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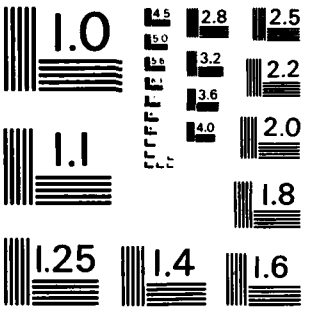

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Numerical Methods for Singular Perturbation Problems

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PREFACE

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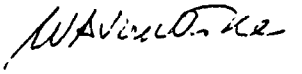

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Singular perturbation equations contain many of the essential difficulties of the Navier-Stokes equations. In this report the weighted-mean scheme for linear equations and the monotone difference scheme for nonlinear equations were adopted. Presented here are fasc iterative techniques for solving large systems of equations that result from discretization. Numerical results are also presented for nonlinear cases using Newton's

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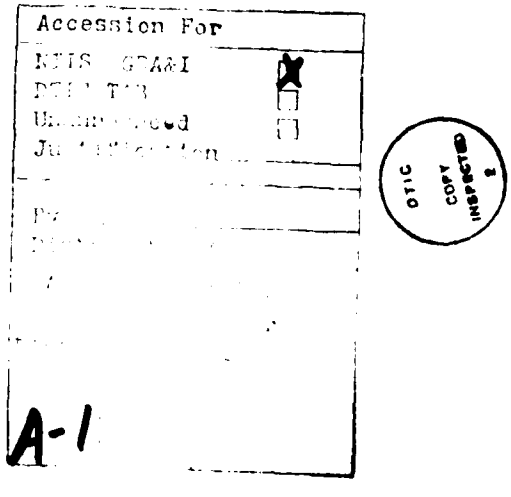
20. ABSTRACT (Cont'd)

method combined with the minimal residual method. The main conclusions are that minimal residual methods with a preconditioning technique and multigrid methods with a special relaxation scheme have proved to be quite reliable and far more efficient than standard iterative methods.

TABLE OF CONTENTS



LIST OF ILLUSTRATIONS

LIST OF TABLES

NUMERICAL METHODS FOR SINGULAR PERTURBATION PROBLEMS

INTRODUCTION

Numerical analysis of singular perturbation problems has been of considerable interest recently since these problems mimic difficulties encountered with the Navier-Stokes equations. The existence of a small parameter, ε, in singular perturbation problems causes the appearance of a thin boundary layer in their solutions. If ε tends to zero, an infinite number of grid points need to be clustered near the physical boundary so that the boundary layer can be properly resolved. Moreover, in the nonlinear case, the location of the boundary layer is not known a priori, and this renders the problem more difficult.

Finite difference approximations of singular perturbation problems lead to unsymmetric matrices. Reliable and fast iterative methods will be presented here for linear and nonlinear problems. The assumption is that matrices are diagonally dominant, and the methods do not require the symmetry property of matrices. Numerical results will be compared with solutions from standard algorithms.

THE LINEAR PROBLEM

Consider the linear advection-diffusion equation in conservative form:

$$\frac{\partial}{\partial x}\left(u\phi - \varepsilon \frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(v\phi - \varepsilon \frac{\partial \phi}{\partial y}\right) = 0 , \qquad (1)$$

where ϕ is the advected quantity, u and v are velocity components in x and y directions respectively, and ε is the diffusivity constant. Fiadeiro and

Veronis[1] proposed the weighted mean (W-M) scheme to discretize equation (1) as

$$W\,\phi_{i-1,j} + E\,\phi_{i+1,j} + S\,\phi_{i,j-1} + N\,\phi_{i,j+1} - C\,\phi_{i,j} = 0\,,$$

where

$$W = \frac{u_i - 1/2}{2\Delta x}\left[\coth\left(\frac{u_i - 1/2\,\Delta x}{2\epsilon}\right) + 1\right].$$

$$E = \frac{u_i + 1/2}{2\Delta x}\left[\coth\left(\frac{u_i + 1/2\,\Delta x}{2\epsilon}\right) - 1\right],$$

