

$$3 \left(w_{E\Delta}^{(i)T} S_{EE}^{(i)} w_{E\Delta}^{(i)} + w_{E\Delta}^{(j)T} S_{EE}^{(j)} w_{E\Delta}^{(j)} + w_{E\Delta}^{(k)T} S_{EE}^{(k)} w_{E\Delta}^{(k)} \right)$$

by using only that $S_{EE}^{(i)} : (S_{EE}^{(j)} + S_{EE}^{(k)}) \leq S_{EE}^{(i)}$, etc. For certain problems, e.g., those with constant coefficients in each subdomain and polyhedral subdomains, we can then obtain respectable bounds even without solving any generalized eigenvalue problems. This typically results in a bound involving a factor $C(1 + \log(H/h))$; cf. [26, Lemma 4.16]. A fully satisfactory proof of this result is given in [9].

Returning to the search for adaptive primal spaces, we note that ideally, we would now like to prove that the three operators

$$\begin{aligned} (3.3) \quad T_E^{(i)} &:= S_{EE}^{(i)} : \left(S_{EE}^{(j)} + S_{EE}^{(k)} \right), \\ T_E^{(j)} &:= S_{EE}^{(j)} : \left(S_{EE}^{(i)} + S_{EE}^{(k)} \right), \\ T_E^{(k)} &:= S_{EE}^{(k)} : \left(S_{EE}^{(i)} + S_{EE}^{(j)} \right) \end{aligned}$$

all can be bounded uniformly from above by

$$(3.4) \quad S_{EE}^{(i)} : S_{EE}^{(j)} : S_{EE}^{(k)} := \left(S_{EE}^{(i)-1} + S_{EE}^{(j)-1} + S_{EE}^{(k)-1} \right)^{-1}.$$

If this were possible, we could use that same matrix for estimates for $w_{E\Delta}^{(i)}$, $w_{E\Delta}^{(j)}$, and $w_{E\Delta}^{(k)}$. But we are not that lucky. Before we look at the details, we note that if we were to use the generalized eigenvalues obtained from two parallel sums with three Schur complements as in (3.4), we could complete our argument by noting that

$$\check{S}_{EE}^{(i)} : \check{S}_{EE}^{(j)} : \check{S}_{EE}^{(k)} \leq \check{S}_{EE}^{(i)}, \quad \text{etc.,}$$

and using similar arguments as in the previous section. Thus, a second parallel sum would be constructed by using the Schur complements of the previous Schur complements, associated with the minimal energy extension given by (3.1).

Let us now make an attempt to find a bound such as

$$S_{EE}^{(i)} : \left(S_{EE}^{(j)} + S_{EE}^{(k)} \right) \leq \text{Const. } S_{EE}^{(i)} : S_{EE}^{(j)} : S_{EE}^{(k)}.$$

The operator on the left equals

$$\left(S_{EE}^{(i)-1} + \left(S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1} \right)^{-1}$$

and the one on the right is given by (3.4). The desired inequality would hold if

$$S_{EE}^{(j)-1} + S_{EE}^{(k)-1} \leq \text{Const. } \left(S_{EE}^{(j)} + S_{EE}^{(k)} \right)^{-1},$$

but by using the eigensystem of the generalized eigenvalue problem, $S_{EE}^{(j)}\phi = \mu S_{EE}^{(k)}\phi$, we find that the best constant above would be $\max_{\mu}(\mu + 2 + 1/\mu)$. If $S_{EE}^{(i)-1}S_{EE}^{(j)}$ and $S_{EE}^{(i)-1}S_{EE}^{(k)}$ were well-conditioned, then we would obtain a good bound. In our experience, this is not at all the case for many problems.

