ENERGY OPTIMIZATION OF ALGEBRAIC MULTIGRID BASES*

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Abstract. We propose a fast iterative method to optimize coarse basis functions in algebraic multigrid by minimizing the sum of their energies, subject to the condition that linear combinations of the basis functions equal to given zero energy modes, and subject to restrictions on the supports of the coarse basis functions. The convergence rate of the minimization algorithm is bounded independently of the meshsize under usual assumptions on finite elements. The first iteration gives exactly the same basis functions as our earlier method using smoothed aggregation. The construction is presented for scalar problems as well as for linear elasticity. Computational results on difficult industrial problems demonstrate that the use of energy minimal basis functions improves algebraic multigrid performance and yields a more robust multigrid algorithm than smoothed aggregation.

1. Introduction. This paper is concerned with aspects of the design of Algebraic Multigrid Methods (AMG) for the solution of symmetric, positive definite linear algebraic systems arizing from finite element discretization of elliptic boundary value problems. Multigrid methods achieve their efficiency through the complementary effects of smoothing by relaxation and the coarse level correction, using a hierarchy of coarse meshes. Unlike classical, geometrical multigrid, where the fine meshes are obtained by successive refinement of a given coarse mesh, algebraic multigrid strives to build artificial coarse spaces and the associated operators from a matrix associated with a given fine mesh. For further general information, see, e.g., [3, 10, 13, 15, 17, 27].

First generation multigrid convergence theories [1, 2, 9] were based mainly on the concept of approximation properties between the grids and elliptic regularity. Early in multigrid history, it was recognized that a class of multigrid algorithms can be seen as a successive minimization of the energy in a set of directions consisting of coordinate vectors on the finest grid and of directions given by coarse grid coordinate vectors, transferred via interpolation onto the finest grid [14]. A similar idea has become the background for a new generation of multigrid theory based on energy estimates for successive subspace corrections [4]; see also [3, 28] for overview of related results and relations to domain decomposition methods. In this approach, the role of approximation properties is lessened and an important place is taken by an upper bound on the energy of the basis functions in the grids hierarchy.

The classical approach to the design of algebraic multigrid methods [5, 8, 16, 17] has been to attempt to have the intergrid transfer operators possess approximation properties similar to geometric multigrid. In [22, 23], we have proposed an alternative set of objectives, which includes

- *minimization of energy:* the basis functions on the coarse levels should have as small energy as possible;

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- *preservation of nullspace:* the span of basis functions on each coarse level should contain zero energy modes, at least away from the boundary; and
- *limited overlap:* the supports of the basis functions on the coarse levels should overlap as little as possible, or, equivalently, the system matrices on the coarse levels should have as few nonzero entries as possible.

These objectives are then used to build coarse space basis functions, or, equivalently, the prolongation operators. The objectives were motivated by the multigrid theory of [4], recognition of the need to represent zero energy modes in the coarse space exactly [11, 12], and early work on algebraic multigrid with prolongations by smoothed aggregation [18, 19].

In [6, 22, 23, 24], we have proposed the prolongation by smoothed aggregation as an attempt to satisfy the above objectives approximately. The energy of the basis functions - and convergence of the resulting multigrid method - can be further improved by more smoothing of the coarse basis functions, but at the cost of increasing their supports, and thus the number of nonzeros in coarse level matrices and the computational complexity of the multigrid algorithm [6, 20, 24]. An efficient method to reduce the energy of the coarse basis functions without increasing their supports has been therefore of interest.

Another way to satisfy the above objectives is to set up a minimization problem and to define coarse basis functions as its solution. The issues are then the properties of such coarse basis functions, and how to compute them efficiently. Construction of basis function by minimization of the quadratic function equal to the sum of their energies, subject to the constraint that the basis functions sum up to a constant, was proposed in [25] and further developed in [7, 26]. The constrained minimization problem was solved by Lagrange multipliers. In [26], it was proved that in one dimension, the resulting multigrid method has convergence rate independent of jumps in coefficients and mesh size, the performance of such method for oscilatory and discontinuous coeffients in two dimensions was investigated numerically, and it was demonstrated that, in some cases, the coarse basis functions obtained from energy minimization coincide with standard finite element basis functions.

In this paper, we present a general approach to building coarse basis functions by the minimization of the sum of their energies, subject to the condition that their linear combinations equal to given zero energy modes, and subject to restrictions on their supports. We develop a fast projected gradient descent algorithm for the solution of the minimization problem, and prove that its convergence rate is bounded independently of the meshsize under usual assumptions on finite elements. The first iteration of the projected gradient descent algorithm coincides with our earlier smoothed aggregation method. The construction and the algorithm are presented here for scalar as well as vector problems, such as linearized elasticity. In the scalar case, our abstract minimization problem essentially reduces to that of [25]. Our algorithm for its solution as well its application to basis functions derived from aggregation are different.

Our computational results show that in many situations, the first iteration of the minimization algorithm, that is, smoothed aggregation, results in a quite acceptable algebraic multigrid method already and additional iterations have only marginal effect. But additional iterations of the energy minimization algorithm make the multigrid method more robust and result in an improvement in multigrid performance for difficult problems, especially in the case of vector problems, such as elasticity. To approximate minimization of the maximum of the energies of the coarse basis

functions, we have tried to minimize also the sum of powers of order p of the energies, $p > 1$. This, however, did not yield an additional benefit.

In Sec. 2, we recall the matrix notation used here. Algebraic multigrid with coarse bases by smoothed aggregation is summarized in Sec. 3. For ease of exposition, the new method is first presented in Sec. 4 for the scalar case and with some simplifications. The minimalization algorithm in the general case, including vector problems and preconditioning, is given in Sec. 5. The choice of the initial approximation and application to algebraic multigrid in specific situations is discussed in Sec. 6. Finally, Sec. 7 contains computational results and Sec. 8 our conclusions.

