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QMR METHODS IN COMPUTATIONAL FLUID DYNAMICS*

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We examine the application of QMR methods to the solution of linear systems of equations arising from the use of implicit solution methods in computational fluid dynamics. We will deal with implicit finite difference schemes for solving the Euler equations. These schemes may arise from the implicit treatment of the time dependent equations or from the use of Newton's method for the solution of the steady state equations. In both situations it is necessary to solve a large sparse nonsymmetric linear system of equations at each iteration. We will examine the effectiveness of QMR in the solution of these systems. We compare the resulting methods to methods which rely on some other simplifying technique to solve the linear systems. Our goal is to show that the QMR method is a viable alternative to the more ad-hoc schemes for solving implicit computational fluid dynamics problems.

KEY WORDS: Beam-Warming approximation, Euler equations, iterative methods, QMR

1. INTRODUCTION

We wish to examine the use of the Quasi-Minimal Residual (QMR) method due to Freund and Nachtigal[4] for the solution of large sparse linear systems of equations arising from the discretization of fluid dynamics problems. In particular, we considered the solution of the Euler equations of compressible flow in two dimensions via implicit finite difference methods as described by Pulliam[8]. This method is based on the implicit discretization of the time dependent Euler equations, and it requires the solution of a large banded system of equations at each iteration. Pulliam addresses the problem of solving this large sparse system by using the Beam and Warming[1] approximate factorization technique, which replaces the two-dimensional operator with an approximate factorization into two one-dimensional operators. This factorization, though approximate, is still relatively accurate. Nonetheless, the iterate obtained in this fashion does not exactly satisfy the original linear system; we view this as an ad-hoc method of solving the original system to reduced accuracy. Instead, we propose to investigate the use of the QMR method as an alternative to the Beam and Warming method for solution of the linear systems of equations.

The remainder of the paper is organized as follows. In Section 2 and Section 3, we present the background material on the solution of the Euler equations and on the quasi-minimal residual algorithm, respectively. We describe the basic algorithm and its application to the problem under investigation. In Section 4, we show some numerical examples, and in Section 5, we make some concluding remarks.

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2. CFD BACKGROUND

2.1 THE EULER EQUATIONS

The flow of an inviscid, compressible fluid is governed by the Euler equations. These equations written in generalized curvilinear coordinates are

$$\partial_\tau Q + \partial_\xi E + \partial_\eta F = 0, \tag{1}$$

where

$$Q = J^{-1}\begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{bmatrix}, \; E = J^{-1}\begin{bmatrix} \rho U \\ \rho u U + \xi_x p \\ \rho v U + \xi_y p \\ U(e+p) \end{bmatrix}, \; F = J^{-1}\begin{bmatrix} \rho V \\ \rho u V + \eta_x p \\ \rho v V + \eta_y p \\ V(e+p) \end{bmatrix}.$$

The contravariant velocities are $U = \xi_x u + \xi_y v$, and $V = \eta_x u + \eta_y v$. The independent variables are the fluid density ρ, the Cartesian components of velocity u and v, the total energy e, and the pressure p. The equation of state is taken to be

$$p = (\gamma - 1)(e - \frac{1}{2}\rho(u^2 + v^2)),$$

where γ is the ratio of specific heats. The transformation to curvilinear coordinates $\xi = \xi(x, y)$ and $\eta = \eta(x, y)$ is chosen so that the spacing in the curvilinear coordinates is uniform and of unit length. The quantity $J^{-1} = (x_\xi y_\eta - x_\eta y_\xi)$ appearing in the above equation is the inverse of the Jacobian of the transformation. In Eq. (1), ∂_τ, ∂_ξ and ∂_η represent differentiation with respect to time, the ξ coordinate, and the η coordinate, respectively. Eq. (1) relates the time derivative of the conservative variables Q to the spatial differences of the flux vectors E and F.

