SIAM J. SCI. COMPUT.
Vol. 17, No. 2, pp. 439-453, March 1996

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# TOWARDS AUTOMATIC MULTIGRID ALGORITHMS FOR SPD, NONSYMMETRIC AND INDEFINITE PROBLEMS*

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**Abstract.** A new multigrid algorithm is constructed for the solution of linear systems of equations which arise from the discretization of elliptic PDEs. It is defined in terms of the difference scheme on the fine grid only, and no rediscretization of the PDE is required. Numerical experiments show that this algorithm gives high convergence rates for several classes of problems: symmetric, nonsymmetric and problems with discontinuous coefficients, nonuniform grids, and nonrectangular domains. When supplemented with an acceleration method, good convergence is achieved also for pure convection problems and indefinite Helmholtz equations.

**Key words.** convection-diffusion equation, discontinuous coefficients, elliptic PDEs, indefinite Helmholtz equation, automatic multigrid method

**AMS subject classifications.** 65F10, 65N22, 65N55

## 1. Introduction.

The multigrid method is a powerful tool for the solution of linear systems which arise from the discretization of elliptic PDEs [4], [5]. In a multigrid iteration the equation is first relaxed on a fine grid in order to smooth the error; then the residual equations are transferred to a coarser grid, to be solved subsequently and to supply correction terms. Recursion is used to solve the coarser grid problem in a similar way. In order to implement this procedure the PDE has to be discretized on all grids and restriction and prolongation operators must be defined in order to transfer information between fine and coarse grids. The basic multigrid method works well for the Poisson equation in the square, but difficulties arise with nonsymmetric and indefinite problems and problems with variable coefficients, complicated domains, or nonuniform grids. In these cases, an effective discretization of the PDE on coarse grids becomes more complicated than that provided by a naive approach. Some suggestions on handling discontinuous coefficients are given in [1], while the nonsymmetric case is analyzed in [9] and [10]. A projection method for the solution of slightly indefinite problems is developed in [7]. Another projection method for such problems is presented and analyzed in [3]. These approaches, however, involve specialized and problem-dependent treatment, and the need for a uniform approach is not yet fulfilled.

Present multigrid procedures are not able to serve as "black box" solvers. Special attention has to be given to the neighborhood of the boundary and to the presence of discontinuities. In [6], [20], and [21] the algebraic multigrid (AMG) method is developed. This method is algebraic in the sense that it depends on the discrete system of equations and not on the original PDE or the difference scheme for it. It automatically chooses the coarse level variables and constructs the coarse level equations and the restriction and prolongation operators; hence it applies to general linear systems of equations. However, the set-up time required is large (equivalent to about 10 $V$-cycles).

Multigrid versions whose definition depends on the difference scheme on the original grid only also exist; these methods, which are called automatic methods in the sequel, reduce the original grid to further coarse grids and automatically construct the coarse-grid coefficient matrix and the restriction and prolongation operators. The black-box multigrid method of [11] applies to problems with discontinuous coefficients and nonrectangular domains and also to nonsymmetric problems [12]. Another robust automatic method is presented in [34].

*Received by the editors November 23, 1993; accepted for publication (in revised form) October 25, 1994.

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None of these methods, however, handles highly indefinite equations; they use coarse-grid operators which are derived from a Galerkin approach, resulting in highly indefinite coarse-grid equations.

All the automatic multilevel methods mentioned above suffer from the disadvantage that for $d$-dimensional PDE discretizations the coarse-grid operators involve stencils with $3^d$ coefficients, even when the original difference equation has a $(2d + 1)$-coefficient stencil. This significantly enlarges the amount of arithmetic operations and storage required to generate and store coarse-grid operators (in comparison to algorithms which use $(2d + 1)$-coefficient stencils at all levels). Moreover, it enlarges the cost of a multigrid $V$-cycle (implemented, e.g., with a Gauss–Seidel smoother) by roughly 25% and 40% for 2-d and 3-d problems, respectively. When $W$-cycles or more expensive smoothers are used the overhead may be even larger; in particular, the red-black Gauss–Seidel relaxation is not applicable any more and $2^d$-color relaxation (whose parallel and vector implementations are more complicated) must be used instead. Furthermore, since the coarse coefficient matrices lack property A, most of the analysis of [33] for the successive over-relaxation (SOR) method does not apply (the SOR smoother in multigrid methods is considered in [32]). These difficulties are partially relaxed in the algorithm of [31], where $(2^{d+1} - 1)$-coefficient coarse-grid stencils are used; this version, however, is not satisfactory for nonsymmetric problems and problems with discontinuous coefficients.

The aim of this work is to present an automatic multigrid method which does not suffer from the above difficulties; that is, it uses $(2d + 1)$-coefficient stencils only and can be used to solve indefinite problems and several other important classes of problems, e.g., nonsymmetric problems and problems with discontinuous coefficients and nonrectangular domains. Moreover, coarse-grid, restriction, and prolongation operators are obtained from the linear system of equations by a simple and inexpensive recursive process; actually, the cost of this recursion is approximately one work unit, that is, it is equivalent to one fine-grid Gauss–Seidel sweep (compared to five work units for the method of [31]). This fact is especially important for implicit time marching in evolution problems with differential operator or boundary varying in time, where coarse-grid operators are to be reconstructed at every time level. In addition, the fact that operators on different levels are of the same stencil allows easy programming, with data structures and smoothing procedures for coarse-grid equations similar to those used for the finest-grid equation. Like the methods of [11] and [34], the algorithm is robust with respect to the number of fine-grid points, boundary condition type, and shape of the domain. Unlike these methods, however, it is not applicable to schemes which use $3^d$-coefficient stencils on the finest grid. We call this algorithm AutoMUG (automatic multigrid).

Our numerical experiments show that, for some difficult problems, the basic AutoMUG iteration may be efficiently accelerated by a Lanczos-type method. It is likely that the existing automatic multigrid methods can also profit from such techniques; indeed, it is shown in [22] that even for highly indefinite, nearly singular Helmholtz equations the two-level implementation of both modified black-box multigrid and AutoMUG can be efficiently accelerated.