$$S = \frac{v_j - 1/2}{2\Delta y}\left[\coth\left(\frac{v_j - 1/2\,\Delta y}{2\epsilon}\right) + 1\right],$$

$$N = \frac{v_j + 1/2}{2\Delta y}\left[\coth\left(\frac{v_j + 1/2\,\Delta y}{2\epsilon}\right) - 1\right],$$

$$C = W + E + S + N.$$

The W-M scheme retains the five-point operator character of central difference except that, in the limit, it tends to central difference for strongly diffusive cases and to upwind difference for strongly advective cases. This scheme is derived by using the flux conserving principle; the discretization error is $0\,(\Delta x^2, \Delta y^2)$. Significant advantages of the scheme are that there are no local instabilities in the solution with respect to central difference and that no testing is required at each grid point with respect to upwind difference. Its stability for all grid spacings has been found to result in fast convergence when using the preconditioned minimal residual method and the multigrid method. For comparative purposes, the successive line over-relaxation (SLOR) algorithm, which serves as a standard iterative method, is briefly described.

SUCCESSIVE LINE OVER-RELAXATION (SLOR) METHOD

Equation (1) can be rewritten as

$$L\phi = 0,$$

where L is a differential operator. The SLOR method[2] can be implemented as follows:

$$\left(\alpha + \delta_{yy} + \delta_{xx}\right) \quad e_{ij}^{n} = - \omega \, L \, \phi_{ij}^{n} \quad ,$$

where $e_{ij}^{n} = \phi_{ij}^{n+1} - \phi_{ij}^{n}$ and ω is the relaxation parameter.

The scheme is implicit in the sense that in the x and y directions an inversion of a tridiagonal matrix equation for a given value of i or j is required. In these numerical examples an optimal relaxation factor, ω, is assumed.

THE PRECONDITIONED MINIMAL RESIDUAL (PMR) METHOD

The discretization of equation (1) yields a large system of linear equations

$$Ax = b, \tag{2}$$

where A is a large, sparse, and nonsymmetric coefficient matrix; x is the solution vector; and b contains boundary terms.

Introduced now is a nonsingular matrix, C, called the preconditioning matrix. Equation (2) is thus equivalent to

$$\hat{A}\hat{x} = \hat{b}, \tag{3}$$

where $\hat{A} = C^{-1}A$, $\hat{x} = x$ and $\hat{b} = C^{-1}b$. This case is denoted as PMR I. A more general choice for equation (2) is $\hat{A} = PAQ$, $\hat{X} = Q^{-1}x$, and $\hat{b} = Pb$, where

P and Q are nonsingular matrices. The second case is called PMR II. The procedure for transforming equation (2) into equation (3) is known as a preconditioning technique. Once the matrix C or the matrices P and Q have been chosen, the standard minimal residual (MR) method[3] can be applied to the transformed equation. A different choice for C or for P and Q, therefore, leads to a different preconditioned MR method and, in consequence, different rates of convergence.

To accelerate the convergence rate of the PMR method, it is desirable to find matrices such that $K(C^{-1}A) \ll K(A)$ or $K(PAQ) \ll K(A)$, where $K(M)$ is the condition number of matrix M. The PMR I method can be implemented by the following algorithm:

Let $K = 0$, $r_o = \hat{b} - \hat{A}\hat{X}$. For $K = 0, 1, 2, \ldots$, compute the vectors $\hat{X}_{K+1}$, r_{K+1} from

$$\hat{X}_{K+1} = \hat{X}_K + \alpha_K r_K \text{ , where } \alpha_K = \frac{\left(\hat{A}r_K , r_K\right)}{\left(\hat{A}r_K , \hat{A}r_K\right)} ,$$

$$r_{K+1} = \hat{b} - \hat{A}\hat{X}_{K+1} = r_K - \alpha_K \hat{A}r_K .$$

A similar procedure can be applied to the PMR II method. To minimize the computational work involved in the preconditioning technique, the matrix C should easily be invertible. In general, C is chosen to be the product of lower and upper triangular matrices; i.e., $C = LU$. The inverse can therefore be obtained through simple forward and backward substitutions.

