ITERATIVE SUBSTRUCTURING METHODS FOR SPECTRAL ELEMENTS IN THREE DIMENSIONS

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Abstract. Iterative substructuring methods form an important family of domain decomposition algorithms for elliptic finite element problems. The p-version finite element method based on continuous, piecewise Q_p functions is considered for second order elliptic problems in three dimensions; this special method can also be viewed as a spectral element method. An iterative method is designed for which the condition number of the relevant operator grows only in proportion to $(1 + \log p)^2$.

Key words. p-version finite elements, spectral approximation, domain decomposition, iterative substructuring

AMS(MOS) subject classifications. 41A10, 65N30, 65N35, 65N55

1. Introduction.

Domain decomposition has developed into an active research area over the last few years; a seventh, annual, international symposium is being held October 27-30, 1993 at The Pennsylvania State University; cf. [17,7,8,18,9,21].

The iterative substructuring methods form an important family of domain decomposition methods for elliptic problems. They are based on a decomposition of the given region into nonoverlapping subregions, and as all other domain decomposition methods, provide preconditioners for conjugate gradient type methods. The preconditioners are constructed from solvers for local problems and, in addition, a solver of a coarse problem similar to that used in a multi-grid algorithm. However, the global, coarse problem can be quite exotic; cf. e.g. Dryja, Smith, and Widlund [11].

When an iterative substructuring method is used, data is only exchanged between neighboring local problems through their boundary values. In this they differ from the Schwarz methods that use overlapping subregions; cf. e.g. Dryja and Widlund [13,15] for a discussion of recent work on this other major family of methods.

All these iterative methods are thus two-level methods and convincing arguments have been put forward supporting the opinion that they are particularly well suited for the large, relatively loosely coupled computing systems that are becoming increasingly common; cf Gropp [19]. The best of these algorithms have proven quite powerful and very large and very ill-conditioned systems of linear algebraic equations, arising when elliptic problems are discretized by finite elements and finite differences, have been solved quite economically; cf. e.g. Gropp and Smith [20] and Smith [33].

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A well known bound on the error, after k steps, of the standard preconditioned conjugate gradient method is given by the formula

$$2(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1})^k \text{ where } \kappa = \frac{\lambda_{max}(B^{-1}A)}{\lambda_{min}(B^{-1}A)}.$$

Here A is the coefficient matrix of the original system, and B that of the preconditioner. Therefore, the principal goal of domain decomposition theory is to provide a good upper bound on the condition number of the preconditioned operator.

Earlier work on iterative substructuring methods focused on the h-version finite element methods; see e.g. Bramble, Pasciak, and Schatz [5], Dryja [10], Dryja and Widlund [12], and Smith [31,32,33] for work on three-dimensional elliptic problems. A recent paper by Dryja, Smith, and Widlund [11] summarizes our knowledge of the h-version case. The best of these results show that the condition number of the relevant preconditioned operator grows only linearly with the logarithm of the number of degrees of freedom of an individual subregion. It is important to note that these bounds are independent of the number of subproblems and that they are independent of jumps in the coefficients across subregion boundaries. We also note that there are considerable differences between good iterative substructuring algorithms for two and three dimensional problems; some algorithms that are successful for problems in two dimensions are quite mediocre in three.

The development of iterative methods for higher order and spectral methods poses a special challenge since the stiffness matrices can be much more ill conditioned than for lower order methods. The domain decomposition methods that have been proposed are also less well understood. Since the number of degrees of freedom per element increases rapidly with p, it is natural to use individual elements as subregions to be assigned to individual processors of a parallel computing system. In this paper, we design an algorithm for which we have been able to establish a polylogarithmic bound in the degree p of the spectral elements. We note that the method developed here is directly inspired by a method developed by Barry Smith [32,33] for the h-version.

Important progress has previously been reported, for problems in two dimensions, in Babuška, Craig, Mandel, and Pitkäranta [1], in which polylogarithmic bounds for some methods are proved; see also Pavarino [27] for results in two dimensions, which are similar to those of this paper. In three dimensions, pioneering work has been carried out by Jan Mandel [25,24,23,26]. His algorithms, which use global spaces which differ from ours, have also been implemented in industrial software. A number of domain decomposition methods for spectral elements have been considered by Fischer and Rønquist [16] and Rønquist [29,30]; for a general introduction to spectral element methods, we refer to Maday and Patera [22] and to Bernardi and Maday [4]. However, we know of no previous theoretical results that show only polynomial growth, in $\log p$, for problems in three dimensions. We note that other domain decomposition algorithms for higher order methods, based on overlapping subregions, have been considered in Pavarino [28,27].