If we like to prove a bound which does not require any additional assumptions, we have to find a different common upper bound for $T_E^{(i)}$, $T_E^{(j)}$, and $T_E^{(k)}$ defined in (3.3). This can be accomplished by using the trivial inequality

$$T_E^{(i)} \leq T_E^{(i)} + T_E^{(j)} + T_E^{(k)}, \quad \text{etc.}$$

We will therefore define our generalized eigenvalue problem as

$$(3.5) \quad \left(\check{S}_{EE}^{(i)} : \check{S}_{EE}^{(j)} : \check{S}_{EE}^{(k)} \right) \phi = \lambda \left(T_E^{(i)} + T_E^{(j)} + T_E^{(k)} \right) \phi.$$

This is the recipe that we have used in most of our numerical experiments to select primal constraints by using a selection of eigenvectors. We note that these eigenvalue problems are different from those of Section 2.2 and less attractive; see further the next section. Given the success of others with using parallel sums of each of the two sets of three Schur complements, we have also carried out experiments with that alternative generalized eigenvalue problem although we have not been able to justify this choice theoretically. We have also tested an additional alternative.

We note that in their recent paper, Kim, Chung, and Wang [12] used an approach similar to ours but using the operator

$$(3.6) \quad \begin{aligned} & S_E^{(j)} \left(S_E^{(i)} + S_E^{(j)} + S_E^{(k)} \right)^{-1} S_E^{(i)} \left(S_E^{(i)} + S_E^{(j)} + S_E^{(k)} \right)^{-1} S_E^{(j)} \\ & + S_E^{(k)} \left(S_E^{(i)} + S_E^{(j)} + S_E^{(k)} \right)^{-1} S_E^{(i)} \left(S_E^{(i)} + S_E^{(j)} + S_E^{(k)} \right)^{-1} S_E^{(k)} \end{aligned}$$

in place of our $T_E^{(i)}$, etc.

An alternative generalized eigenvalue problem could be obtained by replacing the sum on the right hand side of (3.5) by $S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)}$. Since $T_E^{(i)} \leq S_{EE}^{(i)}$, we see that we again can obtain a solid bound. But we would then be one step further away from the expression of the energy of $(P_D w)|_E$.

We can now write down a bound similar to the one of (2.3) in terms of a tolerance for the eigenvalues of (3.5) by using that

$$\check{S}_{EE}^{(i)} : \check{S}_{EE}^{(j)} : \check{S}_{EE}^{(k)} \leq \check{S}_{EE}^{(i)}, \quad \text{etc.}$$

We have the following lemma:

LEMMA 3.1. *Let λ_{tol}^E be the smallest eigenvalue of (3.5) not chosen when selecting the primal constraints for a subdomain edge E shared by three subdomains Ω_i, Ω_j , and Ω_k . We then have*

$$\|(P_D w)|_E\|_{\check{S}}^2 \leq \frac{3}{\lambda_{tol}^E} (a_i(w, w) + a_j(w, w) + a_k(w, w)),$$

where $a_i(\cdot, \cdot)$ is the bilinear form associated to (1.1) and the subdomain Ω_i , etc.

We can now combine the estimates of Lemmas 2.2 and 3.1 into what is our main theoretical result. Our result is similar to that of [12, Lemma 4.1].

THEOREM 3.2. *Assume that all subdomain edges are common to no more than three subdomains. The \check{S} -norm of the operator P_D then satisfies*

$$\|P_D w\|_{\check{S}}^2 \leq \left(\frac{2N_F^2}{\min_F \lambda_{tol}^F} + \frac{6N_E^2}{\min_E \lambda_{tol}^E} \right) \|w\|_{\check{S}}^2.$$

Here N_F is the maximum number of faces of any subdomain, and N_E is the maximum number of edges. Therefore, the condition number of the deluxe BDDC algorithm satisfies

$$\kappa \left(M_{BDDC}^{-1} \hat{S} \right) \leq \frac{2N_F^2}{\min_F \lambda_{tol}^F} + \frac{6N_E^2}{\min_E \lambda_{tol}^E}.$$

Proof. We first note that we can write $P_D w$ as the sum of the sum of $(P_D w)|_F$ over all subdomain faces of the interface Γ and the sum of $(P_D w)|_E$ over all subdomain edges of Γ . By an elementary estimate, we find that $\|P_D w\|_{\check{S}}^2$ can be bounded by 2 times the sum of the squares of the norms of the two sums. We next consider the square of the $S^{(i)}$ -norm of the sum of $(P_D w)|_F$ over the faces of Ω_i . The fact that there are at most N_F such faces introduces an additional factor N_F in front of the sum of $\|(P_D w)|_F\|_{S^{(i)}}^2$. Lemma 2.2 shows that each such term can be bounded by $\frac{1}{\lambda_{tol}^F} (a_i(w, w) + a_j(w, w))$. We find that the factor multiplying $a_i(w, w)$ is bounded by $\frac{2N_F^2}{\min_F \lambda_{tol}^F}$.