ROW-SUM AGREEMENT FACTORIZATION

Wong[4] suggested an incomplete factorization based on the principle of agreement of row-sum between the preconditioning matrix C and the original matrix A:

Row-sum (A) = Row-sum (C) = Row-sum (LU)

A = LU+R, where R is the defect matrix; hence Row-sum (R) = 0

Therefore, matrix C resembles matrix A in the sense that their eigenvalues have the same bound, namely the norm of A. Different algorithms can be found in Wong[4] for constructing L and U. The row-sum agreement factorization is shown schematically in figure 1. L and U have non-zero elements in these positions which correspond to the nonzero elements in the lower and upper triangular parts of A. The off-diagonal elements of C, whose locations correspond to the nonzero off-diagonal elements of A, are set to those values. If $||R||$ is small, LU will be a good approximation to A; consequently, a fast convergence can be achieved by the PMR method.

THE MULTIGRID PROCEDURE

The <<Cycle C>> algorithm with correction storage is used here, as presented by Brandt.[5] The initial approximate solution is defined on the finer grid, and then relaxed. When the relaxation is found to be inefficient, a correction is projected on a coarser grid. When the relaxation converges on any grid, the values on the finer grid are updated, and relaxation performed at this finer level. The sequence of grids used is not defined a priori, but depends on the efficiency and convergence of the relaxation just completed. Data are transferred from fine to coarse grids