2. Notation. For a matrix $M = (m_{ij})$, denote by m_{*k} and m_{k*} the k-th column and row, respectively. If the matrix M has a block structure, M_{*k} and M_{k*} are the k-th block column and row, respectively. For a square matrix M, $\mathrm{tr}(M)$ is its trace and $\mathrm{diag}(M) = \mathrm{diag}(m_{ii})$ is the diagonal matrix with the same diagonal elements as M. For a collection of matrices $\{D_k\}$, $\mathrm{diag}(D_k)$ is the block diagonal matrix with D_k as diagonal blocks.

For two matrices X and Y of the same dimensions, define the term-by-term product $X * Y(x_{ij}y_{ij})$ and the Frobenius matrix inner product

$$(X, Y) = \sum_{i,j} x_{ij}y_{ij} = \mathrm{tr}(X^t Y).$$

The associated Frobenius matrix norm is $\|X\| = (X, X)^{1/2}$. If D is symmetric, positive definite matrix, we define the matrix inner product $(X, Y)_D = (DX, Y)$.

The symbol $\mathbb{M}^{m\times n}$ will denote the space of all $m \times n$ real matrices. The canonical unit vectors in $\Re^n$ are denoted by e_i and $\mathbf{1}$ is the vector of all ones.

We will use matrix-to-matrix mappings, with the notation like $Z : P \mapsto Q$ or $Z(P) = Q$. We will always enclose the argument of a matrix-to-matrix mappings in parentheses because application of a matrix-of-matrix map and multiplication of matrices do not commute, $Z(AB) \neq Z(A)B$. Composition of matrix-to-matrix mappings will be denoted by $\circ$, as in $(W \circ Z)(P) = W(Z(P))$. We believe that the matrix-to-matrix mapping notation makes the paper easier to read than if the tensor notation was used.

The spectral radius of M is $\rho(M)$, and M^+ denotes the Moore-Penrose pseudoinverse of M.

3. Algebraic multigrid by smoothed aggregation. We briefly recall the concept of smoothed aggregation prolongators as we have previously applied it to solving a system of algebraic equations

$$Ax = b, \tag{3.1}$$

where A is the $n \times n$ symmetric positive definite matrix arising from a finite element discretization of the second order elliptic problem. For simplicity, consider the model problem

$$a(u, v) \equiv \int_\Omega \alpha(x)\,\mathrm{grad}\,u\,\mathrm{grad}\,v\;dx = \int_\Omega fv\;dx + \int_{\partial\Gamma_N} gv\;ds \tag{3.2}$$

$\alpha(x) > 0$ in Ω, discretized by P1 or Q1 conforming Lagrange elements, and assume that the finite element basis $\{\varphi_i\}$ is scaled so that

$$\|\varphi_i\|_{L^\infty(\Omega)} = 1. \tag{3.3}$$

On input, our method requires the system of algebraic equations (3.1), the set of functions which are to be captured precisely on the coarse level, and the system $\{\mathcal{A}_i\}_{i=1}^m$ of node aggregates forming a disjoint covering of the set of all unconstrained nodes,

$$\bigcup_{i=1}^{m} \mathcal{A}_i = \{1, \ldots, n\}, \quad \mathcal{A}_i \cap \mathcal{A}_j = \emptyset \text{ for } i \neq j. \tag{3.4}$$

Let the set of functions we want to be represented exactly by the coarse space functions be denoted by $\{b^i\}_{i=1}^{n_k}$. For the model problem, $n_k = 1$ and b^1 is the constant function. Thus, assuming the scaling (3.3), the discrete representation of b^1 with respect to the finite element basis is i$\mathbf{1}$. The tentative prolongator is now defined by

$$\hat{P}_{ij} = \begin{cases} 1 & \text{if } i \in \mathcal{A}_j \\ 0 & \text{otherwise.} \end{cases}$$

(See Sec. 6 of this paper and [21] for the construction in the general case.) In order to eliminate high energy components from the range of $\hat{P}$, we introduce an $n \times n$ *prolongator smoother* $\mathcal{S}$ and define the final prolongator P by

$$P = \mathcal{S}\hat{P}, \tag{3.5}$$

where $\mathcal{S} = q(D^{-1}A)$, D is symmetric positive definite and q is a polynomial such that $q(0) = 1$.

The energy of the discrete coarse level function $\Phi_i = \mathcal{S}\hat{P}e_i$, can be bounded by

$$\langle \Phi_i, \Phi_i \rangle_A = \langle p^2(A)A\hat{P}e_i, \hat{P}e_i \rangle \leq \varrho(p^2(A)A)\langle \hat{P}e_i, \hat{P}e_i \rangle.$$

cf., [21]. The polynomial q is then chosen to minimize an estimate of $\varrho(q^2(A)A)$. This corresponds to minimizing the maximum of the energies of the coarse basis functions. In this paper, we advocate minimization of the the quadratic functional equal to the sum of the energies of the coarse basis functions. This functional is easier to minimize, and in the practically important case $\deg q = 1$, the first step of the projected descent method for its minimization will be seen to give exactly the same result as (3.5). We will also investigate the minimization of $\sum_i \langle \Phi_i, \Phi_i \rangle_A^p$, $p > 1$, to approximate the minimization of $\max_i \langle \Phi_i, \Phi_i \rangle_A$.

The prolongation operator based on the technique of smoothed aggregation yields very good convergence properties of the multigrid method, but it leads to increased computational complexity for small aggregates and high degree of $\mathcal{S}$. In the case of coarsening by a factor of about 3 in each direction [23], one is forced to use a smoother $\mathcal{S}$ of degree 1 in order to assure sparsity of the coarse level matrices. Minimizing energy of the coarse space basis functions without the penalty of increased computational complexity is the subject of this paper.