The estimate of the edge terms can be derived very similarly. The factor will be larger since we have an extra factor 3 in Lemma 3.1. \square

We note that we have found this bound to be quite pessimistic given the quadratic factors $2N_F^2$ and $6N_E^2$. A similar bound is provided in Section 3.2 for the case when the maximum number of the subdomains common to a subdomain edge equals 4; the factor 6 in the second term will be replaced by 8.

3.1. Some eigenvalue distributions. Following the example of Section 2.2, we have computed the eigenvalues of $S_{EE}^{(i)-1} (S_{EE}^{(i)} - \check{S}_{EE}^{(i)})$. The four plots provide information on the eigenvalues of the generalized eigenvalue problem defined by $S_{EE}^{(i)}$ and $\check{S}_{EE}^{(i)}$ in four different cases.

We note that while in all cases we have one eigenvalue equal to 1, the decay of the rest of the spectra is much less pronounced than for the faces. We note that a subdomain edge typically will be associated with much fewer degrees of freedom than a subdomain face and that therefore the need for a very rapid decay of these eigenvalues might be less important.

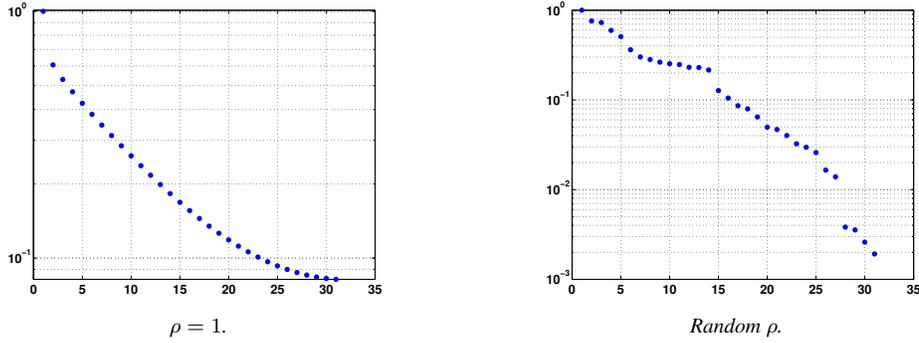


FIG. 3.1. Eigenvalues of $S_{EE}^{(i)-1}(S_{EE}^{(i)} - \check{S}_{EE}^{(i)})$ for an edge with 31 nodes of 3D problems with cubic subdomains.

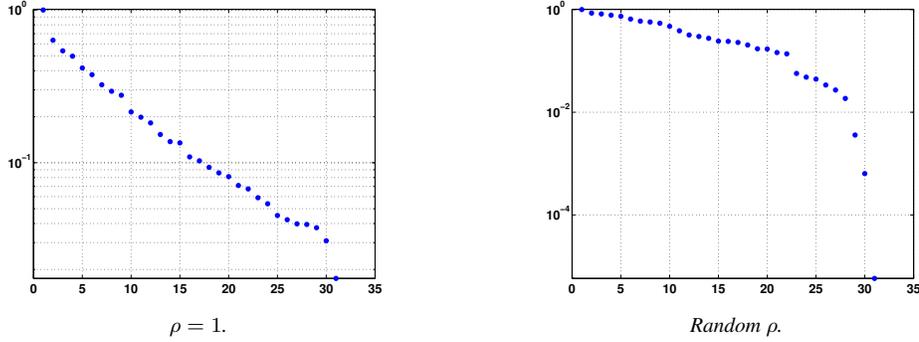


FIG. 3.2. Eigenvalues of $S_{EE}^{(i)-1}(S_{EE}^{(i)} - \check{S}_{EE}^{(i)})$ for an edge with 32 nodes of 3D problems with METIS subdomains.