2.2 DISCRETIZATION

Eq. (1) is differenced in time by the first order implicit scheme

$$Q^{n+1} - Q^n + h(E_\xi^{n+1} + F_\eta^{n+1}) = 0 \tag{2}$$

where $h = \Delta t$ is the time step. The flux vector terms in this equation are linearized in time about Q^n

$$E^{n+1} = E^n + A^n \Delta Q^n + \mathcal{O}(h^2) \tag{3}$$
$$F^{n+1} = F^n + B^n \Delta Q^n + \mathcal{O}(h^2) \tag{4}$$

where $A = \partial E/\partial Q$ and $B = \partial F/\partial Q$ are the flux Jacobians and $A,\ B \in \Re^{4\times 4}$. Substituting these relations into Eq. (2) gives

$$[I + h\partial_\xi A^n + h\partial_\eta B^n]\Delta Q^n = -h(\partial_\xi E^n + \partial_\eta F^n).$$

The spatial derivatives ∂_ξ and ∂_η are approximated by centered differences δ_ξ and δ_η respectively, where $\delta_\xi u_{i,j} = (u_{i+1,j} - u_{i-1,j})/2$ and $\delta_\eta u_{i,j} = (u_{i,j+1} - u_{i,j-1})/2$.

This results in the fully discretized form of the Euler equations

$$[I + h\delta_\xi A^n + h\delta_\eta B^n]\Delta Q^n = -h(\delta_\xi E^n + \delta_\eta F^n). \tag{5}$$

Artificial dissipation is added to Eq. (5) for stability reasons. Implicit second and mixed explicit second and fourth difference operators are used. The full details of the implementation can be found in Pulliam[7], and a complete description of boundary condition treatment and artificial dissipation can be found in Pulliam[8].

2.3 MATRIX FORMS

The expression $[I + h\delta_\xi A^n + h\delta_\eta B^n]$ in Eq. (5) represents a large sparse matrix, with the following structure:

$$G = \begin{bmatrix}
I & A & & & B & & & & & & & \\
-A & \cdot & \cdot & & & \cdot & & & & & & \\
 & \cdot & \cdot & A & & & \cdot & & & & & \\
 & & -A & I & & & & \cdot & & & & \\
-B & & & & I & A & & & \cdot & & & \\
 & \cdot & & & -A & \cdot & \cdot & & & \cdot & & \\
 & & \cdot & & & \cdot & \cdot & \cdot & & & \cdot & \\
 & & & \cdot & & & \cdot & \cdot & & & & B \\
 & & & & \cdot & & & & I & A & & \\
 & & & & & \cdot & & & -A & \cdot & \cdot & \\
 & & & & & & \cdot & & & \cdot & \cdot & A \\
 & & & & & & & -B & & & -A & I
\end{bmatrix}.$$

The system $Gx = b$ is usually not solved directly because of the large computational cost. Instead, the amount of work required can be greatly reduced by approximately factoring the matrix into the product of two block tridiagonal systems, $G \approx G_1 G_2$, where $G_1 G_2 x = b$ is easier to solve than the original system. The matrices G_1 and G_2 have the form

$$G_1 = \begin{bmatrix}
I & A & & & & & & & & & & \\
-A & \cdot & \cdot & & & & & & & & & \\
 & \cdot & \cdot & A & & & & & & & & \\
 & & -A & I & & & & & & & & \\
 & & & & I & A & & & & & & \\
 & & & & -A & \cdot & \cdot & & & & & \\
 & & & & & \cdot & \cdot & \cdot & & & & \\
 & & & & & & \cdot & \cdot & & & & \\
 & & & & & & & & I & A & & \\
 & & & & & & & & -A & \cdot & \cdot & \\
 & & & & & & & & & \cdot & \cdot & A \\
 & & & & & & & & & & -A & I
\end{bmatrix}$$

and

$$G = \begin{bmatrix} I & B & & & \\ & \ddots & \ddots & & \\ -B & & \ddots & & \\ & \ddots & & \ddots & B \\ & & & -B & I \end{bmatrix}.$$

This is the basis of the approximate factorization method proposed by Beam and Warming[1]. It amounts to a decoupling of the coordinate directions. The solution is obtained by solving the two block tridiagonal linear systems in succession by LU decomposition: first $G_1 y = b$ is solved for y, and then $G_2 x = y$ is solved for x.