4. Coarse bases by minimization of energy: Simple case. In this section, we consider the scalar problems such as (3.2). Although Section 4 also covers this case, this will allow us to explain more clearly the main idea unobscured by technical details.

Let $N = (n_{ij}) \in \mathbb{M}^{m \times n}$ be a given 0-1 matrix corresponding to the nonzero structure of the sought prolongator P: $n_{ij} = 0 \Longrightarrow p_{ij} = 0$, and define the space

$$\mathcal{N} = \{P \in \mathbb{M}^{n \times m} : p_{ij} = 0 \text{ if } n_{ij} = 0\}$$

equipped with the Frobenius matrix inner product (P,Q). Note that $\mathcal{N} = \{P \in \mathbb{M}^{n\times m} : N * P = P\}$, and $(S, N * Q) = (N * S, Q)$ for all S and Q.

We will construct our prolongator to satisfy the general requirements postulated in [23], cf. the summary in Section 1.

Our first requirement is that the coarse space basis reproduces zero modes of the bilinear form. In the scalar case, the modes are constants, which means that $\sum_i P_{ij} = 1$ for all j such that node j and its neighbors do not have a Dirichlet constraint. The selection is implemented by the $0-1$ vector $F = (f_i)$, Vector F will be used for identification of strictly interior nodes: we will set

$$\left.\begin{array}{ll} f_i = 0 & \text{if node } i \text{ belongs to element with Dirichlet constraint} \\ f_i = 1 & \text{otherwise} \end{array}\right\} \tag{4.1}$$

The energy of the i-th coarse-space basis function equals $\langle APe_i, Pe_i\rangle = p_{*i}^t A p_{*i}$. We will minimize the sum of the energies

$$J(P) = \frac{1}{2}\sum_i p_{*i}^t A p_{*i} = \frac{1}{2}(P, AP) \to \min \tag{4.2}$$

subject to

$$\left.\begin{array}{l} P \in \mathcal{N} \\ \sum_j p_{ij} = 1 \quad \text{if } f_i = 1, \end{array}\right\} \tag{4.3}$$

cf., [25]. Since A is symmetric positive definite, this problem has a unique solution, which we denote by P^*. Define the subspace $\mathcal{Z} \subset \mathcal{N}$ by

$$\begin{aligned} \mathcal{Z} &= \{Q_1 - Q_2 \mid Q_1, Q_2 \text{ satisfy (4.3)}\} \\ &= \{Q \in \mathcal{N} \mid \sum_j q_{ij} = 0 \quad \text{if } f_i = 1\}. \end{aligned}$$

To write an iterative method for the solution of the problem (4.2), (4.3), we will need the gradient of $J(P)$ in the space $\mathcal{N}$ and the orthogonal projection onto $\mathcal{Z}$.

LEMMA 4.1. *The gradient of the functional J in the space $\mathcal{N}$ is*

$$\operatorname{grad}_{\mathcal{N}} J(P) = N * (AP).$$

Proof. The gradient is defined by

$$J(P + tQ) = J(P) + t(Q, \operatorname{grad}_{\mathcal{N}} J(P)) + o(t), \quad t \to 0, \quad \forall Q \in \mathcal{N}.$$

Since

$$\frac{1}{2}(P + tQ, A(P + tQ)) = \frac{1}{2}(P, AP) + t\,(Q, AP) + o(t) \quad t \to 0,$$

it holds that $(Q, \operatorname{grad}_{\mathcal{N}} J(P)) = (Q, AP) = (Q, N * (AP))$, for all $Q \in \mathcal{N}$. □

LEMMA 4.2. *The orthogonal projection in $\mathcal{N}$ onto $\mathcal{Z}$ is $Z : S \mapsto Q$, where*

$$q_{ij} = s_{ij} - f_i \frac{(s_{i*}, n_{i*})}{(n_{i*}, n_{i*})}.$$

Proof. Since n_{ij} is 0 or 1, and $q_{ij} = 0$ if $n_{ij} = 0$, the constraint $\sum_j q_{ij} = 0$, for all i such that $f_i = 1$, is equivalent to a collection of independent constraints $(q_{i*}, n_{i*}) = 0$ for all i such that $f_i = 1$. If $f_i = 0$, there is no constraint on q_{i*}, so $q_{i*} = s_{i*}$. Let $f_i = 1$. Since $(X, Y) = \sum_i (x_{i*}, y_{i*})$, it follows that $q_{i*} = s_{i*} + \lambda_i n_{i*}$, with $\lambda_i = -(s_{i*}, n_{i*})/(n_{i*}, n_{i*})$. □

Given P_0 satisfying (4.3), the problem (4.2) is now equivalent to finding P such that

$$P - P_0 \in \mathcal{Z} \quad \text{and} \quad Z(\operatorname{grad}_{\mathcal{N}} J(P)) = Z(N * (AP)) = 0. \tag{4.4}$$

We compute the prolongation operators by the projected steepest descent method.

ALGORITHM 1.

1. *Choose* P_0 *satisfying* (4.3) *and* $\omega \in (0, 2/\varrho(A))$.

2. $P_{n+1} = P_n - \omega Z(N * (AP_n))$, $n = 0, 1, 2, \ldots$

We now derive a bound on the convergence of Algorithm 1.