3.2. Equivalence classes with four subdomain boundaries. This case very closely parallels the previous. The average defined by (3.2) is replaced by

$$\bar{w}_E := \left(S_{EE}^{(i)} + S_{EE}^{(j)} + S_{EE}^{(k)} + S_{EE}^{(\ell)} \right)^{-1} \left(S_{EE}^{(i)} w_E^{(i)} + S_{EE}^{(j)} w_E^{(j)} + S_{EE}^{(k)} w_E^{(k)} + S_{EE}^{(\ell)} w_E^{(\ell)} \right).$$

We find that the energy of $P_D w$ can be estimated by the sum of four terms, the first two of which are

$$4w_{E\Delta}^{(i)T} S_{EE}^{(i)} : \left(S_{EE}^{(j)} + S_{EE}^{(k)} + S_{EE}^{(\ell)} \right) w_{E\Delta}^{(i)}$$

and

$$4w_{E\Delta}^{(j)T} S_{EE}^{(j)} : \left(S_{EE}^{(i)} + S_{EE}^{(k)} + S_{EE}^{(\ell)} \right) w_{E\Delta}^{(j)}.$$

If a bound of $S_{EE}^{(i)}$ in terms of $\check{S}_{EE}^{(i)}$ and similar bounds for the other pairs of Schur complements were available, then we could obtain a bound right away for the BDDC algorithm, without adaption, with a factor 4. This is also an improvement as far as the constant is concerned in comparison to previous results. But here we will focus on selecting the primal constraints adaptively.

With four subdomains in the equivalence class, we use four operators

$$T_E^{(i)} := S_{EE}^{(i)} : \left(S_{EE}^{(j)} + S_{EE}^{(k)} + S_{EE}^{(\ell)} \right), \quad T_E^{(j)} := S_{EE}^{(j)} : \left(S_{EE}^{(i)} + S_{EE}^{(k)} + S_{EE}^{(\ell)} \right), \quad \text{etc.}$$

All these operators are symmetric, positive definite, and they appear directly in our estimate of the energy of $P_D w$. We can now use the trivial inequality

$$T_E^{(i)} \leq T_E^{(i)} + T_E^{(j)} + T_E^{(k)} + T_E^{(\ell)}$$

and very similar bounds for the other terms and arrive at the generalized eigenvalue problem

$$(3.7) \quad \left(\check{S}_{EE}^{(i)} : \check{S}_{EE}^{(j)} : \check{S}_{EE}^{(k)} : \check{S}_{EE}^{(\ell)} \right) \phi = \lambda \left(T_E^{(i)} + T_E^{(j)} + T_E^{(k)} + T_E^{(\ell)} \right) \phi.$$

Both operators of (3.7) are symmetric with respect to the Schur complements. What will be featured in the final bound would be the smallest eigenvalue not taken into account, i.e., with eigenvectors not associated with the primal space, and a fixed factor similar to what appears in the bounds of Lemmas 2.2 and 3.1 and Theorem 3.2.

LEMMA 3.3. *Let λ_{tol}^E be the smallest eigenvalue of (3.5) not chosen when selecting the primal constraints for a subdomain edge E shared by four subdomains $\Omega_i, \Omega_j, \Omega_k$, and Ω_ℓ . We then have*

$$\|(P_D w)|_E\|_{\check{S}}^2 \leq \frac{4}{\lambda_{tol}^E} (a_i(w, w) + a_j(w, w) + a_k(w, w) + a_\ell(w, w)),$$

where $a_i(\cdot, \cdot)$ is the bilinear form associated to (1.1) and the subdomain Ω_i , etc.

We can now combine the estimates of Lemmas 2.2 and 3.3 into what is our main theoretical result for this case.

THEOREM 3.4. *Assume that all subdomain edges are common to no more than four subdomains. The \check{S} -norm of the operator P_D then satisfies*

$$\|P_D w\|_{\check{S}}^2 \leq \left(\frac{2N_F^2}{\min_F \lambda_{tol}^F} + \frac{8N_E^2}{\min_E \lambda_{tol}^E} \right) \|w\|_{\check{S}}^2.$$

Here N_F is the maximum number of faces of any subdomain, and N_E is the maximum number of edges. Therefore, the condition number of the deluxe BDDC algorithm satisfies

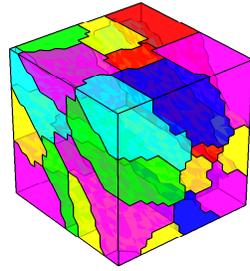
$$\kappa \left(M_{BDDC}^{-1} \hat{S} \right) \leq \frac{2N_F^2}{\min_F \lambda_{tol}^F} + \frac{8N_E^2}{\min_E \lambda_{tol}^E}.$$

The proofs of this lemma and theorem follow exactly the same lines as those of Lemma 3.1 and Theorem 3.2.