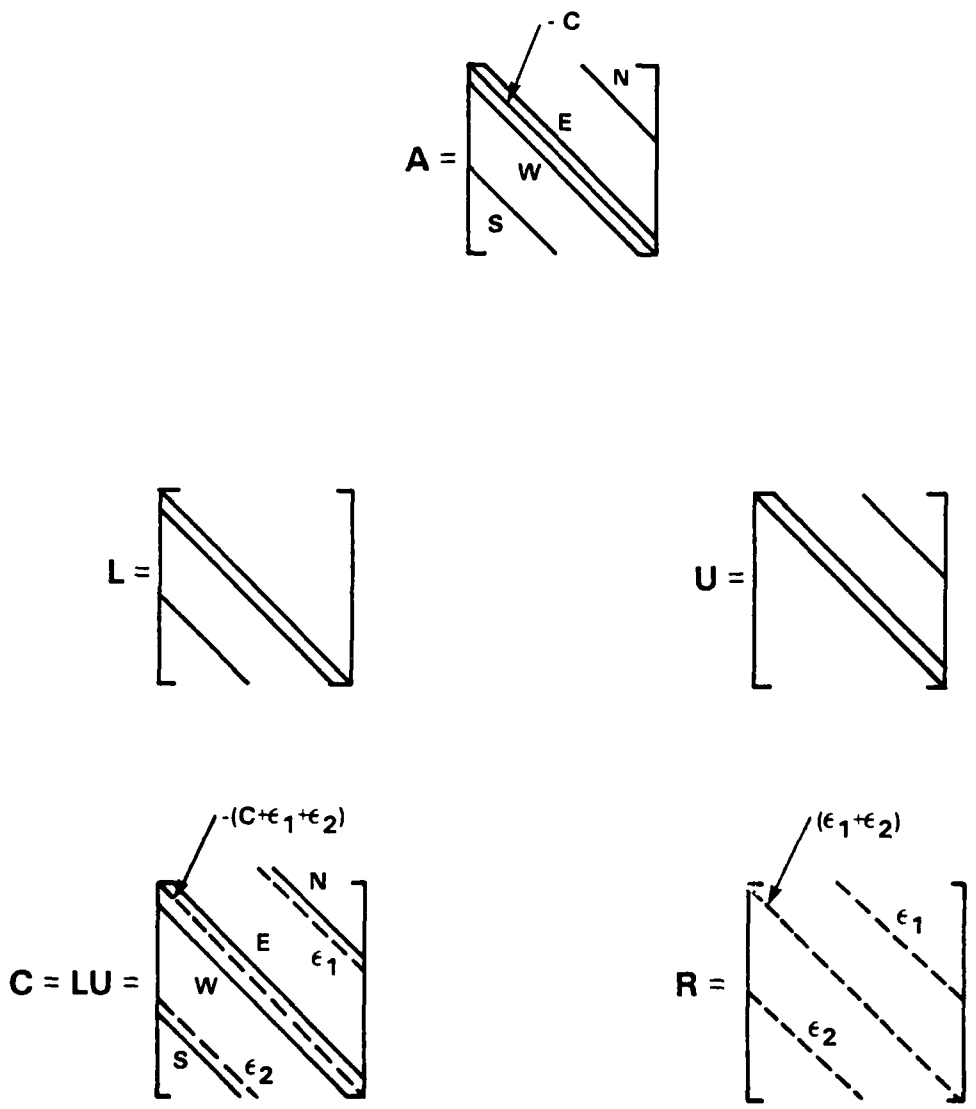


Figure 1. Row-Sum Agreement Factorization

by projection, and from coarse to fine grids by linear interpolation. The relaxation performed is point Gauss-Seidel. Since the problem is linear and the velocity field is explicitly given, the coefficients N, S, E, W are explicitly computed at each level, using the appropriate location (x,y) and Δx, Δy.

Used here for an efficiency criterion is:

residual at present relaxation $\leq$ 0.6 (residual at former relaxation); and for a convergence criterion:

$$\left(\frac{\text{residual on "coarse" grid K}}{h_K^2}\right) \leq 0.3 \left(\frac{\text{residual on "fine" grid K + 1}}{h_{K+1}^2}\right).$$

This scaling takes into account the fact that the method is second order, i.e., error $\sim h^2$.

A simple local analysis produces an interesting result for variable flow fields. Consider the smoothing rate for Gauss-Seidel relaxation in the usual ordering, with both x and y increasing:

$$\bar{\mu} = \underset{\frac{\pi}{2} \leq \xi,\ \eta \leq \pi}{\text{MAX.}} \left| \frac{E\, e^{i\xi} + N e^{i\eta}}{C - We^{-i\xi} - Se^{i\eta}} \right| .$$

Since $\bar{\mu}$ is the reduction factor for high frequency modes, it should be as small as possible. But, from the explicit expression for N, S, E, W, it can be seen that if u or v is negative and large in magnitude, E >> W and N >> S, as they should be in an upstream differentiation formulation. This produces a smoothing rate very near to one. Thus, if u is negative, relaxation should not be in the direction of increasing x.

If the flow field is reasonably simple, so that the relaxation can be explicitly performed following the flow, i.e., x, y, increasing if only u, v > 0, then the convergence is much faster.

It wasn't necessary to use this method on these test problems as u, v > 0 everywhere, but there are results showing speedup of convergence of a Bénard cell type problem solved by Lustman, et al.[6] In any case, multigrid iteration is evidently faster than SLOR, even when the best overrelaxation parameter is used, as table 1 shows.

NUMERICAL RESULTS OF A LINEAR EXAMPLE

Consider the following model problem:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\phi - P\left[\frac{\partial}{\partial x}\left(u\,\phi\right) + \frac{\partial}{\partial y}\left(v\,\phi\right)\right] = 0\ ,$$

where $u = U(1 - X/L)$, $v = UY/L$, and $P = UL/K$, with boundary conditions:

$\phi = 0$ at left and bottom,

$\phi = 1$ at right and top.