THEOREM 4.3. *Let* A_j *denote the square matrix obtained by selecting rows and columns of* A *with indices* $\{i \mid n_{ij} = 1\}$. *Further let* $c_1 = \min_j \lambda_{\min}(A_j)$, $c_2 = \max_j \lambda_{\max}(A_j)$. *Then Algorithm 1 converges for all* $\omega \in (0, 2/c_2)$, *and*

$$\|P_{n+1} - P^*\| \le \max\{|1 - \omega c_1|, |1 - \omega c_2|\} \|P_n - P^*\|.$$

Proof. From the definition of c_1, c_2, we have $c_1 P_{*j}^t P_{*j} \le P_{*j}^t A P_{*j} \le c_2 P_{*j}^t P_{*j}$, for all $P \in \mathcal{N}$ and all j, hence

$$c_1(P, P) \le (P, AP) \le c_2(P, P), \quad \forall P \in \mathcal{N}. \tag{4.5}$$

Let $P_n \in \mathcal{N}$. Then $P_n - P^* \in \mathcal{Z}$. Using this, the facts that Z is projection onto $\mathcal{Z}$, and that P^* solves (4.4), hence $Z(N * (AP^*)) = 0$, we have

$$\begin{aligned} P_{n+1} - P^* &= P_n - P^* - \omega Z(N * (AP_n)) \\ &= Z(P_n - P^*) - \omega Z(N * (A(P_n - P^*))) \\ &= (Z \circ (I - \omega \tilde{A}) \circ Z)(P_n - P^*), \end{aligned}$$

where $\tilde{A} : \mathcal{N} \to \mathcal{N}$, $\tilde{A}(P) = \operatorname{grad}_{\mathcal{N}} J(P) = N * (AP)$. Since Z is an orthogonal projection, it follows that

$$\|P_{n+1} - P^*\| \le \|I - \omega \tilde{A}\| \|P_n - P^*\|.$$

Because $\tilde{A}$ is a symmetric operator in $\mathcal{N}$, and, from (4.5), $c_1 \le \lambda_{\min}(\tilde{A}) \le \lambda_{\max}(\tilde{A}) \le c_2$, it follows that

$$\|I - \omega \tilde{A}\| = \rho(I - \omega \tilde{A}) = \max\{|1 - \omega c_1|, |1 - \omega c_2|\},$$

which concludes the proof. □

REMARK 4.4. **(Convergence independent of meshsize)** Under the assumption that the fine mesh is locally quasiuniform, and the coefficients of the differential operator are uniformly elliptic and bounded, the convergence rate of Algorithm 1 does not deteriorate with decreasing meshsize. Indeed, each A_j is a (small) submatrix of A corresponding to a Dirichlet boundary value problem on a mesh with nodes i such that $n_{ij} = 1$, thus we have $\lambda_{\max}(A)/c_1 \le C$. Choosing

$\omega = \frac{1}{\bar{\lambda}}$, where $\bar{\lambda} \geq \lambda_{\max}(A)$ is an easy to compute estimate, we obtain a fast and practical algorithm.

REMARK 4.5. **(Relation to smoothed aggregations)** Let P_0 be the result of unknowns aggregation, and choose N so that nonzeros are allowed only at the nodes of the aggregates and at their immediate neighbors. In terms of the underlying finite element mesh, we allow $p_{ij} \neq 0$ only on elements forming the aggregate plus one strip of elements around. Then the prolongator P_1 resulting from one iteration of Algorithm 1 is identical to the smoothed aggregation prolongator from [23], described in Sec. 3 of this paper. Indeed, with our selection of N, we have $P_0 \in \mathcal{N}$ and $AP_0 \in \mathcal{N}$. Recalling that in (4.1), f was chosen so that $f_i = 1$ except at the Dirichlet boundary and at its immediate neighbors, we have

$$\sum_j a_{ij} = 0 \quad \text{for} \quad f_i = 1.$$

Since $\sum_j (P_0)_{ij} = 1$ if $f_i = 1$, we have $(AP_0\mathbf{1})_i = (A\mathbf{1})_i = 0$ if $f_i = 1$, hence $AP_0 \in \mathcal{Z}$. Consequently, $ZAP_0 = AP_0$, and $P_1 = P_0 - \omega AP_0 = (I - \omega A)P_0$, the original smoothed aggregation prolongator for the smoother of degree 1.

5. Coarse bases by minimization of energy: General Case. We will now discuss an extension of the method described in Section 4 suitable in the case of systems of equations such as three-dimensional linear elasticity.

We will find it convenient to work in terms of blocks corresponding to degrees of freedom associated with a single node. That is, we will identify all degrees of freedom on a node as a single entity. Let n denote the number of nodes on the current fine level, and d be the number of degrees of freedom per node. The matrix A will be understood as an $n \times n$ block matrix with $d \times d$ blocks. Let B be a given $(nd) \times r$ matrix whose columns are discrete representation of the zero energy modes of the problem. That is, the columns of B span the nullspace of the stiffness matrix for the related problem with no essential boundary conditions imposed. For example, in the case of 3D elasticity, columns of B are formed by discrete representation of the 6 rigid body modes with respect to the current fine level basis. We wish to capture the column space of B exactly in the range of the prolongation. The number r will play the role of the number of degrees of freedom per node on the coarse level.

The matrix B will be viewed as a block column formed by $d \times r$ blocks:

$$B = \begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_n \end{pmatrix}.$$

We will view the prolongator P as an $n \times m$ block matrix $P = (P_{ij})$ with $d \times r$ blocks. Further, let

$$R = \begin{pmatrix} R_1 \\ R_2 \\ \vdots \\ R_m \end{pmatrix}$$

be a given a block column matrix with $r \times r$ blocks storing the discrete representation of the zero energy modes on the coarse level. That is, we will require that $PR = B$

with a modification in rows that correspond to points near the boundary. Again, let N be a given $0-1$ matrix with 1 where nonzeros of P are allowed, and define

$$\mathcal{N} = \{P \in \mathbb{M}^{nd \times mr} : p_{ij} = 0 \text{ if } n_{ij} = 0\}.$$

Next, assume there is given a block diagonal symmetric positive definite matrix $D = \operatorname{diag}(D_{ii})$ with $d \times d$ diagonal blocks D_i, which will play the role of a preconditioner for A. We assume D to preserve the nonzero pattern, i.e., $D : \mathcal{N} \to \mathcal{N}$. This will be true when the blocks N_{ij} are matrices of all zeros or all ones.