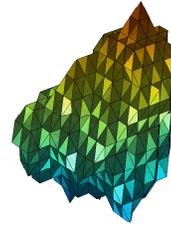
3.3. Recipes of some previous work. Several other generalized eigenvalue problems have been employed quite successful but so far lack full theoretical justifications.

Scacchi and Zampini have used what would correspond to the operators $S_{EE}^{(i)} : S_{EE}^{(j)} : S_{EE}^{(k)}$ and $\check{S}_{EE}^{(i)} + \check{S}_{EE}^{(j)} + \check{S}_{EE}^{(k)}$ or $\check{S}_{EE}^{(i)} : \check{S}_{EE}^{(j)} : \check{S}_{EE}^{(k)}$ for difficult, very ill-conditioned problems arising in isogeometric analysis. Stefano Zampini has also used $S_{EE}^{(i)} : S_{EE}^{(j)} : S_{EE}^{(k)}$ and $\check{S}_{EE}^{(i)} : \check{S}_{EE}^{(j)} : \check{S}_{EE}^{(k)}$ successfully for subdomain edges and three-dimensional $H(\mathbf{curl})$ problems; see [28]. So far, we have not found as full a justification for these recipes as for the one based on using the generalized eigenvalue problems (2.2), (3.5), and (3.7).

4. Numerical results. We present some numerical results for our adaptive BDDC deluxe algorithm. We consider a triangulation of the unit cube into tetrahedral elements and decompositions of this domain into cubic subdomains or subdomains obtained by using a METIS mesh partitioner; see Figure 4.1.

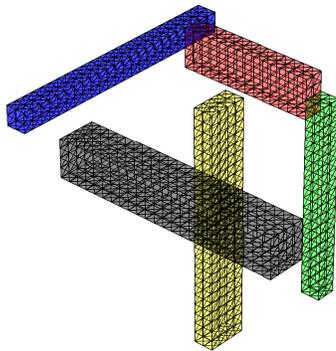


METIS decomposition.

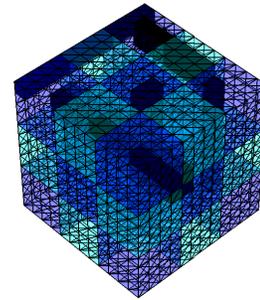


One of the METIS subdomains.

FIG. 4.1. Domain decomposition obtained by METIS for the unit cube, $N = 27$.



Channels with $\rho = 10^3$.



Coefficient distribution.

FIG. 4.2. Coefficient distribution with channels: black elements on the right have $\rho = 10^3$, and all the other elements have $\rho = 1$.

We solve the resulting linear systems with random right-hand sides using BDDC preconditioners to a relative residual tolerance of 10^{-6} . We always use a zero initial guess. The number of iterations and condition number estimates (in parentheses) are reported for each experiment.

EXAMPLE 4.1. We first consider the scalability of the BDDC deluxe algorithm for a cubic subdomain partitioning of the unit cube and for different standard choices of the primal space. The column label “Corners” represents the common choice with only primal constraints for the subdomain vertices. “Edges” adds the average over each edge to the set of primal constraints while “Edges and Faces” additionally uses the averages over each face; see Table 4.1. We then compare these results with adaptive algorithms based on generalized eigenvalue problems; see Table 4.2. The numbers in its first two columns represent the fraction of the range of the eigenvalues related to the subdomain edges that are incorporated into the primal space through their eigenvectors. Thus, given the interval between the smallest and the largest eigenvalues, we use, as primal constraints, the eigenvectors of all the eigenvalues that lie in the leftmost 5% or 50% of this interval. For the faces, we always use a fixed 5%. Finally, for the last column, “Adaptive”, we use $\lambda_{tol}^F = (1 + \log(H/h))^{-1}$, $\lambda_{tol}^E = (kH/h)^{-1}$, where k is the number of subdomains that share the edge E to select the eigenvalues. These formulas are borrowed from [12] and have allowed us to make direct comparisons with results of that study. We have also found that this recipe selects a relatively small number of effective primal constraints.