P is the Péclet number which measures the intensity of advection relative to diffusion. U, L, and K (diffusivity constant) are quantities used for nondimensionalization. Figure 2 depicts the flow pattern where streamlines enter along the left boundary and leave through the top boundary. Plots of isotherms are shown in figures 3 and 4 for P = 1 and 100, respectively. Observe the thin boundary layer developed near x = L and y = L for strong advective cases. In table 1 the number of iterations for P from 10 to 400

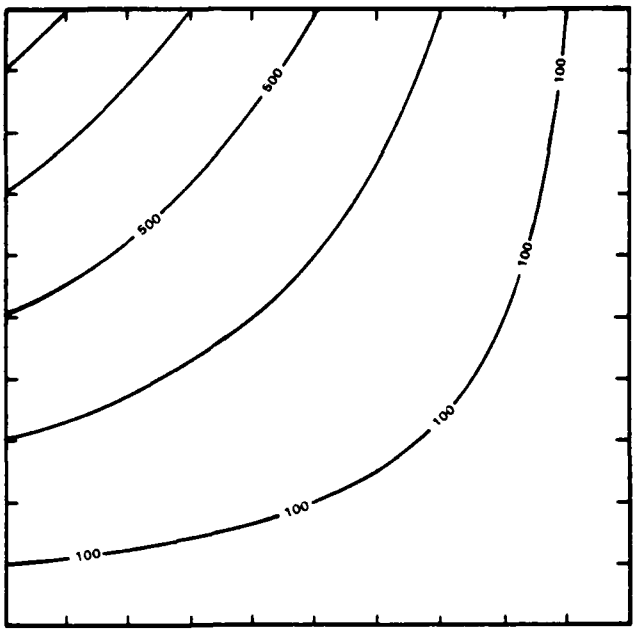


Figure 2. Flow Pattern

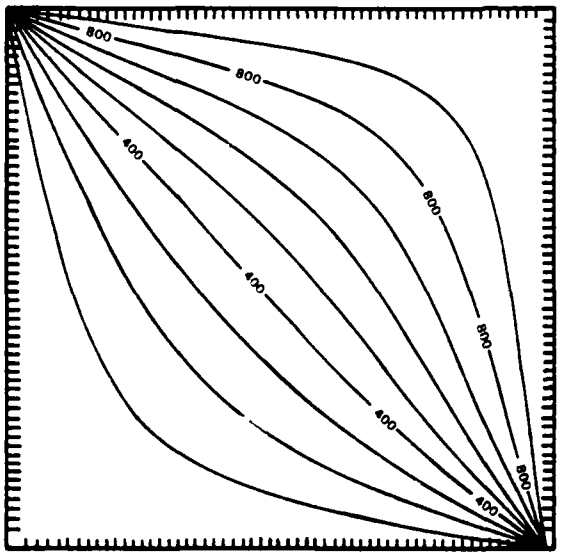


Figure 3. Isotherms for P = 1

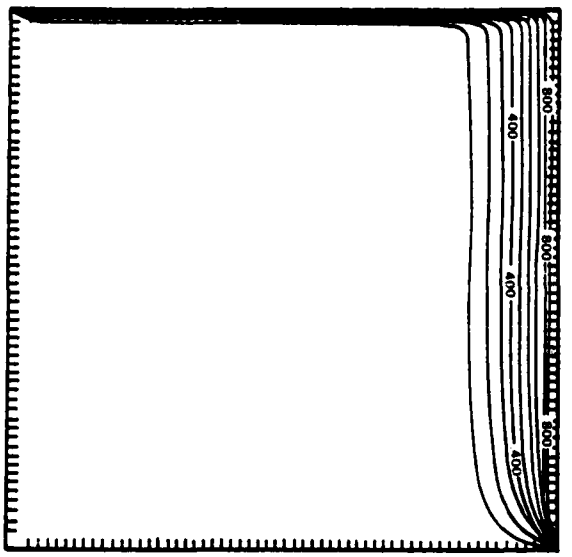


Figure 4. Isotherms for P = 100

Table 1. Number of Iterations with Different Relaxation Methods

Relaxation Method \ Pećlet No.	10	50	100	400
SLOR in x and y Directions*	120	73	60	23
PMR I	45	48	37	22
PMR II	93	45	35	21
Multigrid, WU†	95.6	77.2	64.0	45.2

*One SLOR iteration is a sweep in the x direction, followed by a sweep in the y direction. It is approximately equal to the work done by one PMR iteration.