Finally, to treat the nodes close to essential boundary condition, associate with each node i a given $r \times r$ matrix F_i. The purpose of the matrix F_i is to select the subspace of zero energy modes that are to be captured by the range of P at node i.

Let $p \geq 1$ and consider the problem

$$J(P) = \frac{1}{p} \sum_k (p_{*k}^t A p_{*k})^p = \frac{1}{p} \operatorname{tr}(\operatorname{diag}(P^t A P))^p \to \min \tag{5.1}$$

subject to the constraint

$$\left.\begin{array}{c} P \in \mathcal{N} \\ (P_{i*} R - B_i) F_i = 0 \quad \text{for all nodes } i. \end{array}\right\} \tag{5.2}$$

The simple case, discussed in Section 4, is obtained by setting $p = 1$, $d = 1$, $r = 1$, $B = b_{*1} = \mathbf{1}$, and $F_i = f_i = 0$ or 1.

Again, denote

$$\begin{aligned} \mathcal{Z} &= \{Q_1 - Q_2 \mid Q_1, Q_2 \text{ satisfy (5.2)}\} \\ &= \{Q \in \mathcal{N} \mid Q_{i*} R F_i = 0 \text{ for all } i\}, \end{aligned} \tag{5.3}$$

and compute the gradient of $J(P)$ in $\mathcal{N}$ and the orthogonal projection onto $\mathcal{Z}$, now in the matrix inner product $(\cdot,\cdot)_D$.

LEMMA 5.1. *The gradient of J in the space $\mathcal{N}$ with the inner product $(\cdot,\cdot)$ is*

$$\operatorname{grad}_D J(P) = D^{-1}(N * (AP((\operatorname{diag}(P^t A P))^{p-1}). \tag{5.4}$$

Proof. By a direct computation,

$$\begin{aligned} (Q, \operatorname{grad}_D J(P))_D &= \frac{d}{dt} J(P + tQ)|_{t=0} \\ &= \frac{1}{2p} \sum_j p(p_{*j}^t p_{*j})^{p-1} 2 q_{*j}^t A p_{*j} \\ &= (Q, AP((\operatorname{diag}(P^t A P))^{p-1}) \\ &= (Q, D^{-1}(N * (AP((\operatorname{diag}(P^t A P))^{p-1}))_D, \end{aligned}$$

for all $Q \in \mathcal{N}$. ∎

LEMMA 5.2. *The $(\cdot,\cdot)_D$–orthogonal projection in $\mathcal{N}$ onto the subspace $\mathcal{Z}$ is $Z : S \mapsto Q$, defined by*

$$Q_{i*} = S_{i*}(I - \tilde{R}_i (\tilde{R}_i^t \tilde{R}_i)^+ \tilde{R}_i^t),$$

where $\tilde{R}_i = N_{i*}^t * (RF_i)$.

Proof. We have $Q_{i*}RF_i = (Q_{i*} * N)(RF_i) = Q_{i*}(N_{j*}^t * (RF_i))$, for all $Q \in \mathcal{N}$. Therefore, (5.3) can be written as $\mathcal{Z} = \{X \in \mathcal{N} \mid X_{i*}\tilde{R}_i = 0 \text{ for all } i\}$, where the constraints $X_{i*}\tilde{R}_i = 0$ are independent. Since also

$$(X, Y)_D = \sum_i (D_i X_{i*}, Y_{i*}),$$

it follows that $Z : S \mapsto Q$ is equivalent to $Z_i : S_{i*} \mapsto Q_{i*}$, where Z_i are the $(D_i X_{i*}, Y_{i*})$-orthogonal projections in the space of block row vectors onto the subspaces $\{X_{i*} \mid X_{i*}\tilde{R}_i = 0\}$. So, we only need to find the matrix form of $Z_i : S_{i*} \mapsto S_{i*}Z_i$. Let s be a row of (a block row) S_{i*}. It is easy to see that the mapping $s \mapsto s\tilde{Z}_i$, $\tilde{Z} = I - \tilde{R}_i(\tilde{R}_i^t\tilde{R}_i)^+\tilde{R}_i^t$, is an orthogonal projection onto the subspace $\{q : q\tilde{R}_i = 0\}$ in the inner product (x, y). Since

$$(X_{i*}, Y_{i*}) = \sum_{\text{rows } x_j \text{ of } X_{i*}} (x_j, y_j),$$

the mapping $S_{i*} \mapsto S_{i*}\tilde{Z}_i$ is the orthogonal projection in the inner product (X_{i*}, Y_{i*}) onto $\{X_{i*} \mid X_{i*}\tilde{R}_i = 0\}$. Because the mappings $X_{i*} \mapsto D_i X_{i*}$ and $S_{i*} \mapsto S_{i*}\tilde{Z}_i$ commute, $S_{i*} \mapsto S_{i*}\tilde{Z}_i$ is symmetric also in the inner product $(D_i X_{i*}, Y_{i*})$, hence an orthogonal projection. □

Note that Lemma 5.2 implies that the projection Z does not depend on the preconditioning matrix D as long as D is symmetric positive definite and has the assumed block diagonal structure.

We are now ready to write the general algorithm for computation of the improved prolongator.

ALGORITHM 2.

1. *Choose* P_0 *satisfying* (5.2)

2. *For* $n = 0, 1, 2, \ldots$, *choose* ω_n *and set*

$$P_{n+1} = P_n - \omega Z(D^{-1}(N * AP_n(\text{diag}(P_n^t AP_n)^{p-1}))).$$

In Algorithm 2, the values ω_n are to be chosen sufficiently small so that $J(P_{n+1}) < J(P_n)$ except at the solution. In the practically important case $p = 1$, we have the following direct generalization of Algorithm 1.

ALGORITHM 3.

1. *Choose* P_0 *satisfying* (5.2) *and* $\omega \in (0, 2/\varrho(D^{-1}A))$.