TABLE 4.1

Performance for different choices of primal constraints with $H/h = 8$ and cubic subdomains. NE is the number of subdomain edges, and DOF is the number of degrees of freedom of the problem.

ρ	N	Corners		Edges		Edges and Faces		NE	DOF
		$I(\kappa)$	$ W_{\Pi} $	$I(\kappa)$	$ W_{\Pi} $	$I(\kappa)$	$ W_{\Pi} $		
1	3^3	12(14.9)	8	12(13.9)	44	12(13.9)	98	36	15626
	4^3	17(16.6)	27	17(15.6)	135	17(15.6)	279	108	35937
	5^3	24(17.2)	64	24(16.1)	304	23(16.1)	604	240	68921
	6^3	26(17.6)	125	25(16.5)	575	25(16.5)	1115	450	117649
R	3^3	23(42.9)	8	21(39.2)	44	23(39.1)	98	36	15626
	4^3	34(77.9)	27	33(64.8)	135	37(62.3)	279	108	35937
	5^3	51(83.4)	64	48(75.5)	304	51(75.2)	604	240	68921
	6^3	68(106)	125	66(90.0)	575	61(90.0)	1115	450	117649
S	3^3	24(176)	8	24(174)	44	23(173)	98	36	15626
	4^3	37(1068)	27	37(985)	135	33(981)	279	108	35937
	5^3	60(1994)	64	59(1812)	304	55(1804)	604	240	68921
	6^3	74(2234)	125	71(2022)	575	64(2013)	1115	450	117649

TABLE 4.2

Scalability for adaptive primal constraints with $H/h = 8$ and cubic subdomains.

ρ	N	Primal 5%		Primal 50%		Adaptive	
		$I(\kappa)$	$ W_{\Pi} $	$I(\kappa)$	$ W_{\Pi} $	$I(\kappa)$	$ W_{\Pi} [f]$
1	3^3	6(1.5)	98	6(1.5)	122	8(2.2)	50 [0.6]
	4^3	6(1.5)	279	6(1.5)	333	8(2.2)	189[0.8]
	5^3	7(1.5)	604	6(1.5)	700	8(2.2)	460[0.9]
	6^3	7(1.5)	1115	7(1.5)	1265	8(2.1)	905[0.9]
R	3^3	14(5.9)	115	11(3.2)	213	10(2.5)	237[2.6]
	4^3	16(7.4)	336	13(7.3)	622	11(3.1)	746[3.0]
	5^3	19(12.1)	765	13(4.0)	1361	11(3.1)	1698[3.1]
	6^3	22(20.9)	1368	14(5.5)	2534	11(3.5)	3140[3.2]
S	3^3	9(10.5)	102	9(10.5)	119	10(10.6)	65[0.7]
	4^3	10(14.3)	285	10(13.8)	340	11(11.6)	197[0.8]
	5^3	11(15.2)	612	11(14.5)	708	11(15.2)	473[0.9]
	6^3	12(15.3)	1125	12(14.6)	1272	12(15.3)	918[0.9]

However, we note that in numerical experiments not reported here, we have found that the smallest eigenvalues of the generalized eigenvalue problems for the subdomain edges remain above a positive constant when H/h increases.

The number $[f]$ in square brackets represents the ratio of the dimension of the primal space and the total number of edges and faces. Different choices of ρ are considered in all cases: $\rho = 1$, $\rho = R$ (random values for each element), and $\rho = S$ (a distribution with rods and with jumps in the coefficients; see Figure 4.2). In the case of random values, we use a uniform distribution to pick a number r in the interval $[-3, 3]$ and then assign to each element the value 10^r .

These experiments show that the standard choices of primal constraints can fail quite badly for problems with a coefficient that varies considerably inside the subdomains. The results for the adaptive choices of primal constraints are much more satisfactory. We also find that we can have success with only a small number of primal constraints even for the

TABLE 4.3

Performance for different choices of primal constraints with $H/h = 8$ and METIS subdomains. NE is the number of subdomain edges.