AutoMUG is described in §2. In §3 numerical examples are presented. In §4 the algorithm and the numerical results are discussed.

**2. The AutoMUG (automatic multigrid) method.** In this section we define the AutoMUG method for the solution of finite difference equations which have $(2d + 1)$-coefficient stencils (for $d = 1, 2$) and examine the properties of its coarse-grid coefficient matrices.

**2.1. Abstract definition of AutoMUG.** We begin with an abstract definition of AutoMUG for the solution of the linear system of equations

$$Ax = b.$$

The notation of this definition will be useful in the sequel. In the following, "$\leftarrow$" means replacement, $S_1$ and $S_2$ are some smoothing procedures, and $\epsilon$, $\nu_1$, $\nu_2$, and $o$ are nonnegative integers denoting, respectively, the cycle index, the number of presmoothings, the number of postsmoothings, and the minimal order of $A$ for which AutoMUG is called recursively. The operators $R$, $P$, and $Q$ will be defined later.

$$
\begin{aligned}
&\text{AutoMUG}(x_{\text{in}}, A, b, x_{\text{out}}):\\
&\quad \text{if order}(A) < o\\
&\qquad\qquad x_{\text{out}} \leftarrow A^{-1}b\\
&\quad \text{otherwise:}\\
&\qquad\qquad x_{\text{in}} \leftarrow S_1 x_{\text{in}} \quad (\text{repeat } \nu_1 \text{ times})\\
&\qquad\qquad e \leftarrow 0\\
&\qquad\qquad \left.\begin{array}{l}\text{AutoMUG}(e, Q, R(Ax_{\text{in}} - b), e_{\text{out}})\\ e \leftarrow e_{\text{out}}\end{array}\right\} \text{ repeat } \epsilon \text{ times}\\
&\qquad\qquad x_{\text{out}} \leftarrow x_{\text{in}} - Pe\\
&\qquad\qquad x_{\text{out}} \leftarrow S_2 x_{\text{out}} \quad (\text{repeat } \nu_2 \text{ times}).
\end{aligned}
\tag{1}
$$

For simplicity, we assume in this paper that the method is implemented with a $V$-cycle ($\epsilon = 1$) and a maximal number of levels ($o = 2$). An iterative application of AutoMUG is given by

$$
\begin{aligned}
&x_0 = 0,\ k = 0\\
&\text{while } \|Ax_k - b\|_2 \geq \text{threshold} \cdot \|Ax_0 - b\|_2\\
&\text{AutoMUG}(x_k, A, b, x_{k+1})\\
&k \leftarrow k + 1\\
&\text{endwhile}
\end{aligned}
\tag{2}
$$

Below we define the operators $R$, $P$, and $Q$ of (1) for the case in which $A$ is a tridiagonal matrix. Although this is of little significance in itself, it is crucial in the development of the algorithm for other more complicated cases that arise in practical applications and are treated next in this paper.

**2.2. The tridiagonal case.** In this subsection we define the operators $R$, $P$, and $Q$ used in (1) for linear systems which arise, for example, from finite-difference discretization of the ODE

$$(au')' + cu' + \beta u = f \tag{3}$$

where $a$, $c$, $\beta$, $u$, and $f$ are functions defined on $\Omega \subset R$ and suitable boundary conditions are imposed on $\partial\Omega$ (this illustrative example will be used in the sequel).

For any matrix $B$, $B = (b_{i,j})_{1\le i\le K,\ 1\le j\le L}$, define

$$\text{rowsum}(B) \equiv \text{diag}\left(\sum_{j=1}^{L} b_{i,j}\right)_{1\le i\le K}.$$

For a diagonal matrix $B$, $B = \text{diag}(b_i)_{1\le i\le K}$, let

$$\text{even}(B) \equiv \text{diag}(b_{2i})_{1\le i\le \lfloor K/2\rfloor} \text{ and } \text{odd}(B) \equiv \text{diag}(b_{2i-1})_{1\le i\le \lceil K/2\rceil}.$$

Let $I$ denote an identity matrix of a suitable order. Let $N$ be a positive integer, $n = \lfloor \log_2 N \rfloor$, $h \equiv 1/(N+1)$ be the mesh size, and $A$ be a tridiagonal matrix of order $N$ resulting, for

example, from a difference scheme approximating (3). For any positive integer $K$, let $M(K)$ be the permutation matrix which reorders the variables of a $K$-dimensional vector such that odd-numbered variables appear in the first block and even-numbered variables appear in the second block. Define

$$A_0 = A \text{ and } M_i = M(N/2^i), \quad 0 \le i \le n, \tag{4}$$

where, here and in the sequel, $N/2^i$ means an integer division, that is, $\lfloor N/2^i \rfloor$. In the following we give some motivation for the definition of the operators $R$, $P$, and $Q$ used in (1). Suppose $A$ has no vanishing diagonal element and let $D = \text{diag}(A)$. Then, for some bidiagonal matrices $B$ and $C$, we have

$$A = DM_0^T \begin{pmatrix} I & -B \\ -C & I \end{pmatrix} M_0 = M_0^T (M_0 D M_0^T) \begin{pmatrix} I & -B \\ -C & I \end{pmatrix} M_0 = R^{-1} Q P^{-1},$$

where

$$R = (M_0 D M_0^T) \begin{pmatrix} I & 0 \\ C & I \end{pmatrix} (M_0 D M_0^T)^{-1} M_0, \quad Q = (M_0 D M_0^T) \begin{pmatrix} I & 0 \\ 0 & I - CB \end{pmatrix},$$

$$P = M_0^T \begin{pmatrix} I & B \\ 0 & I \end{pmatrix}.$$

Suppose these operators are used in (1). Since $Q$ is tridiagonal, one may repeat the above procedure with $A$ replaced by $Q$ to generate suitable operators for the recursive call in (1). With $\nu_1 = \nu_2 = 0$ in (1) this yields a direct solver which is equivalent to the cyclic reduction method [2].

