COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING 47 (1984) 357–367
NORTH-HOLLAND

OPTIMUM ACCELERATION FACTORS FOR ITERATIVE SOLUTION OF LINEAR AND NONLINEAR DIFFERENTIAL SYSTEMS

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Received 26 April 1984

A new acceleration concept for iterative schemes is described. The concept is based on elementary variational calculus, and can be readily implemented in the iterative solution of a wide variety of linear and nonlinear differential systems. The method is not limited to finite difference, finite element or finite volume discretization schemes, but only to schemes that are inherently iterative. Most importantly, the method is exact in the sense that optimal relaxation/acceleration factors can be analytically determined for a class of commonly encountered systems possessing simple nonlinearity. For systems exhibiting complex nonlinearity, the method can be applied in a semi-exact but highly accurate fashion using truncated Taylor series. Without any modification, this acceleration method can be directly applied to existing iterative schemes using either orthogonal or completely arbitrary non-orthogonal computational grids, since the formulation of the method is dependent only on the governing differential system. The described method belongs to the general class of minimal residual techniques, but can be applied to nonlinear systems.

1. Introduction

The numerical solution of linear and nonlinear ordinary and partial differential equations has recently become one of the most important aspects of applied research in science and engineering. Large coupled systems of differential equations are now being solved routinely on today's supercomputers [1–3]. Nevertheless, the differential systems that are being solved are usually approximations to exact mathematical models. In addition, the complexity of the physical geometries that are studied are somewhat limited by computer storage and time considerations, even on Class VI machines. Thus, it is imperative that new methods for accelerating the convergence of numerical schemes be developed, allowing the numerical study of complex fully three-dimensional problems governed by exact mathematical models.

Presently, there are several methods for accelerating the convergence of numerical schemes. In the nonlinear case these methods include the multiple grid method [4, 5], and approximate determination of the dominant eigenvalue of nonlinear relaxation matrices [6, 7]. There is an abundance of literature related to linear problems, including Young's pioneering work on optimal relaxation factors [8], conjugate gradient methods [9], and minimal residual methods [9, 10]. The multiple grid methods have been shown to offer significant increases in convergence rates but are somewhat difficult to implement. Acceleration schemes that depend on determination of the dominant eigenvalue of very large iteration matrices have two basic disadvantages: (a) the methods are inherently approximate, and (b) the assumption that a strongly dominant eigenvalue exists is not always true for nonlinear problems. Large linear

systems can be solved efficiently with the use of existing linear theory [2, 3, 11, 12]. However, most problems of practical interest in, say, fluid dynamics are strongly nonlinear, and the linear theory can only be applied by first linearizing the governing equations.

It is the objective of this paper to introduce a new and very general concept for the analytic determination of optimal relaxation and aceleration factors for the numerical solution of both linear and nonlinear ordinary and partial differential equations. This new method is based on minimizing the residual at each step of the iteration process by analytically determining an optimal acceleration factor.

Several numerical examples of the acceleration method are shown with particular applications to solution of Burgers' equation, the heat equation and the full potential compressible flow equation.

2. Analysis

Assume that we are solving a system of coupled (non-) linear algebraic equations resulting from a discretization of a set of differential equations. For demonstrative purposes, we will confine the analysis to a system of differential equations in one dependent variable on a two-dimensional computational domain. Note that the analysis is valid for an N-dimensional system in any number of dependent variables. The differential system to be solved is given by

$$L\Phi = F, \tag{1}$$

where L is a (non-) linear differential operator, Φ is the dependent variable and F is the usual right-hand side (or forcing term). After discretization, the system can be written as

$$l\phi_{ij} = f, \tag{2}$$

where ϕ_{ij} is the exact solution of the discrete system at the grid point defined by the indices i and j for $1 \leq i \leq p$ and $1 \leq j \leq q$, l is the discrete analog of L, and f is the discrete representation of F. As in all iterative schemes, we assume an initial guess for ϕ and iterate the solution until the desired convergence is achieved.

Now, assume that given ϕ^n we can calculate a temporary value $\bar{\phi}^{n+1}$ from

$$\bar{\phi}^{n+1} = \phi^n + M\phi^n, \tag{3}$$

where M is a scheme-dependent operator that gives the correction

$$\delta\phi^n \equiv \bar{\phi}^{n+1} - \phi^n = M\phi^n \tag{4}$$

which is to be added to ϕ^n to obtain $\bar{\phi}^{n+1}$ at each grid point of the domain. Some iterative techniques are implicit meaning that the correction is dependent on the new iterate.

$$\delta\phi^n \equiv M(\phi^n, \bar{\phi}^{n+1}). \tag{5}$$

Let the actual value of the new iterate ϕ_{ij}^{n+1} be given by

$$\phi_{ij}^{n+1} = \phi_{ij}^n + \omega\delta\phi_{ij}^n, \tag{6}$$

where the iterative acceleration factor ω is a constant over the domain Ω but changes from one iteration to the next. Our objective is to determine an optimal value of ω.