We note that it is known that certain collocation methods result in coefficient matrices which are spectrally equivalent to the stiffness matrices derived from the

Galerkin procedure considered here; cf. Bernardi and Maday [4]. It therefore appears likely that our algorithm could be of use for collocation problems as well.

2. The elliptic problem and block-Jacobi methods. We consider a linear, elliptic problem on a bounded domain $\Omega \subset R^3$ formulated variationally as

$$a(u,v) = \int_\Omega \rho(x) \nabla u \cdot \nabla v \, dx \quad = \quad f_\Omega(v), \; \forall \; v \in \; V.$$

V is an appropriate subspace of $H^1(\Omega)$. $\rho(x) > 0$ can be discontinuous, with very different values for different subregions, but we allow this coefficient to vary only moderately within each subregion Ω_i. In fact, without decreasing the generality of our results, we will only consider the piecewise constant case of $\rho(x) = \rho_i, x \in \Omega_i$.

The region is the union of elements, which are cubes or images of a reference cube under reasonably smooth mappings; no element can be "too distorted". Almost all our technical work can in fact be carried out on a single reference cube.

The discrete space $V^p \subset V$ is the space of continuous, piecewise Q_p elements. This is a conforming Galerkin method; the finite element problem is obtained by restricting u and the test functions to the space V^p. The finite element solution is a projection of the exact solution onto the finite element space; the projection is orthogonal with respect to the bilinear form $a(\cdot,\cdot)$.

The finite element variational problem is turned into a linear system of algebraic equations, $Kx = b$, in the usual way. Here K is the stiffness matrix, and b the load vector. $K^T = K > 0$, a property inherited from the bilinear form $a(\cdot,\cdot)$.

Here we view our iterative substructuring method as a block-Jacobi/conjugate gradient method; cf. Dryja and Widlund [15]. The stiffness matrix K is preconditioned by a matrix K_J, which is the direct sum of diagonal blocks of K. We can also replace some of these blocks by spectrally equivalent (or almost spectrally equivalent) block matrices in an attempt to speed up the computation. However, to arrive at a successful method, we must first carry out a suitable change of basis and select the blocks carefully. Each block of the Jacobi splitting corresponds to a set of degrees of freedom that define a subspace V_i. In the case considered, the space V^p is the direct sum of these subspaces.

Block-Jacobi methods such as these can also be viewed differently. For each subspace V_i, we introduce an orthogonal projection P_i given by

$$a(P_i u, v) = a(u,v), \quad \forall v \in V_i, \quad u \in V^p,$$

or an approximation thereof, defined by a different inner product,

$$\tilde{a}_i(T_i u, v) = a(u,v), \quad \forall v \in V_i, \quad u \in V^p.$$

In a simple case, when a subspace corresponds to a set of adjacent degrees of freedom of a finite element scheme, P_i simply corresponds to the inverse of the relevant diagonal block of K, padded with zero blocks, times K; the sum of these operators represents $K_J^{-1}K$. To obtain T_i, the special block of K is replaced by an approximate solver for

the given operator restricted to the subregion. We will see that our successful method results from selecting one of the subspaces quite differently from that of this simple example.

The spectrum relevant for this iterative method is that of the operator

$$T = \sum_{i=0}^{N} T_i.$$

The eigenvalues of $K^{-1}K_J$, which are identical to those of the inverse of the operator T, are given in terms of the Rayleigh quotient

$$\frac{\sum_{i=0}^{N} \tilde{a}_i(u_i, u_i)}{a(u,u)}, \quad u = \sum_{i=0}^{N} u_i, \quad u_i \in V_i.$$

Providing an upper bound of this Rayleigh quotient is the most challenging part of our work. Success is tied to estimating the approximate energies $\tilde{a}_i(u_i, u_i)$ uniformly, or almost uniformly, in terms of the strain energy $a(u,u)$. An upper bound on $a(u_i, u_i)/\tilde{a}(u_i, u_i), u_i \in V_i$, also enters the bound on $\kappa(K_J^{-1}K)$ if inexact solvers are used for some or all of the subspaces.

In this study, we use the block-Jacobi framework but there is also a more general theory; cf. Dryja and Widlund [14]. Thus, any block-Jacobi method can be viewed as an *additive Schwarz* method based on a direct sum of subspaces. There are also Gauss-Seidel-like, *multiplicative*, as well as *hybrid Schwarz* algorithms; cf. Dryja, Smith, and Widlund [11] for a general discussion.

3. A choice of subspaces. A method of this kind is primarily defined by a set of subspaces; the mathematical description of the method is complete when, in addition, the bilinear forms $\tilde{a}_i(\cdot,\cdot)$ have been specified. In designing methods, we can learn from the h-version case. The first lesson is that we cannot obtain a good bound if $V_0 = Q_1$ and the elements of the other subspaces all vanish at the vertices of the elements. We must then choose $u_0 \in V_0$ in the decomposition, $u = \sum u_i$, as the interpolant onto V_0. In three dimensions, the norm of this interpolant can be much larger than the norm of u itself and any upper bound on the Rayleigh quotient must be disappointing. This point is discussed in detail in Dryja, Smith, and Widlund [11] where remedies, and their consequences, are discussed for the piecewise linear case.