Suppose odd-numbered variables are red-colored. If $\nu_1 = 0$, $\nu_2 = 1$, and the smoothing procedure $S_2$ of (1) corresponds to the red leg of a red-black Gauss–Seidel relaxation, then an equivalent algorithm is obtained when the definition of $R$, $Q$, and $P$ is modified to read

$$\tilde{C} = \text{even}(D) C \text{odd}(D)^{-1}, \quad R = \begin{pmatrix} \tilde{C} & I \end{pmatrix} M_0, \quad Q = \text{even}(D)(I - CB), \quad P = M_0^T \begin{pmatrix} B \\ I \end{pmatrix}.$$

Moreover, $Q = RAP$ still holds; hence this is an appropriate choice for the operators in (1). This procedure is equivalent to that used in [26] for tridiagonal systems.

Note that $Q$ is the Schur complement of $A$ relative to the even-numbered variables. These variables may be viewed as abstract coarse-grid points. Then $Q$ is a coarse-grid operator, $R$ is a fine-to-coarse-grid restriction, and $P$ is a coarse-to-fine-grid prolongation.

We come now to a precise definition of the operators $R$, $P$, and $Q$ used in (1). For $0 \le i < n$, define the matrices $D_i$, $B_i$, $C_i$, $P_{A,i+1}$, $\tilde{C}_i$, $R_{A,i+1}$, $A_{i+1}$, and $S_{A,i+1}$, in this order, by

$$\begin{aligned}
D_i &= \text{diag}(A_i), \\
A_i &= D_i M_i^T \begin{pmatrix} I & -B_i \\ -C_i & I \end{pmatrix} M_i, \\
P_{A,i+1} &= M_i^T \begin{pmatrix} B_i \\ I \end{pmatrix}, \\
\tilde{C}_i &= \text{even}(D_i) C_i \text{odd}(D_i)^{-1}, \\
R_{A,i+1} &= \begin{pmatrix} \tilde{C}_i & I \end{pmatrix} M_i, \\
A_{i+1} &= I - C_i B_i, \\
S_{A,i+1} &= \text{rowsum}(2I - A_{i+1}), \\
A_{i+1} &\leftarrow \text{even}(D_i) A_{i+1}.
\end{aligned} \tag{5}$$

Note that all the $A_i$ are tridiagonal, hence $B_i$ and $C_i$ are well defined (vanishing of a diagonal element of $D_i$, for some $i$, is discussed at the end of §2.3). The operator $S_{A,i+1}$ is not used in the present case, but will be helpful in §2.4, where it serves as an approximation to $R_{A,i+1}P_{A,i+1}$. Indeed, when $D_0$ is a multiple of the identity,

$$
\begin{aligned}
S_{A,1} - R_{A,1}P_{A,1} &= \text{rowsum}(I + C_0B_0) - (I + C_0B_0) \\
&= \begin{pmatrix} -C_0 & \text{rowsum}(C_0B_0) \end{pmatrix} \begin{pmatrix} B_0 \\ I \end{pmatrix} \sim \frac{h^2}{|a|} \left( \frac{d}{dx} a \frac{d}{dx} + c \frac{d}{dx} \right),
\end{aligned} \tag{6}
$$

which is negligible when operating on functions $u$ for which $(au')'$ and $cu'$ are not too large. This condition is fulfilled for the solution of the ODE (3), according to the assumptions made in [1].

*Remark.* The above definition of $S_{A,i+1}$ may be replaced by $S_{A,i+1} = \text{rowsum}(H_i)$, with

$$
H_i = R_{A,i+1}P_{A,i+1}, \quad H_i = R_{A,i+1} \text{ or } H_i = \begin{pmatrix} C_i & I \end{pmatrix}.
$$

This yields no essential change in either the theory or the numerical results presented in this paper. The third version is slightly better for indefinite problems, and is used in [23], [24], and [25].

The AutoMUG procedure, namely

$$
\text{AutoMUG}(x_{\text{in}}, A, b, x_{\text{out}}),
$$

defined in (1), is called $n+1$ times per iteration. In the $(n+1)$st time the AutoMUG procedure is a direct solver. For $1 \le i \le n$, the $i$th call to the AutoMUG procedure is accomplished with the operators

$$
Q \leftarrow A_i, \quad P \leftarrow P_{A,i}, \quad R \leftarrow R_{A,i}.
$$

**2.3. Properties of the coarse-grid operators.** In this subsection we show that the coarse-grid operators $A_i$ defined in (5) preserve some desirable properties of $A$. To this end, we prove the following lemmas.

For any matrix $T$ let $T^{(i)}$ and $T^{[j]}$ denote its $i$th row and $j$th column, respectively, $|T|$ denote the matrix defined by $|T|_{i,j} = |T_{i,j}|$, and $T \ge 0$ ($T$ is nonnegative) hold if all the elements of $T$ are positive or zero. For any two matrices $T$ and $S$ of the same size let $T \ge S$ hold if $T - S \ge 0$. Let $(\cdot, \cdot)$ denote the $l_2$ inner product and $e$ be the vector whose components are all equal to 1.

LEMMA 2.1. *Assume $T$ and $S$ are two matrices for which the number of rows of $S$ is equal to the number of columns of $T$. Then*

$$
\text{rowsum}(|S|) \le I \;\Rightarrow\; \text{rowsum}(|TS|) \le \text{rowsum}(|T|).
$$

*Furthermore, if* $\text{rowsum}(|S|) \le I$ *and for some* $i_0$ $\text{rowsum}(|S|)_{i_0,i_0} < 1$ *and* $T^{[i_0]} \ne 0$ *then*

$$
\exists\, j_0 \text{ s.t. } \text{rowsum}(|TS|)_{j_0,j_0} < \text{rowsum}(|T|)_{j_0,j_0}.
$$

*Proof.* Suppose $T \ge 0$ and $S \ge 0$. Then

$$
\text{rowsum}(TS)_{i,i} = \left( T^{(i)}, \sum_j S^{[j]} \right) \le (T^{(i)}, e) = \text{rowsum}(T)_{i,i}.
$$

For the second part of the lemma, by assumption there exists a $j_0$ such that $T_{j_0,i_0} > 0$. Consequently,

$$
\text{rowsum}(TS)_{j_0,j_0} = (T^{(j_0)}, \sum_j S^{[j]}) < (T^{(j_0)}, e) = \text{rowsum}(T)_{j_0,j_0}.
$$

For the general case, the lemma follows from

$$\text{rowsum}(|TS|) \leq \text{rowsum}(|T||S|).$$

This completes the proof of the lemma.