ρ	N	Corners		Edges		Edges and Faces		NE
		$I(\kappa)$	$ W_{\Pi} $	$I(\kappa)$	$ W_{\Pi} $	$I(\kappa)$	$ W_{\Pi} $	
1	3^3	17(7.0)	51	16(6.4)	169	15(6.3)	268	126
	4^3	20(7.4)	164	19(6.4)	516	17(6.3)	793	389
	5^3	22(8.2)	417	25(11.2)	1265	23(11.1)	1886	951
	6^3	26(10.0)	658	28(10.1)	1977	25(9.9)	2912	1458
R	3^3	21(15.5)	51	32(44.1)	169	31(54.9)	268	126
	4^3	27(14.7)	164	46(124)	516	48(236)	793	389
	5^3	34(19.5)	417	64(384)	1265	61(383)	1886	951
	6^3	39(24.1)	658	68(108)	1977	71(242)	2912	1458
S	3^3	29(147)	51	50(173)	169	56(171)	268	126
	4^3	35(263)	164	64(242)	516	69(232)	793	389
	5^3	52(254)	417	110(1911)	1265	117(1859)	1886	951
	6^3	57(398)	658	161(1125)	1977	160(1121)	2912	1458

TABLE 4.4

Scalability for adaptive primal constraints with $H/h = 8$ and METIS subdomains.

ρ	N	Primal 5%		Primal 50%		Adaptive	
		$I(\kappa)$	$ W_{\Pi} $	$I(\kappa)$	$ W_{\Pi} $	$I(\kappa)$	$ W_{\Pi} [f]$
1	3^3	7(2.0)	252	8(2.0)	299	9(2.4)	108[0.5]
	4^3	8(1.9)	732	7(1.8)	855	9(2.4)	363[0.5]
	5^3	12(5.9)	1697	12(5.9)	1884	13(6.0)	927[0.6]
	6^3	15(5.7)	2688	14(5.7)	2967	14(5.7)	2319[0.9]
R	3^3	15(15.1)	275	12(4.9)	379	13(4.8)	264[1.2]
	4^3	16(12.9)	798	14(7.9)	1143	21(24.3)	834[1.2]
	5^3	23(15.3)	1852	19(11.8)	2607	20(13.1)	2036[1.2]
	6^3	24(16.0)	3003	22(15.7)	4216	20(15.8)	4115[1.7]
S	3^3	15(47.9)	263	14(37.8)	300	14(32.4)	143[0.6]
	4^3	20(50.8)	748	20(50.3)	864	20(31.3)	402[0.6]
	5^3	23(86.0)	1723	25(85.9)	1908	23(86.6)	981[0.6]
	6^3	33(55.0)	2710	33(55.0)	3019	35(55.0)	2379[0.6]

subdomain edges. We also note that adaptive choices of the primal constraints can result in much smaller condition numbers even for the case of a constant coefficient ρ .

EXAMPLE 4.2. We verify the scalability of our algorithm for METIS subdomains with the same coefficient distribution as in Example 4.1; see Tables 4.3 and 4.4. The results are in many cases quite similar to those for cubic subdomains.

EXAMPLE 4.3. This example is used to study the behavior of our algorithm for increasing values of H/h with 27 cubic subdomains; see Table 4.5. We find the results, all obtained with the tolerances used in the "Adaptive" columns of Tables 4.2 and 4.4, quite satisfactory.

EXAMPLE 4.4. This example is used to compare the behavior of different eigenvalue problems with 27 cubic subdomains and $H/h = 16$; see Table 4.6. Here, E_T refers to the generalized eigenvalue problem (3.7), E_{par} refers to

$$\left(\check{S}_{EE}^{(i)} : \check{S}_{EE}^{(j)} : \check{S}_{EE}^{(k)} : \check{S}_{EE}^{(\ell)} \right) \phi = \lambda \left(S_{EE}^{(i)} : S_{EE}^{(j)} : S_{EE}^{(k)} : S_{EE}^{(\ell)} \right) \phi,$$

TABLE 4.5
Results for the adaptive algorithm with 27 cubic subdomains for increasing values of H/h .