†One WU (work unit) is equivalent to one point relaxation sweep over a 61 x 61 grid. It is about half the work done in one SLOR relaxation.

is compared for a grid 61 x 61. Convergence was reached when the norm of the residual vector was less than 10^{-6}.

For all four iteration methods considered, it was found that the W-M scheme converges faster for more convective flows since the preconditioning matrix C becomes closer to the original matrix A as the Péclet number becomes larger. The PMR and multigrid methods need about the same storage and are efficient for high as well as low Péclet numbers. Furthermore, no parameter is required for the PMR algorithm. The multigrid program involves some complexity since the various sizes of the arrays represent the same quantity and there is a need for interpolations. On the other hand, the PMR method needs an efficient LU decomposition.

THE NONLINEAR PROBLEM

Consider the following 2-D Burger's equation in a unit square in R^2:

$$\Omega = \left\{ (x, y) \;\middle|\; 0 \le x \le 1, \quad 0 \le y \le 1 \right\}$$

$$- \frac{1}{2} \left(u^2\right)_x - \frac{1}{2} \left(u^2\right)_y + \varepsilon \nabla^2 u = 0 , \tag{4}$$

with boundary conditions:

u = 0 at left and bottom,

u = 1 at right and top.

For standard upwind differencing of the convective terms, the nonlinearity might cause instabilities and convergence to the incorrect (nonphysical) solution. Hence, the monotone difference scheme of Engquist and Osher[7] is used here to approximate the nonlinear convective terms, and central difference is used to discretize the Laplacian operator. For the

1-D singular perturbation equation, Osher[8] has proved, via the time-dependent equation, that convergence to a unique steady-state solution occurs. Moreover, computational evidence of the 1-D case in Osher's paper indicates that the method is very useful in accurately locating regions of large gradient even for complicated problems. For nonuniform grids, Abrahamsson and Osher[9] have proved general convergence results and have shown that the Engquist-Osher scheme reproduces essential properties of the true solution.

Next, the monotone difference scheme is described briefly. Let $f(u) = \frac{1}{2} u^2$. The Engquist-Osher scheme is based on the approximation

$$\left[f(u)\right]_x \longrightarrow \frac{1}{\Delta x} \left[\Delta_+ f_- \left(u_i\right) + \Delta_- f_+ \left(u_i\right)\right] , \tag{5}$$

where

$$\Delta_+ u_i = u_{i+1} - u_i \ , \quad \Delta - u_i = u_i - u_{i-1} \ ,$$

and

$$f_+ \left(u_i\right) = f\left[\max \left(u_i, o\right)\right] , \quad f_- \left(u_i\right) = f\left[\min \left(u_i, o\right)\right] .$$

For each grid point, the discretized form of equation (4) reads:

$$\begin{aligned} &\varepsilon \left[u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,\,j+1} - 4\, u_{i,j}\right] \\ &- h \left[f - \left(u_{i+1,j}\right) - 2\, f_- \left(u_{i,j}\right) + 2\, f_+ \left(u_{i,j}\right)\right. \\ &\left. - f_+ \left(u_{i-1,j}\right) + f_- \left(u_{i,j+1}\right) - f_+ \left(u_{i,\,j-1}\right)\right] = 0, \end{aligned} \tag{6}$$

where h is the uniform grid size and

$$f_-(u) = \begin{cases} \frac{u^2}{2}, & u < 0 \\ 0, & u \geq 0 \end{cases}$$

$$f_+(u) = \begin{cases} \frac{u^2}{2}, & u > 0 \\ 0, & u \leq 0 \end{cases} .$$

Convergence to steady-state solution will be accomplished via artificial time stepping and Newton's method.

METHOD OF TIME STEPPING AND NEWTON'S METHOD

$$u_t = -\tfrac{1}{2}(u^2)_x - \tfrac{1}{2}(u^2)_Y + \epsilon \nabla^2 u \qquad (7)$$

with boundary conditions and initial conditions.