LEMMA 2.2. *Let $I_m$ be the identity matrix of order $m$. For some positive integers $k$ and $l$ let $W$ be a matrix of the form*

$$W = \begin{pmatrix} I_k & -S \\ -T & I_l \end{pmatrix},$$

*where either $T$ and $S$ are bidiagonal matrices satisfying $T_{i,j} = 0 \Leftrightarrow S_{j,i} = 0$ and $|k-l| \leq 1$ or $T$ and $S$ are nonnegative matrices. Then if $W$ is irreducible, so is $I_l - TS$.*

*Proof.* For any square matrix $U$ of order $m$ let $G[U]$ be the directed graph defined by

$$G[U] \equiv \{1, 2, \ldots, m\},\ \{(i, j) \mid U_{j,i} \neq 0\}$$

where the first set denotes the nodes and the second one the edges of the graph. Irreducibility of $U$ is equivalent to strong connectivity of $G[U]$, which is equivalent to strong connectivity of $G[I - U]$ (see [30]). From the assumptions of the lemma, there follows, at least for $i \neq j$,

$$((I_{k+l} - W)^2)_{j,i} \neq 0 \ \Leftrightarrow\ \{\exists\, m,\ (I_{k+l} - W)_{j,m} \neq 0,\ (I_{k+l} - W)_{m,i} \neq 0\}.$$

Consequently,

$$\{1, 2, \ldots, k+l\},\ \{(i, j) \mid i \neq j \text{ and } \exists\, m \text{ s.t. } (I_{k+l} - W)_{j,m} \neq 0, (I_{k+l} - W)_{m,i} \neq 0\}$$

$$\subset G[(I_{k+l} - W)^2].$$

Let $i_1$ and $i_2$ be some integers satisfying $k+1 \leq i_1, i_2 \leq k+l$. Since $G[I_{k+l} - W]$ is strongly connected, there exists a path in $G[I_{k+l} - W]$ leading from $i_1$ to $i_2$. From the structure of $I_{k+l} - W$ this path must include an even number of edges. Hence $i_1$ is connected to $i_2$ also in $G[(I_{k+l} - W)^2]$. The lemma follows from

$$(I_{k+l} - W)^2 = \begin{pmatrix} ST & 0 \\ 0 & TS \end{pmatrix}.$$

This completes the proof of the lemma.

LEMMA 2.3. *Assume $T$ is an $M$-matrix and* $\text{diag}(T) = I$. *Then $(2I - T)T$ is an $M$-matrix.*

*Proof.* From the assumptions of the lemma, we have $I - T \geq 0$, and, by Theorem 3.10 of [30], $\rho(I - T) < 1$, where $\rho$ denotes the spectral radius. Hence $(I - T)^2 \geq 0$ and $\rho((I - T)^2) < 1$. Since

$$(2I - T)T = I - (I - T)^2$$

the lemma follows from Theorem 3.8 of [30]. This completes the proof of the lemma.

THEOREM 2.4. *Assume $A$ is tridiagonal and one of the following*: (a) *an $M$-matrix,* (b) *a nonsingular weakly diagonally dominant matrix, or* (c) *an irreducibly diagonally dominant matrix. Then so are all the matrices $A_{i+1}$ defined in* (4) *and* (5); *moreover, the matrices $D_i$ defined in* (5) *are symmetric positive definite* (*SPD*) *and, in case* (a), *so are the matrices $S_{A,i+1}$.*

*Proof.* The proof is by induction on $i$ in (5). For case (a), the SPD property of $D_i$ follows from $A_i$ being an $M$-matrix, and the $M$-matrix property of $A_{i+1}$ follows from Lemma 2.3 and

$$(2I - D_i^{-1}A_i)D_i^{-1}A_i = M_i^T \begin{pmatrix} I & B_i \\ C_i & I \end{pmatrix} \begin{pmatrix} I & -B_i \\ -C_i & I \end{pmatrix} M_i$$
$$= M_i^T \begin{pmatrix} I - B_iC_i & 0 \\ 0 & I - C_iB_i \end{pmatrix} M_i.$$

For case (b), the SPD property of $D_i$ follows from the nonsingularity and weak diagonal dominance of $A_i$, the nonsingularity of $A_{i+1}$ follows from

$$D_i^{-1}A_i = M_i^T \begin{pmatrix} I & -B_i \\ -C_i & I \end{pmatrix} M_i$$
$$= M_i^T \begin{pmatrix} I & 0 \\ -C_i & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & I - C_iB_i \end{pmatrix} \begin{pmatrix} I & -B_i \\ 0 & I \end{pmatrix} M_i,$$

and the weak diagonal dominance of $A_{i+1}$ follows from Lemma 2.1. For case (c), the SPD property of $D_i$ follows from irreducible diagonal dominance of $A_i$, and the irreducible diagonal dominance of $A_{i+1}$ follows from Lemmas 2.1 and 2.2. The last part of the theorem follows from $A_i$ being an $M$-matrix. This completes the proof of the theorem.

When its assumption holds, Theorem 2.4 ensures that the matrices $B_i$ and $C_i$ of (5) are well defined and that no division by zero occurs. Otherwise, a diagonal element of $D_i$ (for some $i$) may vanish; this may be handled by a reasonable definition of the corresponding line of $C_i$ and column of $B_i$, and, similarly, of the off-diagonal elements in the corresponding line of $R_{A,i+1}$ and column of $P_{A,i+1}$ (e.g., the templates [0, 1, 0] for restriction and [0, 1, 0]$^t$ for prolongation).