H/h	$\rho = 1$		$\rho = R$		$\rho = S$	
	$I(\kappa)$	$ W_{\Pi} [f]$	$I(\kappa)$	$ W_{\Pi} [f]$	$I(\kappa)$	$ W_{\Pi} [f]$
4	5(1.2)	62[0.7]	7(1.7)	154[1.7]	5(1.2)	62[0.7]
8	8(2.2)	50[0.6]	10(2.5)	237[2.6]	10(10.7)	65[0.7]
12	9(2.7)	50[0.6]	12(4.0)	265[2.9]	11(19.7)	89[1.0]
16	10(3.1)	50[0.6]	13(4.3)	270[3.0]	12(5.4)	60[0.7]

TABLE 4.6
Results for different eigenvalue problems with N cubic subdomains and $H/h = 8$.

ρ	N	E_T		E_{par}		E_{mix}	
		$I(\kappa)$	$ W_{\Pi} [f]$	$I(\kappa)$	$ W_{\Pi} [f]$	$I(\kappa)$	$ W_{\Pi} [f]$
1	3^3	8(2.1)	50[0.6]	8(2.1)	50[0.6]	8(2.2)	38[0.5]
	4^3	8(2.1)	189[0.8]	8(2.1)	189[0.8]	8(2.2)	141[0.6]
	5^3	8(2.1)	460[0.8]	8(2.1)	460[0.8]	8(2.2)	352[0.7]
	6^3	8(2.1)	905[0.9]	8(2.1)	905[0.9]	9(2.2)	713[0.7]
R	3^3	10(2.5)	237[2.6]	13(4.3)	71[0.8]	13(4.3)	59[0.7]
	4^3	11(7.3)	746[3.0]	15(9.6)	246[1.0]	14(4.4)	198[0.8]
	5^3	11(3.1)	1698[3.1]	16(8.8)	604[1.1]	14(4.8)	496[0.9]
	6^3	11(3.5)	3140[3.2]	18(10.3)	1158[1.2]	17(8.5)	966[1.0]
S	3^3	10(10.6)	65[0.7]	10(12.0)	57[0.7]	11(13.6)	41[0.5]
	4^3	11(11.6)	197[0.8]	14(30.0)	189[0.8]	14(29.1)	140[0.6]
	5^3	11(15.2)	473[0.9]	15(30.0)	463[0.9]	14(29.1)	354[0.7]
	6^3	12(15.3)	918[0.9]	17(30.0)	906[0.9]	16(29.4)	713[0.7]

and E_{mix} to

$$\left(\check{S}_{EE}^{(i)} + \check{S}_{EE}^{(j)} + \check{S}_{EE}^{(k)} + \check{S}_{EE}^{(\ell)} \right) \phi = \lambda \left(S_{EE}^{(i)} : S_{EE}^{(j)} : S_{EE}^{(k)} : S_{EE}^{(\ell)} \right) \phi.$$

5. Conclusions. We have developed adaptive choices for the primal spaces for BDDC deluxe methods and elliptic problems and a theoretical bound for the condition number of the preconditioned system. We have first observed that adaptivity can considerably improve the performance since classical choices with primal vertices, edge averages, and faces averages can fail in case of large variations in the coefficients; see Table 4.1 and 4.3. Second, numerical experiments show that the primal constraints related to the subdomain faces generally are easy to handle; this is supported by the discussion in Section 2.2. Therefore, the 5%-option has been used in many of the experiments resulting in just one or two constraints per face in most of the cases. For the subdomain edges, we note that there is no significant difference in the case of constant coefficients if we use 5% or 50% of the interval. For the other two cases considered, extending this interval beyond 5% can be more important; it is clear that such an increase will improve the condition number and the iteration count as illustrated in Tables 4.2 and 4.4. Here, the results in the "Adaptive" column show that we can keep the primal space small.

As we have already observed, the tolerances used for subdomain faces and edges seem to work well since they produce small primal spaces with good condition numbers. In most of the cases, the ratio between the dimension of the primal space and the total number of edges and faces $[f]$ is smaller than 1, which means that, on average, we use fewer than one constraint

per subdomain face/edge. Finally, Table 4.6 exemplifies that different eigenvalue problems considered by others can have a similar performance as ours.

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