2.1. Optimum acceleration factor

Let the residual left by the nth iterate of ϕ be defined by

$$R_{ij}^n \equiv l\phi_{ij}^n - f. \tag{7}$$

The residual at the new iteration level $n+1$ is given by

$$R_{ij}^{n+1} = R(\phi_{ij}^{n+1}) = R(\phi_{ij}^n + \omega\delta\phi_{ij}^n). \tag{8}$$

We will seek the minimum of the L^2-norm of R^{n+1} with respect to ω.

If we assume that the residual obeys the relation

$$\iint_\Omega (R^{n+1})^2 \, d\Omega < \iint_\Omega (R^n)^2 \, d\Omega$$

for all n greater than some m, then a method in which we seek to minimize the residual at iteration $n+1$ will produce a sequence of iterates which will converge to the exact solution ϕ. within some given tolerance. Define the cost function $J(\omega)$ by

$$J(\omega) \equiv \iint_\Omega (R^{n+1})^2 \, d\Omega, \tag{9}$$

and thus

$$\min[J(\omega)] \quad \text{implies} \quad \frac{\partial J}{\partial \omega} = 0 \text{ and } \frac{\partial^2 J}{\partial \omega^2} > 0. \tag{10}$$

For governing differential systems (1) possessing simple nonlinearity (i.e., terms in the governing system are simple polynomials in the dependent variables), the new residual is a polynomial of degree N in ω,

$$R_{ij}^{n+1} = a_0 + a_1\omega + a_2\omega^2 + \cdots + a_N\omega^N, \tag{11}$$

where the a_m, $0 \leq m \leq N$, are functions of the known quantities ϕ_{ij}^n and $\delta\phi_{ij}^n$. If the system possesses any nonsimple (complex) nonlinearity, we can approximate the complex nonlinearity with a simple truncated Taylor series. This approach produces a residual of the form given in (11), where the equality should be replaced by an approximate equality. The order of the Residual Polynomial (RP) given by (11) depends on the system (1). The order of the RP does not depend on the differential order of the governing equations but only on the order of their nonlinearity and/or the number of terms in the truncated Taylor series expansion of any complex nonlinearity. This fact will be demonstrated in the examples below.

From (9) and (10) it follows that

$$\frac{\partial J}{\partial \omega} = 2 \iint_\Omega R^{n+1} \frac{\partial}{\partial \omega}(R^{n+1}) \, d\Omega = 0 \tag{12}$$

and

$$\frac{\partial^2 J}{\partial \omega^2} = 2 \iint_\Omega \left\{ R^{n+1} \frac{\partial^2}{\partial \omega^2}(R^{n+1}) + \left[\frac{\partial}{\partial \omega}(R^{n+1}) \right]^2 \right\} d\Omega. \tag{13}$$

Substitution of (11) in (12) results in

$$\frac{\partial J}{\partial \omega} = A_0 + A_1\omega + A_2\omega^2 + \cdots + A_{2N-1}\omega^{2N-1} = 0 \tag{14}$$

and

$$\frac{\partial^2 J}{\partial \omega^2} = A_1 + 2A_2\omega + \cdots + (2N-1)A_{2N-1}\omega^{2N-2} > 0\,, \tag{15}$$

where the A_m, $0 \leq m \leq 2N-1$, are known functions of the a_m, $0 \leq m \leq N$. For example,

$$A_0 = 2\iint_{\Omega} (a_0 a_1)\,\mathrm{d}\Omega\,. \tag{16}$$

For a discrete problem the integrals can be approximated with appropriately weighted sums over the grid points.

The solution of the minimization problem (10) is thus reduced to finding the $2N-1$ roots of the Minimizing Polynomial (MP) given by (14). Each of the real roots is tested to find which ones produce local minima using (15). Of these roots, the optimal value of ω is chosen as the one producing the minimal value in the L^2-norm of the residual (11).

The general procedure for accelerating an iterative scheme can be summarized as follows:

Step 1. Calculate temporary values of $\bar{\phi}^{n+1}$ at all grid points using (3).
Step 2. From ϕ^n and $\bar{\phi}^{n+1}$ calculate $\delta\phi^n$ from (4).
Step 3. Form the RP and MP from (11) and (14) and find all roots of the MP.
Step 4. Test the roots of the MP using (15) and (11) to find the optimum value of ω.
Step 5. Calculate the actual new iterates ϕ^{n+1} from (6).