2. $P_{n+1} = P_n - \omega ZD^{-1}(N * AP_n)$, $n = 0, 1, 2, \ldots$

We have a straightforward generalization of Theorem 4.3.

THEOREM 5.3. *Let* $\|\cdot\|_D = (\cdot, \cdot)_D$ *and* A_j^D *be the square matrix obtained by selecting the rows and columns of* $D^{-1/2}AD^{-1/2}$ *with indices* $\{i : n_{ij} = 1\}$. *Further, let* $c_1 = \min_j \lambda_{\min}(A_j^D)$, $c_2 = \max_j \lambda_{\max}(A_j^D)$. *Then, for any initial guess* P_0 *satisfying the constraint* (5.2) *and* $\omega \in (0, 2/c_2)$, *Algorithm 3 creates a sequence* $P_1, P_2 \ldots$ *such that*

$$\|P_{k+1} - P^*\|_D \leq \max\{|1 - \omega c_1|, |1 - \omega c_2|\}\|P_k - P^*\|_D.$$

Proof. From the definition of c_1, c_2,

$$c_1 P_{*j}^t P_{*j} \leq P_{*j}^t D^{-1/2} A D^{-2} P_{*j} \leq c_2 P_{*j}^t P_{*j}.$$

The rest of the proof follows by replacing in the proof of Theorem 4.3 $(\cdot,\cdot)$, $\|\cdot\|$, A, by $(\cdot,\cdot)_D$, $\|\cdot\|_D$, $D^{-1}A$, respectively. □

Similarly as in the simple case, this implies that the convergence of Algorithm 3 is independent of mesh size in the case of quasiuniform mesh and a uniformly elliptic problem.

6. Specification of Algorithm Components and Applications. To use the method of Section 5 in a practical situation, we need to specify the choice of the nonzero structure N of P, as well as the matrices F_i, R, B, and P_0.

First let us specify the blocks F_i. For each node i, let U_i denote the list of nodes adjacent to node i in the graph of matrix A. i.e.

$$U_i = \{j \mid A_{ij} \neq 0\},$$

where A_{ij} is the $d \times d$ block of the matrix A corresponding to the nodes i, j. Let A_{U_i} be the local stiffness matrix associated with the nodes of U_i, and $B(U_i)$ be the corresponding block row selection of B. Then, we define F_i to be the matrix such that

$$A_{U_i} B(U_i) F_i = 0.$$

In other words, the columns of F_i specify the coefficients of the linear combination of the r columns of $B(U_i)$ forming the kernel of A_{U_i} (the so-called local kernel of A at the neighborhood of the node i).

In practice, however, local stiffness matrices A_{U_i} may not be available. In such a case, F_i is constructed as follows: Let $A(U_i, U_i)$ be the submatrix of A obtained by selecting the block rows and columns corresponding to the nodes in U_i and define F_i so that

$$(A(U_i, U_i) B(U_i) F_i)_{i_{\text{local}}} = 0,$$

where i_{local} is the index of node i in the local numbering associated with U_i.

Let $\{\mathcal{A}_i\}_{i=1}^m$ denote the set of aggregates forming disjoint covering of the set of nodes $\{1, \ldots, n\}$ as in (3.4), and let d_i denote the number of degrees of freedom in aggregate i. For the sake of simplicity we assume that the fine level nodes are numbered by consecutive numbers within each aggregate. To find initial P_0 in the case of elasticity problem, we proceed as follows:

1. Recall that B is the matrix representation of the zero energy modes with respect to the fine grid basis, and r denotes the number of columns of B. We partition B into sets of rows $B_k^{\mathcal{A}}$, $k = 1, \ldots, m$, each corresponding to the set of degrees of freedom on an aggregate $\mathcal{A}_k$ (see Figure 6.1).
2. Decompose matrices $B_k^{\mathcal{A}} = Q_k^{\mathcal{A}} R_k^{\mathcal{A}}$, where $Q_k^{\mathcal{A}}$ is $d_k \times r$ orthogonal, and $R_k^{\mathcal{A}}$ is $r \times r$ upper triangular square matrix. These matrices are easily obtained from the QR decomposition of $B_k^{\mathcal{A}}$.
3. Finally, set $P_0 = \text{diag}(Q_k^{\mathcal{A}})$, and $R = \left(R_1^{\mathcal{A}\,t}, \ldots, R_m^{\mathcal{A}\,t} \right)^t$. Here, P_0 is understood to be partitioned into $d_i \times r$ blocks $P_{ij}^{\mathcal{A}}$ corresponding to aggregate degrees of freedom (cf., Fig. 6.2).

Note that this construction guarantees that the action of the projection $\mathcal{Z}$ defined in Lemma 5.2 will be computed inexpensively. Step 3 can be viewed as the Gram-Schmidt orthogonalization of the coarse space basis of rigid body modes, as previously suggested in [23].