**2.4. The two-dimensional case.** In this subsection we define the operators $R$, $P$, and $Q$ used in (1) for linear systems which arise, for example, from finite difference discretization of the PDE

$$(au_x)_x + (bu_y)_y + cu_x + du_y + \beta u = f,$$

where $a, b, c, d, \beta, u$, and $f$ are functions defined on $\Omega \subset R^2$ and suitable boundary conditions are imposed on $\partial\Omega$.

Let $U(K, L)$ be a permutation matrix such that for any vector $v$ defined on a $K \times L$ grid and ordered lexicographically row by row, $U(K, L)v$ is the same vector $v$ ordered lexicographically column by column. Let

$$U_{k,l} \equiv U(N/2^k, N/2^l), \qquad 0 \le k, l \le n,$$

where, here and in the sequel, $N/2^j$ means an integer division, that is, $\lfloor N/2^j \rfloor$. Suppose $A$ is of the form

$$A = \text{blockdiag}(X^{(j)})_{1\le j\le N} + U_{0,0}^T \cdot \text{blockdiag}(Y^{(j)})_{1\le j\le N} U_{0,0} \tag{7}$$

where $X^{(j)}$ and $Y^{(j)}$ are tridiagonal matrices of order $N$. For example, if

$$X^{(j)} = Y^{(j)} = \text{tridiag}\left(\frac{1}{h^2}, \frac{-2}{h^2} + \frac{\beta}{2}, \frac{1}{h^2}\right), \quad 1 \le j \le N$$

for some $\beta \in C$, then $A$ represents a central discretization of the Helmholtz equation

$$u_{xx} + u_{yy} + \beta u = f$$

in the unit square with Dirichlet boundary conditions.

In the following we give some motivation to the definition of the operators $R$, $P$, and $Q$ used in (1). For simplicity, we treat semi-coarsening in the $x$-direction only; the $y$-direction coarsening is implemented analogously.

By replacing $A$ in (4) with $X^{(j)}$ and applying (5) to it one may define

$$R_x = \text{blockdiag}(R_{X^{(j)},1})_{1\le j\le N}, \quad P_x = \text{blockdiag}(P_{X^{(j)},1})_{1\le j\le N}.$$

The natural definition $Q = R_x A P_x$ is undesirable because it spoils the tridiagonal structure of the second term in the right-hand side of (7). In order to avoid this, only the first term in the right-hand side of (7) is multiplied by $R_x$ and $P_x$ from the left and right sides, respectively; the second term is multiplied instead by rowsum$(R_x P_x)$. According to (6), the relative error inserted into $R_x A P_x$ by this approximation is negligible, at least for functions in the neighborhood of the solution.

In order to perform a $y$-direction coarsening, the second term in the right-hand side of (7) is treated similarly (using restriction and prolongation operators $R_y$ and $P_y$), while not spoiling the structure of the first term. (1) is then implemented with the resulting coarse-grid operator $Q$ and the restriction and prolongation operators $R = R_y R_x$ and $P = P_x P_y$.

We come now to a precise definition of the operators $R$, $P$, and $Q$ of (1) for the 2-d case. Define

$$X_0^{(j)} \equiv X^{(j)}, \quad Y_0^{(j)} \equiv Y^{(j)}, \quad 1 \le j \le N.$$

For $i = 1, \ldots, n$, define the matrices $R_i$, $P_i$, and $A_i$, in this order, by

For $1 \le j \le N/2^{i-1}$, do (5) with $A$ and $i$ replaced by $X^{(2^{i-1}j)}$ and $i-1$, respectively,

For $1 \le j \le N/2^{i-1}$, do (5) with $A$ and $i$ replaced by $Y^{(2^{i-1}j)}$ and $i-1$, respectively,

$$R_i \equiv U_{i,i}^T \cdot \text{blockdiag}(R_{Y^{(2^i j)},i})_{1\le j\le N/2^i} U_{i-1,i} \cdot \text{blockdiag}(R_{X^{(2^{i-1}j)},i})_{1\le j\le N/2^{i-1}},$$

$$P_i \equiv \text{blockdiag}(P_{X^{(2^{i-1}j)},i})_{1\le j\le N/2^{i-1}} U_{i-1,i}^T \cdot \text{blockdiag}(P_{Y^{(2^i j)},i})_{1\le j\le N/2^i} U_{i,i},$$

$$\text{blockdiag}(X_i^{(2^i j)})_{1\le j\le N/2^i} \leftarrow$$

$$\leftarrow U_{i,i}^T \cdot \text{blockdiag}(S_{Y^{(2^i j)},i}))_{1\le j\le N/2^i} U_{i,i} \cdot \text{blockdiag}(X_i^{(2^i j)})_{1\le j\le N/2^i}, \tag{8}$$

$$\text{blockdiag}(Y_i^{(2^i j)})_{1\le j\le N/2^i} \leftarrow$$

$$\leftarrow U_{i,i} \cdot \text{blockdiag}(S_{X^{(2^i j)},i}))_{1\le j\le N/2^i} U_{i,i}^T \cdot \text{blockdiag}(Y_i^{(2^i j)})_{1\le j\le N/2^i},$$

$$A_i \equiv \text{blockdiag}(X_i^{(2^i j)})_{1\le j\le N/2^i} + U_{i,i}^T \cdot \text{blockdiag}(Y_i^{(2^i j)})_{1\le j\le N/2^i} \cdot U_{i,i}.$$

As in the tridiagonal case, the $i$th call to the AutoMUG procedure in (1), $1 \le i \le n$, is accomplished with the operators

$$Q \leftarrow A_i, \quad P \leftarrow P_i, \quad R \leftarrow R_i.$$

The following theorem ensures that the coarse-grid operators $A_i$ enjoy a desirable property.