Discretization of equation (7) with respect to time yields

$$u_{i,j}^{n+1} = u_{i,j}^{n} + \Delta t^n \; Lu^n ,$$

where Lu^n represents the right hand side of equation (7) and Δt^n the time increment. In this example, the time steps, Δt^n, which are limited by the Courant-Friedrich-Levy (CFL) condition, are chosen to be fixed for all n, $\Delta t^n = \Delta t^o$ since the finite difference equation satisfies the maximum principle.

Instead of solving the time-dependent equation (7), Newton's method can be used to iterate an initial guess of the steady-state solution. However,

to ensure convergence, the starting guess of solution should be close enough to the exact solution.

Consider now the basic idea of iterative methods for nonlinear systems of equations. Any iterative scheme can be expressed as

$$M\delta u^n = - Lu^n \quad , \tag{8}$$

where $\delta u^n = u^{n+1} - u^n$, Lu^n is the residual vector at the n^{th} iteration, and M is an iterative matrix. It appears that many choices of M are possible. The closer that M is to representing L, the faster convergence is. In general, it is required that M will be chosen in such a way that:

1. M can be computed easily.
2. Only a little storage is needed to store M.
3. δu^n can be computed rapidly from equation (8).
4. The iteration scheme as expressed in equation (8) should converge.

If M is selected to be the Jacobian of L, then equation (8) will be a Newton iterative scheme and the rate of convergence will be quadratic.

In this example the Jacobian of L is given, at n^{th} step, by

$$M\delta u^n = \varepsilon \left(\delta u^n_{xx} + \delta u^n_{yy}\right) - u^n \delta u^n_x - u^n \delta u^n_y - \left(u^n_x + u^n_y\right) \delta u^n \quad . \tag{9}$$

Again the convective and diffusive parts are approximated by the W-M scheme since equation (9) is linear in δu^n. Then the calculations of the correction vectors, δu^n, should invoke the combination of the W-M scheme and the preconditioned minimal residual method for efficiency reasons. Note that in using the PMR method to solve the linearized system of equation (8), only a few iterations are needed for each outer iteration, since the

interest is in the convergence for the whole nonlinear problem. The number of inner iterations is fixed at six in these numerical examples.

A NONLINEAR EXAMPLE

The combined Newton and PMR methods discussed in the previous section result in a very fast converging iterative method for the solution of nonlinear systems of equations that approximate equation (4). In table 2 the number of iterations is compared for the explicit scheme and Newton's method for $\varepsilon = 0.1$, 0.05, and 0.01 with a grid 31 x 31. Note that all calculations were started with the same uniform initial guess of $u = 0.5$, and convergence was reached when the norm of the residual vector was less than 10^{-4}. Table 3 shows the total computing time on a VAX 11/780 computer for the two methods. There are slight changes in the number of Newton's iterations and drastic increases in the number of time steps when ε decreases. Table 4 lists the number of Newton's iterations and the computing time with $\varepsilon = 0.01$ for different starting guesses of solutions.

CONCLUSIONS

The PMR and multigrid methods are very efficient iterative procedures for large as well as small ε. Moreover, numerical results indicate that the stronger the convection is, the faster the convergence is. Finally, it has been shown that Newton's method combined with the PMR method can be applied very successfully to a nonlinear multidimensional problem.

Table 2. Iteration Numbers

ε	0.1	0.05	0.01
Time Steps	68	134	437
Newton Iterations	8	9	7

Table 3. CPU Time

ε	0.1	0.05	0.01
Explicit Scheme	19.72	32.01	1:26.45
Newton's Method	31.99	33.46	29.85

Table 4. Runs with Different Initial Guesses

$\varepsilon = 0.01$	I	II	III
Newton Iterations	9	7	8
Computing Time	32.94	29.85	31.51

I = uniform initial guess of 0

II = uniform initial guess of 0.5

III = uniform initial guess of 1

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