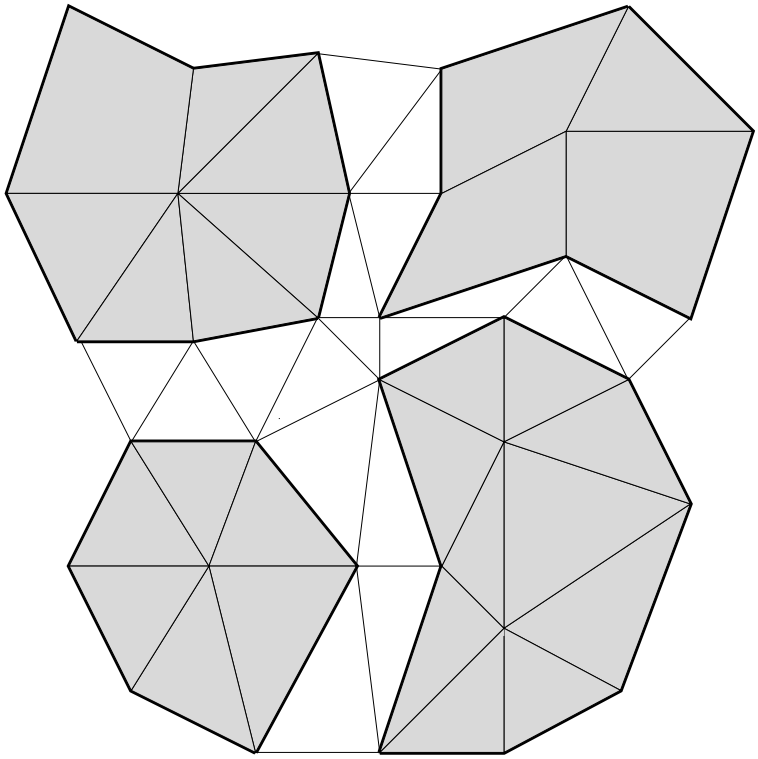

FIG. 6.1. *Example of node aggregation in 2D.*

REMARK 6.1. **(Semi-coarsening)** The coarse matrix fill-in associated with the application of smoothed aggregation method becomes critical when many of the aggregates are "strips" only one element wide. These aggregate types will be encountered when semi-coarsening is used to deal with anisotropic problems. To reduce fill, the supports of coarse basis functions should not extend beyond the aggregate in the short direction of the strips. In [23], we have proposed to modify the result of smoothed aggregation by a heuristic "filtering" process to achieve this. Using the present approach, we can simply specify the desired support of the basis functions, and the method performs the "filtering" in a systematic way.

7. Computational Experiments. The purpose of this section is to demonstrate the performance of the proposed method and compare it to the smoothed aggregation technique of [23]. The sparsity structure N was set to be the nonzero structure of AP_0, so the two methods coincide if only one minimization step is used in the current method.

In all the experiments below, the method is used as a preconditioner for the conjugate gradient method, and the stopping criterion used was

$$\left[\frac{\langle Br^i, r^i\rangle}{\langle Br^0, r^0\rangle}\mathrm{cond}(B,A)\right]^{1/2} \leq 10^{-5},$$

where B is the preconditioner, r^i denotes the residual after i steps of the iteration, and $\mathrm{cond}(B,A)$ is a condition number estimate computed at run time.

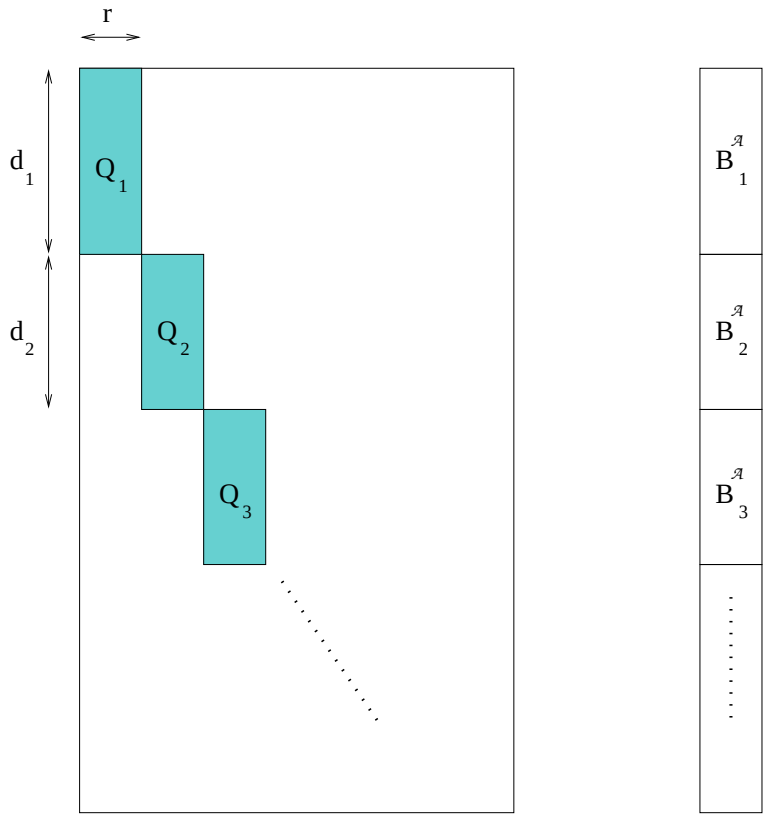

FIG. 6.2. *The structure of P_0 and B corresponding to aggregate degrees of freedom.*

TABLE 7.1
The body of an automobile.

unstructured shell, QUAD4 elements, 43,104 dofs.						
min. steps	setup time	iter. time	total time	num. of iters.	cond estim	time/ time sm. agg.
1	1.56	18.05	19.61	37	119.5	1.00
2	1.93	15.56	17.49	32	92.27	0.89
3	2.11	14.23	16.34	29	81.70	0.83
4	2.21	13.83	16.04	28	78.78	0.81
5	2.33	14.28	16.61	28	78.15	0.84
6	2.45	12.82	16.27	28	77.89	0.82
7	2.74	13.83	16.57	28	77.77	0.84

The system of aggregates and the tentative prolongator P_0 were constructed as described in [23]. The coarsening process was stopped when the number of degrees of freedom on the coarsest level reached 3000.

The experiments we run on 15 R10000 processors of a 16-processor SGI Origin/2000. The results of the experiments are presented in Table 7.1–7.4. The first line of each table corresponds to the smoothed aggregation technique with a smoother of degree 1.