THEOREM 2.5. *Assume $A$ is defined as in* (7) *with $X^{(j)}$ and $Y^{(j)}$ being tridiagonal irreducibly diagonally dominant M-matrices of order $N$. Then all the matrices $A_i$ defined in* (8) *are irreducibly diagonally dominant M-matrices.*

*Proof.* Following the route of the proof of Theorem 2.4, by induction on $i$ in (8) all the tridiagonal matrices $X_i$ and $Y_i$ are irreducibly diagonally dominant $M$-matrices and the diagonal matrices $S_i$ are SPD. Hence the $A_i$ are weakly diagonally dominant, with a strict diagonal dominance for at least one row. Irreducibility of $A_i$ follows from

$$G[A_i] = \{1, 2, \ldots, N/2^i\} \times \{1, 2, \ldots, N/2^i\},$$

$$\{((k, l), (m, l)) \mid (X_i^{(2^i l)})_{m,k} \neq 0\} \cup \{((l, k), (l, m)) \mid (Y_i^{(2^i l)})_{m,k} \neq 0\}.$$

Hence the $A_i$ are irreducibly diagonally dominant matrices. Since the $A_i$ have positive diagonal elements and nonpositive off-diagonal elements, it follows from [30] that they are also $M$-matrices. This completes the proof of the theorem.

The definition (7) of the coefficient matrix $A$ assumes that the grid is logically rectangular. Problems involving complicated domains may be treated by embedding the original grid into a logically rectangular grid [28] and appending trivial equations for the redundant variables. This approach was used in the numerical experiments in §3. Note that these dummy variables, as well as their corresponding equations, do not have to be stored, since they do not influence the values of the original variables.

**3. Numerical experiments.** Our aim in this section is to show the applicability of AutoMUG to several classes of problems, including indefinite Helmholtz equations. We compare the performance of AutoMUG to that of a standard multigrid version which has the same complexity, that is, uses $(2d + 1)$-coefficient coarse-grid stencils only (see §1). This version, denoted by MG, is implemented as follows: coarse-grid operators are generated from the PDE by the same scheme as that used on the finest grid. Full weighting and bilinear interpolation are used for restriction and prolongation, respectively. For both AutoMUG and MG the maximal number of levels (e.g., six levels for $63 \times 63$ grids) is used, which means setting $o = 2$ in (1); the only exceptions are examples 13 and 14, where four levels are used.

When implementing MG one must use $2^{n+1} - 1$ grid points on the finest grid and $2^q - 1$, $1 \leq q \leq n$, for coarser grids in order to preserve uniformity. Here the even points, which are taken as coarse-grid points, are always internal points of the original grid. For $2^n$-point grids, on the other hand, the last fine-grid point appears as a last grid point in all grids. Hence, coarse grids are biased towards the boundary. For AutoMUG, on the other hand, grids of both $2^n$ points or $2^{n+1} - 1$ points may be used, and actually achieve the same convergence rates; this is because in the $2^n$ points case AutoMUG automatically chooses in the coarse-grid schemes the most accurate extrapolation of boundary points. An odd number of points $N = 63$ is used here for an easier comparison between AutoMUG and MG.

On all grids the smoother was either the one provided by the ILU(1,1) decomposition of [18] and [29] (namely, ILU with no fill-in) or the red-black Gauss–Seidel (RB) relaxation. ILU was considered as a smoother in multigrid in [16] and 17]. One presmoothing and one postsmoothing is performed in each level of a $V$-cycle ($\epsilon = \nu_1 = \nu_2 = 1$ in (1)). The initial guess is random in (0, 1). Double-precision arithmetic is used.

AutoMUG and MG are iterated according to (2) with $10^{-12} \leq$ threshold $\leq 10^{-14}$, to avoid the effect of round-off errors. It was checked that the $l_\infty$ norm of the error is reduced during this process by more than 10 orders of magnitude. Convergence factors are computed from the last four iterations, namely

$$\text{convergence factor} = \left( \frac{\|Ax_{\text{last}} - b\|_2}{\|Ax_{\text{last}-3} - b\|_2} \right)^{1/3}$$

where *last* is the index of the last iteration. When the basic iteration (2) by itself diverges (denoted by "$*$") or unsatisfactorily converges, it is also implemented with an acceleration

TABLE 1

*Convergence factors for MG and AutoMUG (in parentheses: averaged convergence factors when the TFQMR acceleration is used).*

| | MG | MG | AutoMUG | AutoMUG |
|---|---|---|---|---|
| example | ILU | RB | ILU | RB |
| 1 | 0.067 | 0.102 | 0.068 | 0.096 |
| 2a | 0.474 (0.148) | 0.96 (0.667) | 0.474 (0.148) | 0.96 (0.667) |
| 2b | 0.005 | 0.99 (0.83) | 0.005 | 0.99 (0.83) |
| 3 | 0.127 | 0.58 (0.330) | 0.127 | 0.58 (0.330) |
| 4 | 0.181 | 0.287 | 0.088 | 0.198 |
| 5a | 0.235 | 0.49 (0.164) | 0.114 | 0.199 |
| 5b | 0.208 | 0.44 (0.159) | 0.112 | 0.198 |
| 6 | 0.196 | 0.574 (0.269) | 0.154 | 0.424 (0.171) |
| 7 | * (0.525) | * | 0.162 | 0.427 (0.192) |
| 8 | 0.573 (0.159) | 0.886 (0.46) | 0.220 | 0.526 (0.215) |
| 9 | * (0.57) | * | 0.196 | 0.526 (0.205) |
| 10a | 0.057 | 0.458 (0.427) | 0.063 | 0.148 |
| 10b | 0.26 | * | 0.120 | * |
| 11 | * | * | 0.691 (0.243) | 0.865 (0.454) |
| 12 | 0.53 (0.246) | 0.79 (0.414) | 0.994 (0.183) | * (0.392) |
| 13 | * | * (0.60) | * (0.70) | 0.95 (0.314) |
| 14 | * | * (0.714) | * (0.543) | 0.85 (0.367) |

method applied to it. We have used the Transpose-free quasi-minimal residual (TFQMR) method (Algorithm 5.2 in [15]) which avoids the computation of the transpose of the coefficient matrix and preconditioner (the latter is only implicitly given in (1), so its transpose is not available). As a matter of fact, the TFQMR method may be considered a modification of the conjugate gradients squared (CGS) method of [27] and [28], which is a generalization of the conjugate gradients (CG) method to nonsymmetric and indefinite problems. We have found that the performance of CGS is similar to that of TFQMR; however, we have preferred the latter because of its smooth convergence curve.