3. QMR BACKGROUND

The quasi-minimal residual method is a Krylov subspace method for the solution of linear systems. It relies on the nonsymmetric Lanczos algorithm to build a basis for the Krylov space, and it then uses the quasi-minimal approach to select an iterate from the space. We will briefly describe the nonsymmetric Lanczos process and the quasi-minimal approach; full details can be found in Freund et al [3,4,5]. In practice, iterative methods are often of little help without a good preconditioner; we will therefore also briefly discuss preconditioning.

3.1 THE LOOK-AHEAD LANCZOS ALGORITHM

Given two starting vectors v_1 and w_1 and a matrix A, the look-ahead Lanczos algorithm is a procedure for building two sets of basis vectors, $\{v_j\}_{j=1}^n$ and $\{w_j\}_{j=1}^n$, for the Krylov spaces $K_n(v_1, A)$ and $K_n(w_1, A^T)$. Here, $K_n(v, A)$ denotes the nth Krylov subspace generated by a vector v and the matrix A,

$$K_n(v, A) = \text{span}\{v, Av, \ldots, A^{n-1}v\}.$$

The two basis sets are generated so that they are block biorthogonal:

$$(W^{(j)})^T V^{(k)} = \begin{cases} D^{(k)} & \text{if } j = k, \\ 0 & \text{if } j \neq k, \end{cases} \qquad j, k = 1, \ldots, l. \tag{6}$$

Here,

$$\begin{aligned} V^{(k)} &= [\, v_{n_k} \quad v_{n_k+1} \quad \cdots \quad v_{n_{k+1}-1} \,], \\ W^{(k)} &= [\, w_{n_k} \quad w_{n_k+1} \quad \cdots \quad w_{n_{k+1}-1} \,], \end{aligned} \qquad k = 1, \ldots, l-1,$$

and

$$V^{(l)} = [\, v_{n_l} \quad v_{n_l+1} \quad \cdots \quad v_n \,],$$
$$W^{(l)} = [\, w_{n_l} \quad w_{n_l+1} \quad \cdots \quad w_n \,],$$

where

$$1 = n_1 < n_2 < \cdots < n_k < \cdots < n_l \leq n < n_{l+1}.$$

The basis vectors are thus grouped in blocks, indexed by k, with the current block denoted by l. The blocks $D^{(k)}$ are nonsingular for $k = 1, \ldots, l-1$, and $D^{(l)}$ is nonsingular if $n = n_{l+1} - 1$. The main advantage of the look-ahead Lanczos process is that the bases can be built with short block recurrences. The vectors v_{n+1} and w_{n+1} are built using the recurrences

$$v_{n+1} = Av_n - V^{(l)}\mu_n - V^{(l-1)}\nu_n,$$
$$w_{n+1} = A^T w_n - W^{(l)}\mu_n - W^{(l-1)}\nu_n.$$

At each step, one attempts to construct the recurrence coefficients μ_n and ν_n so that the new vector v_{n+1} is biorthogonal to all vectors $w_1, w_2, \ldots, w_n$ (and similarly for w_{n+1}). If this succeeds, then v_{n+1} starts a new block, and l is updated accordingly. Otherwise, the algorithm is said to have encountered a breakdown, and one selects the recurrence coefficients μ_n and ν_n so that only the relaxed biorthogonality condition (6) is enforced. In most practical applications, it turns out that typically, each block involves only one vector, thus reducing the recurrences above to a simple three-term recurrence. Thus, the entire process can be described in matrix form as:

$$\begin{aligned} AV_n &= V_{n+1}H_n, \\ A^T W_n &= W_{n+1}H_n, \\ W_n^T V_n &= D_n, \end{aligned} \tag{7}$$

where D_n is a block diagonal matrix with the blocks $D^{(k)}$ on the diagonal, H_n is an $(n+1) \times n$ block tridiagonal unit upper Hessenberg matrix, and

$$V_n := [\, v_1 \quad v_2 \quad \cdots \quad v_n \,].$$

Full details on the implementation of the look-ahead Lanczos algorithm can be found in Freund et al[3,5].