As in the case of h-finite elements, we consider several important geometric objects: *interiors, faces, edges*, and *vertices.* The subspaces will be directly related to them. For higher order methods this is most natural. For whatever choice of the basis functions, we find each of them naturally associated with one of these objects; cf. e.g. Babuška, Griebel, and Pitkäranta [2]. We will merge the edges and vertices of the individual elements, creating *wire baskets* $\mathcal{W}_i$, and use a related *wire basket based* space V_0.

Let Ω_i denote the elements of the partitioning of the given region Ω. Our new method is based on the following subspaces: (some further details are given in the next section)

• An interior space for each element: $Q_p \cap H_0^1(\Omega_i)$.

• A space for each face. These functions vanish on and outside the boundary of $\Omega_{ij} = (\Omega_i \cup \Gamma_{ij} \cup \Omega_j)$. Here the two elements share a common face; $\overline{\Gamma}_{ij} = \overline{\Omega}_i \cap \overline{\Omega}_j$. Since it is crucial to have a good recipe for the extension of the values on the designated face to the interior of the two relevant elements, we use the minimal energy (discrete harmonic) extension.

• A coarse, global space, V_0, of piecewise discrete harmonic functions, is associated with the wire baskets of the elements. Its elements are defined solely by their values on the wire baskets. A central issue is how to define the values on the faces. Once the face values are given, we use a discrete harmonic extension to the interiors of the elements. It is known from the work on the h-version that it is crucial to include the constants in this coarse, global space. We must therefore make sure that an element of V_0, which takes on a constant value on the wire basket of an element, takes on the same value everywhere in the element. This is explained further in the next section.

For the subspace V_0, we use a simple bilinear form,

$$\tilde{a}_0(\cdot,\cdot) \;=\; \sum_i \rho_i \inf_{c_i} \|u - c_i\|^2_{L_2(\mathcal{W}_i)},$$

This leads to a coarse problem with only one essentially global degree of freedom, c_i, per element. These values are found by solving a linear system of finite difference type. In addition, a larger linear system with a convenient diagonal matrix is solved to find all the values on the wire basket.

A complete proof of the following result will be given in a later paper.

THEOREM 1. *For the iterative substructuring method just introduced,*

$$\kappa(T) \leq const.(1 + \log p)^2.$$

Here the constant is independent of the number of elements, their diameters, the degree p, and the size of the jumps of the coefficient $\rho(x)$ across element boundaries.

4. Bases for the subspaces. We will not provide a proof of our main result in this paper but we will introduce the bases of the subspaces which both define our method and are central in our proof. Some of our technical tools come from a paper by Canuto and Funaro [6], but several appear to be new. As in the the h-version case, extension theorems play an important role; cf. also Babuška, Craig, Mandel, and Pitkäranta [1] and Bernardi and Maday [3].

As has been shown by Bramble, et al., and has been clearly explained by Mandel, we can carry out the analysis locally, one element at a time. Thus, the analysis can be reduced to studying a preconditioner for the Neumann problem on a single subregion; see also Dryja, Smith, and Widlund [11]. We can therefore work exclusively on the unit cube $[-1,+1]^3$. The subproblem on the cube, which corresponds to the restriction of the global subspace, must have the same null space as the local finite element problem to make bounds that are independent of the number of subregions possible; cf. Dryja, Smith, and Widlund [11].

It is quite clear from the work of Babuška, Griebel, and Pitkäranta [2], Babuška, Craig, Mandel, and Pitkäranta [1], and others that the choice of bases for the different subspaces is most crucial for p-version finite element methods and in the design of good preconditioners. Our subspaces are constructed from several sets of basic functions defined on the interval $[-1,+1]$. They replace, in a very natural way, the sine and linear combinations of pairs of exponential functions used when solving Laplace's equation in a cube by the method of separation of variables. We denote by P_0^p the space of degree p polynomials that vanish at the ends of the interval. We use:

• A set of eigenfunctions and eigenvalues, $\Phi_i \in P_0^p$ and $\lambda_i, i = 1, \cdots, p-1$, defined by

$$\int_{-1}^{1} \frac{d\Phi_i(x)}{dx} \frac{dv(x)}{dx}\, dx = \lambda_i \int_{-1}^{1} \Phi_i(x) v(x)\, dx, \quad \forall v \in P_0^p.$$

We normalize these functions to have unit H^1-norm. We also use:

• Two sets of degree p polynomials, equal to one at 1 and zero at -1, defined by

$$\int_{-1}^{1} \frac{d\varphi_i(x)}{dx} \frac{dv(x)}{dx}\, dx + \frac{\lambda_i}{2} \int_{-1}^{1} \varphi_i(x) v(x)\, dx = 0, \quad \forall v \in P_0^p,$$

and

$$\int_{-1}^{1} \frac{d\varphi_{i,j}(x)}{dx} \frac{dv(x)}{dx}\, dx + (\lambda_i + \lambda_j) \int_{-1}^{1} \varphi_{i,j}(x) v(x)\, dx = 0, \quad \forall v \in P_0^p.$$

These functions are different from the sine and exponential functions used in the continuous case in several ways; e.g. λ_{p-1} grows approximately as $Cp^{3.5}$, not as Cp^2. We note that similar sets of functions are used in the work of Babuška, Griebel, and Pitkäranta [2] and Canuto and Funaro [6].

In addition, we use:

• The degree p polynomial φ_0 that solves

$$\min \|\varphi\|_{L_2(-1,1)},\ \varphi(1) = 1,\ \varphi(-1) = 0.$$

We are now ready to describe our subspaces. We note that all of them, except the first, consist of discrete harmonic functions.

• The *interior basis functions* are defined by

$$\Phi_i(x)\Phi_j(y)\Phi_k(z), \quad i,j,k = 1, \cdots, p-1.$$

They are $a(\cdot,\cdot)-$ and L_2-orthogonal.

• The *face basis functions* are given by

$$\Phi_i(x)\Phi_j(y)\varphi_{i,j}(z), \quad i,j = 1, \cdots, p-1,$$

for the face defined by $z = 1$.

The wire basket space is given in terms of edge and vertex basis functions. As we will see, the elements of the subspace spanned by these functions are later "corrected" so that they also contain certain components from the face spaces.

- The *edge basis functions* are given by

$$\varphi_i(x)\varphi_i(y)\Phi_i(z), \quad i = 1, \cdots, p-1,$$

for the edge defined by $x = 1, y = 1$.

- One of the eight *vertex basis functions* is given by

$$\varphi_0(x)\varphi_0(y)\varphi_0(z).$$

Six special functions $\kappa_k(x, y, z)$ are now constructed. Each of them belongs to one of the face spaces; each of them vanishes on five of the faces. They are defined in terms of their sum

$$\kappa(x, y, z) = \sum_{k=1}^{6} \kappa_k(x, y, z).$$

In turn, $\kappa(x, y, z)$ is the difference between the constant function 1 and the unique element in the space spanned by the edge and vertex basis functions that equals 1 on the wire basket.

An element in the final *wire basket space* is now obtained by first matching given values on the wire basket with a function in the space of edge and vertex basis functions. We then add six terms which are the products of the averages, of the given function, over the boundary of the kth face and $\kappa_k(x, y, z)$. This process defines an interpolation operator; the range of it defines the wire basket space. It is important to note that this operator has been constructed so that it reproduces constants exactly. The null space condition mentioned previously is therefore fulfilled.

5. A numerical study of the condition number. As we have previously pointed out, an upper bound for the condition number of the whole problem can be obtained by considering a preconditioner for a Neumann problem on the reference element. Thus it becomes possible to compute this bound from the eigenvalues of a matrix pencil defined by the contributions from an individual element to the stiffness matrix and to the preconditioner. Both these matrices are singular and have the same null space; only the space orthogonal to this one dimensional space is relevant in our analysis. We have carried out a series of MATLAB 4.0 experiments, which closely parallel those of Smith [33] for the case of piecewise linear elements. In our table, S denotes the part of the stiffness matrix which is attributable to the discrete harmonic part of the space. This is the only part of the matrix that is relevant. M is its preconditioner. It follows from standard theory for iterative substructuring methods that $\kappa(M^{-1}S)$ provides an upper bound for the condition number of the entire preconditioned operator.

It is interesting to note that the condition number estimates obtained in this way quite closely approach those obtained by Smith [33] for h-version problems, with the same number of degrees of freedom, as the size of the local problem increases. Thus, for the cases which correspond to $p = 7, 8$ and 9, Smith reports condition numbers of $15.86, 17.59$ and 19.23, respectively.

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Local condition numbers

p	3	4	5	6	7	8	9	10	11
$\kappa(M^{-1}S)$	7.21	9.98	12.08	14.20	15.96	17.74	19.23	20.79	22.08
λ_{max}	1.84	1.95	1.98	2.02	2.04	2.06	2.07	2.08	2.09
λ_{min}	0.255	0.196	0.164	0.142	0.128	0.116	0.108	0.100	0.095