All the above acceleration techniques require an amount of storage and arithmetical operations comparable to that of CG, namely an additional $1-1.5$ work units per iteration. For the accelerated iteration the convergence factor defined above often oscillates; hence the averaged convergence factor defined by

$$\text{averaged convergence factor} = \left(\frac{\|Ax_{\text{last}} - b\|_2}{\|Ax_0 - b\|_2}\right)^{1/\text{last}}$$

is considered instead, and displayed in parentheses in Table 1. When the accelerated iteration stagnates, the sign "$*$" alone is presented.

The problems solved are of the form

$$Lu(x, y) = f(x, y), \quad (x, y) \in \Omega \subset R^2,$$

with the exact solution $u = xy$ (except of examples 7, 9, 10b, and 12, for which the exact solution is $u = 0$). Since the initial guess is random and the problem is linear, the rates of convergence are independent of the specific choice of the solution. A second-order central finite difference scheme is used. For most examples the region $\Omega$ is the unit square, Dirichlet boundary conditions are imposed, and uniform grids are used. Exceptions to the above are noted at particular examples.

It is seen from the numerical results that for some examples AutoMUG by itself diverges or unsatisfactorily converges, while when supplemented with an acceleration scheme it converges quickly; this is apparently because the iteration matrix has some isolated eigenvalues of large magnitude, while most of its spectrum is clustered around zero.

**List of examples.**

1. The Poisson equation $L = -\Delta$.
2. The anisotropic equation

$$-u_{xx} - \sigma u_{yy} = 0$$

with (a) $\sigma = 10^{-2}$ and (b) $\sigma = 10^{-4}$. This example is more difficult than the Poisson equation, since error components which are smooth in the $x$-direction and oscillate in the $y$-direction are not easily smoothed by a point Gauss-Seidel smoother; this difficulty may be handled by employing an appropriate line relaxation [4].

The ILU smoother used here is lexicographically ordered; hence oscillations in the $x$-direction are smoothed much better than those of the $y$-direction. According to the above remark, it is likely that an anti-lexicographical ordering is more suitable to this example.

Case (a) is the most difficult one considered in [31]. The convergence factors derived there are similar to those obtained here.

3. The Poisson equation with a Chebyshev-type grid; it is discretized via central differences on the two-dimensional grid

$$P_N(j,k) \equiv \left( \frac{1 - \cos\left(\frac{j\pi}{N+1}\right)}{2}, \frac{1 - \cos\left(\frac{k\pi}{N+1}\right)}{2} \right), \quad 1 \le j,k \le N.$$

The matrix operator for this scheme may be used as a preconditioner for a Chebyshev-collocation discretization of the Poisson equation (see [19]). Coarse-grid operators for MG are obtained from the discretization of the PDE on the grids $P_{\lfloor N/2^i \rfloor}$, $1 \le i \le 5$. As in the previous example, the RB smoother is inferior to ILU; the reason for this is that the equation is locally anisotropic in most of the mesh cells.

4. The Poisson equation in a square with a slit. The actual shape is a $63 \times 63$ grid minus a narrow strip of width 2 points and length 32 points emerging from the center in the $x$-direction. This problem is considered more difficult than the Poisson equation in a square (see [5]).
5. The Poisson and definite Helmholtz equations in a domain approximating the North Atlantic, from about 10° to 53° north. A definite Helmholtz problem of the form

$$-u_{xx} - u_{yy} + \beta u = f$$

stems from explicit time-stepping in the quasi-geostrophic version of the shallow-water equations. The domain is embedded in a Cartesian grid of $45 \times 93$ points. The bounding points are assumed to lie on that grid. The cases under consideration are (a) $\beta = 0$ and (b) $\beta = 20$.

6. The Poisson equation with boundary conditions of the third kind

$$\frac{\partial u}{\partial n} + 1.5u = 0,$$

where $\vec{n}$ denotes the outer normal vector. This example is presented mainly for the sake of comparison with the next one.

For this example MG was implemented with restriction and prolongation operators modified near the boundaries such that their rowsums equal 1 everywhere; otherwise,

much slower convergence occurs. For all other examples, however, MG with this modification was inferior to MG with the standard bilinear interpolation and full-weighting restriction.

7. The diffusion equation

$$-(a(x, y)u_x)_x - (a(x, y)u_y)_y = 0$$

with the discontinuous coefficient

$$a(x, y) = \begin{cases} \gamma & \max(|x - 0.5|, |y - 0.5|) \le 3h, \\ 1 & \text{otherwise,} \end{cases}$$

where $h$ is the mesh size and $\gamma = 10^4$ and the boundary conditions of the previous example. It is known [1] that standard multigrid approaches cannot simulate the problem appropriately on coarse grids.

This problem is similar to Problem 3 in [34] and to the most difficult case of Problem 1 in [1]. The fine-grid (for MG, also the coarse-grid) discretization is done as in [1].

8. The Poisson equation on the L-shaped region

$$\Omega = ((0, 1) \times (0, 0.5)) \cup ((0, 0.5) \times (0.5, 1)).$$

Dirichlet and Neumann boundary conditions are imposed on

$$\Gamma \equiv (\{0.5\} \times [0.5, 1]) \cup ([0.5, 1] \times \{0.5\})$$

and $\partial\Omega \backslash \Gamma$, respectively. This example is presented mainly for the sake of comparison with the next one.

9. A diffusion equation in the spirit of Kershaw's problem (Problem 7 in [34]) is solved in the same L-shaped region as above. The equation is that of example 7 with $\gamma = 10^6$. Boundary conditions of the same type as those of example 8 are imposed.

By comparing the results of examples 7 and 9 to those of examples 6 and 8 (respectively) it may be concluded that the discontinuity inserted in examples 7 and 9 does not affect the efficiency of AutoMUG.