3.2 THE QUASI-MINIMAL RESIDUAL APPROACH

One of the applications of the look-ahead Lanczos algorithm is to the solution of linear systems

$$Ax = b \tag{8}$$

by a Krylov subspace iterative method. Here, A is a nonsingular $N \times N$ matrix, real or complex. Suppose that x_0 is a given guess to the solution x. If one starts the Lanczos process with $v_1 = r_0 = b - Ax_0$, then the Lanczos vectors v_i will span the Krylov space $K_n(r_0, A)$. A Krylov subspace method will then generate iterates x_n from

$$x_n = x_0 + V_n z_n, \tag{9}$$

where z_n is a vector of n coefficients. Using Eqs. (9) and (7), the residual r_n is given by

$$r_n = b - Ax_n = r_0 - AV_n z_n = r_0 - V_{n+1} H_n z_n.$$

Since $v_1 = r_0$, this simplifies to

$$r_n = V_{n+1}(e_1 - H_n z_n).$$

At this point, it would be possible to compute the coefficient vector z_n that minimized the norm of r_n, but this would require $\mathcal{O}(Nn^2)$ work, which quickly becomes too expensive. Instead, the quasi-minimal approach minimizes only the coefficient vector $e_1 - H_n z_n$. This is an $(n+1) \times n$ least squares problem, that is easily solved by constructing (and updating) the QR decomposition of the upper Hessenberg matrix H_n. In addition, even though Eq. (9) constructs the iterate x_n from all the previous Lanczos vectors v_i, it is possible to derive a short block recurrence for the QMR iterates, so that the storage required by the method is low. The quasi-minimal approach turns out to be powerful enough to allow one to prove several important theoretical results about the QMR algorithm, and in particular convergence, making it the first algorithm in the class of Lanczos-based methods for which such strong statements can be made. Once again, full details on the implementation of the method and its properties can be found in Freund and Nachtigal[4,5].

3.3 PRECONDITIONING

As already mentioned, in practice, the convergence of an iterative method such as QMR is often dismal without the use of a preconditioner. This means that, instead of solving the original linear system (8), one solves the equivalent linear system

$$\tilde{A}\tilde{x} = \tilde{b}, \tag{10}$$

where $\tilde{A} = M_1^{-1} A M_2^{-1}$, $\tilde{x} = M_2 x$, and $\tilde{b} = M_1^{-1} b$. The matrices M_1 and M_2 are factors of the preconditioner matrix $M = M_1 M_2$. The preconditioning is called left, if $M_2 = I$, or right, if $M_1 = I$, or two-sided, if neither M_1 nor M_2 is the identity. It is always possible to recover the original iterates x_n from the preconditioned iterates $\tilde{x}_n$, and the hope is that the preconditioned system (10) will converge faster than the original system (8) would. Thus, one obvious requirement is that one must be able to cheaply compute solutions of linear systems involving M_1 and M_2.

It turns out that the convergence of Krylov subspace methods such as QMR can be related to the distribution of the spectrum and to the non-normality of the coefficient matrix A. In particular, convergence properties can be linked to the problem in approximation theory of constructing a polynomial of as low degree as possible, normalized to be 1 at the origin, and whose maximum on a set enclosing the eigenvalues of A is as small as possible. This implies that the QMR method will converge well on a matrix whose spectrum is relatively well clustered and separated from the origin, since it easy to construct a polynomial small on such a spectrum. Conversely, the convergence of the method is expected to be poor if the

spectrum of the matrix A surrounds the origin. Thus, the common wisdom is to design preconditioners that tend to cluster the spectrum of the matrix. However, beyond that, the design of good preconditioners is still somewhat of a black art. For the problems considered here, the QMR method converged well even without a preconditioner, but this need not be the case in general.