TABLE 7.2
The shell model of an automobile wheel (see Fig. 7.1).

unstructured shell, QUAD4 elements, 59,490 dofs.						
min. steps	setup time	iter. time	total time	num. of iters.	cond estim	time/ time sm. agg.
1	1.30	5.00	6.30	9	4.55	1.00
2	1.47	4.53	6.00	8	3.81	0.95
3	2.00	3.98	5.98	7	2.91	0.94
4	2.08	3.56	5.64	6	2.22	0.89
5	2.28	3.57	5.85	6	2.00	0.92
6	2.47	3.46	5.93	6	1.91	0.94

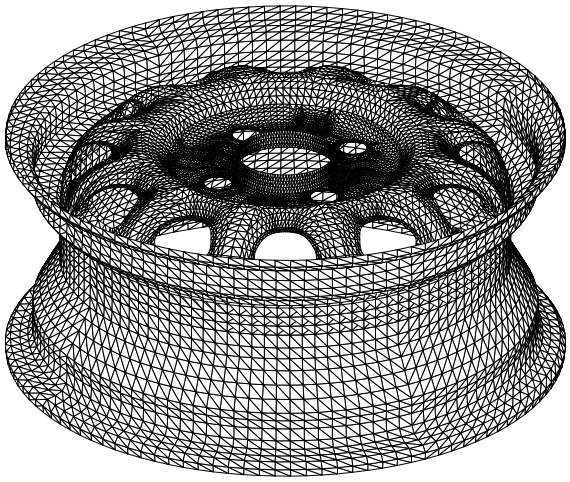

FIG. 7.1. *The mesh of an automobile wheel. (Courtesy of Charbel Farhat, University of Colorado at Boulder.)*

Finally, we have tested the performance of AMG for minimization with $p > 1$ to approximate the minimization of the maximal energy of basis functions. Our algorithm used an (admittedly crude) choice of ω found by replacing ω by $\omega/2$ until the minimization algorithm decreased the value of the objective function. We have found little if any improvement of AMG convergence with increasing p. A sample result is in Table 7.5.

8. Conclusion. We have formulated and tested an algorithm for building algebraic multigrid bases from minimalization of their energies. For minimization of the sum of the energies, the first step of the minimization gives the same result as our previous method, prolongation by smoothed aggregation. Numerical experiments indicate that, in general, adding more minimization steps improves the convergence properties of the solver, but the benefit is partially offset by the expense of the additional minimization steps. In the case of more complicated problems, such as shells, performing more minimization steps results in better computational times. For less complicated problems, the computational time grows, but only insignificantly, because the minimization process is relatively cheap. Minimization of the sums of the energies to a power of p, $p > 1$, is more complicated and computationally expensive,

TABLE 7.3
Large unstructured solid.

large unstructures solid, 407,277 dofs.						
min. steps	setup time	iter. time	total time	num. of iters.	cond estim	time/ time sm. agg.
1	12.79	36.37	49.16	13	6.16	1.00
2	15.43	34.05	49.48	12	5.04	1.01
3	18.11	32.06	50.17	11	4.45	1.02
4	20.28	31.19	51.47	11	4.23	1.04
5	22.44	28.43	50.87	10	4.00	1.03
6	24.95	28.56	53.51	10	3.90	1.09

TABLE 7.4
An automobile steering knuckle (see Fig. 7.2).

unstructured solid, TETRA elements. 75,174 dofs.						
min. steps	setup time	iter. time	total time	num. of iters.	cond estim	time/ time sm. agg.
1	8.13	5.36	13.49	8	2.58	1.00
2	8.60	5.37	13.97	8	2.55	1.03
3	8.85	5.40	14.25	8	2.50	1.06
4	8.86	4.79	13.79	7	2.20	1.02
5	9.07	4.78	13.85	7	2.21	1.03
6	9.52	4.78	14.30	7	2.17	1.06

and did not improve the multigrid convergence enough to offset the added cost, and if fact may make it worse in some cases. Our explanation of this fact is that although the maximum of the energies of basis functions appears in theoretical estimates, these estimates are far from being sharp. Therefore, while the principle of minimization of the energies of the basis functions is a useful tool for constructing the coarse basis functions, the actual behavior of AMG is not predicted exactly by the maximum of the energies.

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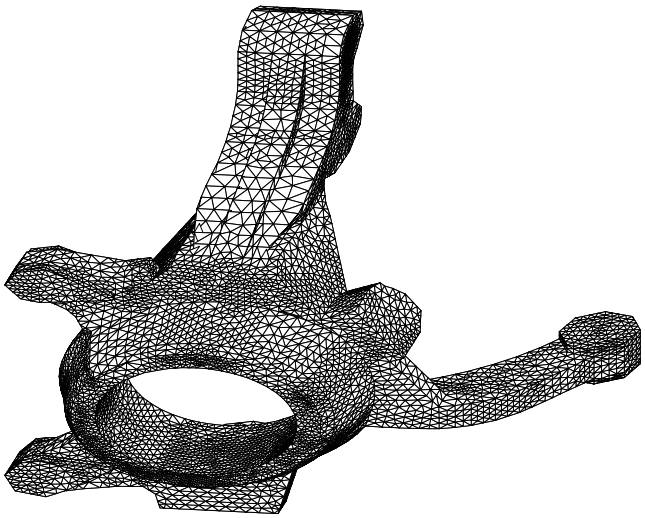

FIG. 7.2. *The mesh of an automobile steering knuckle. (Courtesy of Charbel Farhat, University of Colorado at Boulder.)*

TABLE 7.5

Convergence of the method for different values of p Unstructured solid discretized using PENTA elements. 12125 nodes, 36375 degrees of freedom. Stopping condition: 10^{-6}.

p	min. steps	AMG iters	cond. est.
1	4	27	20.56
1	8	26	19.24
2	4	31	27.17
2	8	30	26.04
3	4	29	26.13
3	8	29	26.06
4	4	29	26.17
4	8	29	26.12
5	4	29	26.18
5	8	29	26.15
10	4	29	26.18
10	8	29	26.18
10	20	29	26.15
10	40	29	26.14
10	80	28	26.02
smoothed agregs.		32	29.11

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