10. The convection-diffusion equation with fan-like streamlines

$$-u_{xx} - u_{yy} + \eta(xu_x + yu_y) = f$$

whose characteristics are rays starting at the origin so that they all intersect a boundary. This kind of equation is hard to solve with the multigrid approach, since error terms which are smooth in the convection direction and oscillate in the perpendicular direction are only half-corrected by the coarse-grid term [9].

Two cases were examined: (a) $\eta = 150$, for which diagonal dominance holds and (b) $\eta = 300$, for which it is violated for most of the equations in the linear system.

Unlike all other examples in this section, MG was implemented with coarse-grid operators derived from an upwind, rather than central, scheme; otherwise, considerably slower convergence (or even divergence) was reported.

11. The circulating flow equation

$$\sin(\pi(y - 0.5))\cos(\pi(x - 0.5))u_x - \sin(\pi(x - 0.5))\cos(\pi(y - 0.5))u_y = f.$$

The region is a square with a $1 \times 1$ point hole at the middle of it. For this region, an upwind scheme is inadequate [8]; following [10], we have thus inserted isotropic

artificial viscosity, the amount of which is locally chosen to be the minimal amount required for weak diagonal dominance. The results for AutoMUG are far better than those of the $V$-cycle in [10]. The coarse-grid operators generated by AutoMUG may thus be used in conjunction with the defect correction approach of [10] to accelerate convergence.

For the MG approach divergence was reported no matter whether coarse-grid operators are derived from the central or upwind scheme.

Convection diffusion equations similar to those considered here are solved efficiently in [34]. The method of [34], however, uses the incomplete line LU (ILLU) smoother; this is a robust smoother, which also achieves high rates of convergence when used as a preconditioner in preconditioned CG (with no multigrid strategy) [28]. Since we are interested in investigating the efficiency of multigrid methods on their own, we avoid implementing AutoMUG with smoothers which are also efficient preconditioners.

The last three examples are of special difficulty, involving oscillating coefficients or indefiniteness.

12. The diffusion equation

$$-(a(x-y)u_x)_x - (a(x-y)u_y)_y = 0$$

with the oscillating coefficient

$$a(t) = 1.05 + \sin\left(\frac{t}{\sqrt{2}h}\right)$$

(see [13]). The discretization is symmetric, as in [30].

13. The indefinite Helmholtz equation

$$-u_{xx} - u_{yy} - \beta u = f$$

with $\beta = 200$. Note that for $h = 1/64$ the $(k, l)$ eigenvalue of the Poisson equation, with $(k, l) \in \{(2, 4), (4, 2)\}$, is equal to

$$\frac{4}{h^2}\left(\sin^2\frac{kh}{2} + \sin^2\frac{lh}{2}\right) = 196.8537;$$

hence, with the above choice for $\beta$, the coefficient matrix has nearly singular eigenvalues (see [7]). Furthermore, eight distinct eigenvalues of the Helmholtz equation are negative; hence the problem is indefinite, and the iteration matrix for either AutoMUG or MG often has eigenvalues of magnitude larger than 1 (see [22]–[24]). The use of an acceleration scheme is thus crucial to ensure convergence.

For the current and the following example only four levels are used, and the fourth-level equation is approximately solved by 100 Kacmarz sweeps. The reason for this is that the coefficient matrix for the fifth-level problem is nonpositive for either AutoMUG or MG, hence cannot serve as a suitable approximation to the PDE (see [23] and [24] for a detailed explanation).

14. The indefinite Helmholtz equation (Example 6.3 in [14])

$$-u_{xx} - u_{yy} - \beta u = f$$

with $\beta = 200$, complex boundary conditions of the third kind

$$\frac{\partial u}{\partial n} + 10iu = g, \quad (x, y) \in [0, 1] \times \{0\},$$

and Dirichlet boundary conditions on the rest of $\partial\Omega$. The mixed boundary conditions are discretized via a first-order scheme as in [14]. Like the previous problem, this problem is indefinite, hence the use of acceleration is crucial.

Unlike most of the examples in this section, for the indefinite examples RB is a better smoother than ILU. We believe this is due to the instability of ILU for coarse-grid equations; this may be handled by adding some positive weights to main diagonal elements in the ILU decomposition which become too small.

**4. Discussion.** AutoMUG is a multilevel method for the solution of finite difference schemes of $(2d+1)$-coefficient stencils which arise, for example, from $d$-dimensional second-order PDEs. It is automatic in the sense that its definition depends on the scheme on the original grid only, and no rediscretization of the PDE is required. Derivation of coarse-grid, restriction, and prolongation operators for AutoMUG is inexpensive and straightforward. In addition, property A of the coefficient matrix is preserved at all levels; this simplifies the programming and enables the use of the RB and SOR smoothers.

The numerical examples show that, when implemented with a suitable smoother, AutoMUG gives high rates of convergence for several classes of problems: symmetric, nonsymmetric and problems with discontinuous coefficients, nonuniform grids, and nonrectangular domains. When supplemented with an acceleration scheme, high rates of convergence also are achieved for pure convection problems and indefinite Helmholtz equations.

For some problems AutoMUG is inferior to nonautomatic multigrid algorithms designed especially for the specific problem. In particular, it is inferior to the method of [7] for slightly indefinite problems and to that of [10] for problems with circulating flow. In these cases, it is recommended that the coarse-grid operators of AutoMUG be used in conjunction with the specific approach, that is, the projection of [7] or the overresidual weighting and defect correction of [10]. Alternatively, accelerating AutoMUG by a Lanczos-type method also yields high rates of convergence. For highly indefinite problems, the use of such acceleration is crucial, since the basic iteration often diverges. Hence for problems which involve several sources of difficulty, e.g., indefiniteness, convection, jumps, singularities, etc., AutoMUG supplemented with an acceleration scheme seems to provide an effective solver.

**Acknowledgment.** We wish to thank Dr. Irad Yavneh for valuable comments and for suggesting examples 4 and 5.

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