4. NUMERICAL EXAMPLES

4.1 TEST CASE

The physical test problem is the flow in a channel with a ten percent circular arc on the lower surface. The inflow mach number is 1.8. The mesh has 80 points in the stream wise direction and 50 points in the cross flow direction. Points are packed on the lower wall, near the circular arc. The linear system is solved for interior points only and so there are 14976 unknowns ($78 \times 48 \times 4$ equations). This large number of points is perhaps overkill for this simple geometry but is used to demonstrate the ability of the iterative solver to address large problems. The flowfield is initialized to free stream conditions and the solution iterated in time for 800 time steps. The time step was taken to be constant over the entire mesh and for this problem was $\Delta t = 0.01$.

The two approaches discussed in Section 2 and Section 3 were used to solve the problem. First, the Beam and Warming method of approximate factorization was used. Recall that in this technique, two block tridiagonal matrices whose product is approximately the matrix in Eq. (5) are solved by LU decomposition. Solutions resulting from this technique do not solve the linear system exactly. The second approach used QMR to solve the original matrix from (5). In particular, we used the transpose-free QMR algorithm, proposed by Freund[2], using the codes from QMRPACK[6]. The key strategy here was to solve each linear system to reduced accuracy. The problem with this strategy lies in determining the required accuracy. The Beam and Warming solutions satisfy $\hat{A}x = b$ where $\hat{A}x = Ax + \mathcal{O}(\Delta t^2)$ and A is the unfactored matrix. From this we conclude that the Beam and Warming iterate gives $||Ax - b|| \approx \mathcal{O}(\Delta t^2)$. It seems reasonable then to require a residual of similar magnitude from the QMR method. Fig. 1 shows the residual norm of the linear system due to the Beam and Warming iterate for the first 100 iterations (time steps). The figure shows that the residual norm is indeed $\mathcal{O}(\Delta t^2)$. The convergence criteria for QMR was selected to reduce the norm of the linear system below Δt^2.

As a result of this convergence criterion, QMR converged in 4 to 8 iterations per linear system. The time required to solve each system in this way was considerably less than that required to solve the two block tridiagonal systems. Fig. 2 shows the relative speeds of the two solution methods. The figure is a plot of Euler residual vs time. Curve A is the approximate factorization method and curve B is the QMR method. The test was run on an IBM RS/6000 530. Solving the linear systems to reduced accuracy with QMR greatly reduces the overall computing time for the problem.

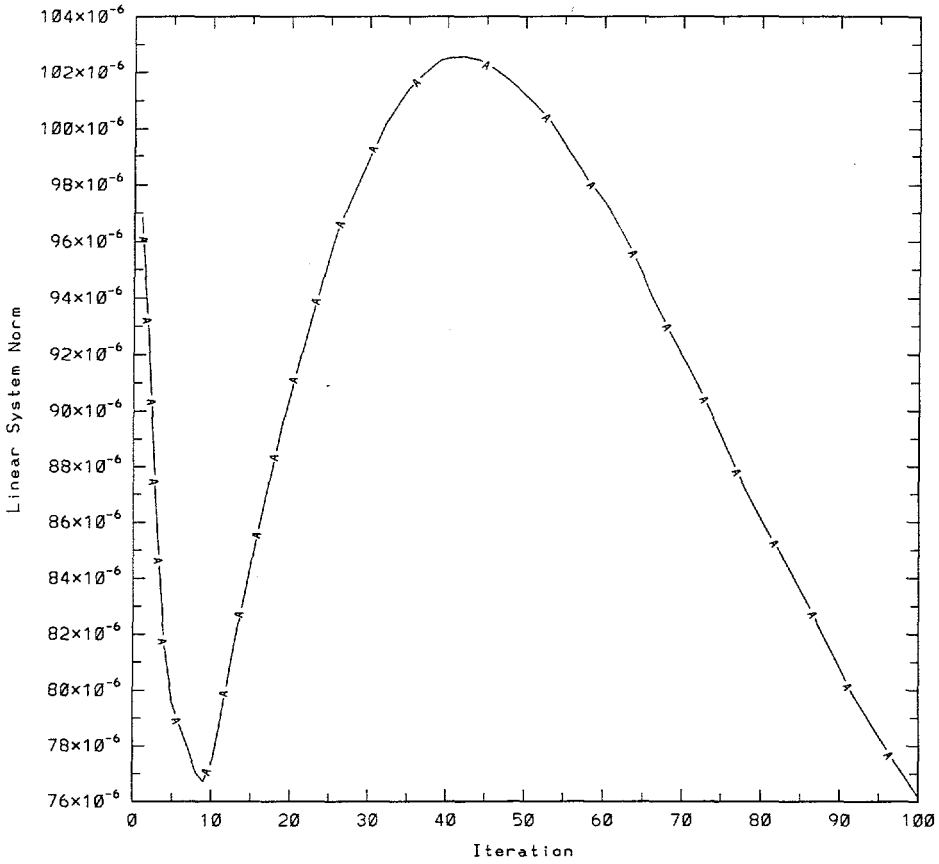

FIGURE 1: Linear system residual norm, Beam and Warming

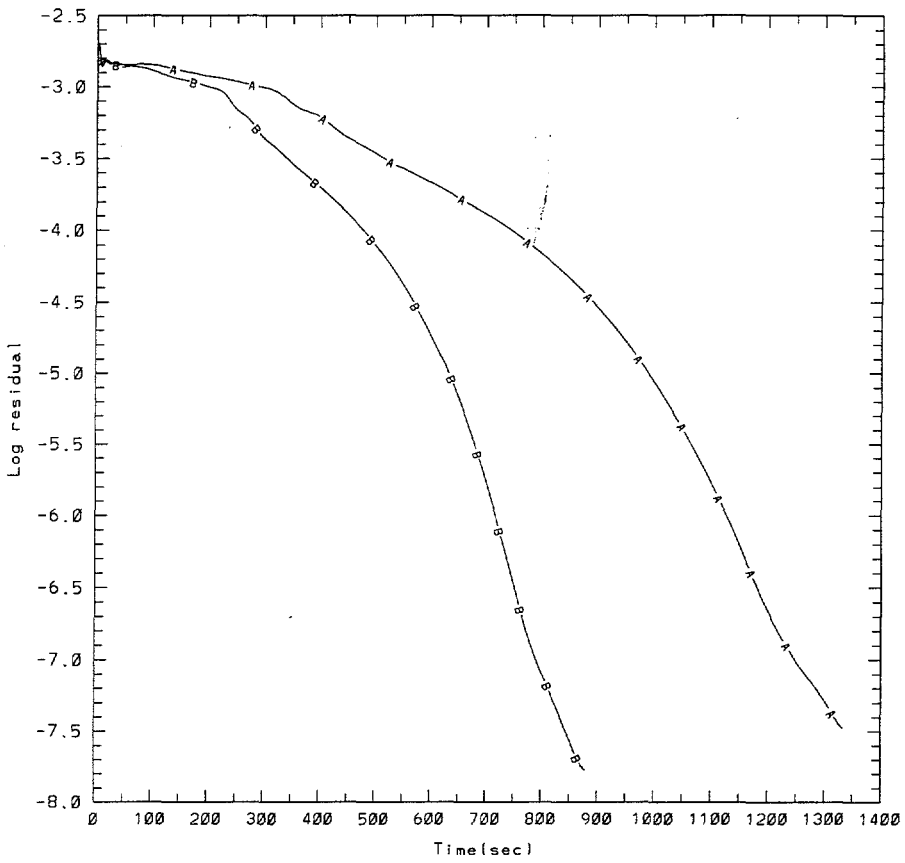

FIGURE 2: Euler residual norm, Beam-Warming (A) vs. QMR (B)

5. CONCLUSION

We examined the use of the quasi-minimal residual method for the solution of linear systems of equations arising from the solution of the compressible two-dimensional Euler equations discretized via implicit finite differences. The method was found to be competitive, even without preconditioning, with the approximate factorization technique proposed by Beam and Warming, at least in the context of computing time-accurate solutions. We plan to further investigate the use of the QMR algorithm for the computation of steady-state solutions; in these cases, preliminary results indicate that preconditioning may be required to improve the convergence of the iterative method.

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