3. Examples of applications

To illustrate how the form of the MP relates to the governing equation, and to demonstrate the acceleration procedure we will look at three examples: Burgers' equation, the two-dimensional heat equation and the two-dimensional full potential equation for compressible flows.

3.1. Burgers' equation

Burgers' equation models a simple one-dimensional convective and diffusive process and is given by

$$\frac{\partial}{\partial t}\phi = -\frac{\partial}{\partial x}\left(\tfrac{1}{2}\phi^2\right) + \nu\frac{\partial^2}{\partial x^2}\phi \equiv R(\phi)\,. \tag{17}$$

The RP is found from

$$R^{n+1} = R(\phi^n + \omega\delta\phi^n) = a_0 + a_1\omega + a_2\omega^2\,, \tag{18}$$

where

$$a_0 = -\frac{\partial}{\partial x}\left[\tfrac{1}{2}(\phi^n)^2\right] + \nu\frac{\partial^2}{\partial x^2}(\phi^n) = R(\phi^n),$$

$$a_1 = -\frac{\partial}{\partial x}(\phi^n\delta\phi^n) + \nu\frac{\partial^2}{\partial x^2}(\delta\phi^n), \tag{19}$$

$$a_2 = -\frac{\partial}{\partial x}\left[\tfrac{1}{2}(\delta\phi^n)^2\right].$$

The MP then becomes

$$\begin{aligned}\mathrm{MP} &= (a_0 + a_1\omega + a_2\omega^2)(a_1 + 2a_2\omega)\\ &= (a_0a_1) + \omega(a_1^2 + 2a_0a_2) + \omega^2(3a_1a_2) + \omega^3(2a_2^2).\end{aligned} \tag{20}$$

Note that the order of the nonlinearity in Burgers' equation is 2 and this produces a MP of order $2(2)-1=3$. Writing (20) for each grid point of a computational domain, and integrating over the domain gives the global MP,

$$\mathrm{MP}_{\mathrm{global}} = A_0 + A_1\omega + A_2\omega^2 + A_3\omega^3 \tag{21}$$

which can easily be solved to find the optimum value of ω.

3.2. The heat equation

The heat equation is given by

$$\frac{\partial}{\partial t}\phi = \alpha\nabla^2\phi \equiv R, \tag{22}$$

where α is the thermal diffusivity. The RP is found from

$$R^{n+1} = R(\phi^n + \omega\delta\phi^n) = \alpha\nabla^2(\phi^n + \omega\delta\phi^n) = a_0 + a_1\omega. \tag{23}$$

Since the heat equation is linear, the RP is a linear function of ω. The MP is also linear and it is given by

$$\mathrm{MP} = (a_0 + a_1\omega)(a_1) = (a_0a_1) + (a_1^2)\omega. \tag{24}$$

Forming the global MP as in (21) we get

$$\mathrm{MP}_{\mathrm{global}} = A_0 + A_1\omega = 0. \tag{25}$$

Thus for this linear equation (as in all linear systems) we can immediately solve for ω_{opt}.

$$\omega_{\mathrm{opt}} = -A_0/A_1. \tag{26}$$

3.3. The full potential equation

The full potential equation is the mathematical model for homentropic, compressible, steady, irrotational flow of a perfect gas. It is derived from the continuity equation

$$(\rho\phi_x)_x + (\rho\phi_y)_y = 0, \tag{27}$$

where ϕ is the velocity potential defined by $V = \nabla\phi$, and the density ρ is given by the

isentropic relation

$$\rho = [\tfrac{1}{2}(\gamma+1) - \tfrac{1}{2}(\gamma-1)(\phi_x^2 + \phi_y^2)]^{1/(\gamma-1)} = \rho(\phi_x, \phi_y)\,. \tag{28}$$

All quantities are normalized by their respective critical conditions. Clearly the density ρ is a highly nonlinear function of ϕ. In this case the residual is given by

$$R^{n+1} = (\rho^{n+1}\phi_x^{n+1})_x + (\rho^{n+1}\phi_y^{n+1})_y\,, \tag{29}$$

where

$$\phi_x^{n+1} = \phi_x^n + \omega\delta\phi_x^n\,, \tag{30}$$

$$\phi_y^{n+1} = \phi_y^n + \omega\delta\phi_y^n\,, \tag{31}$$

$$\rho^{n+1} = \rho(\phi_x^{n+1}, \phi_y^{n+1})\,. \tag{32}$$

The residual is not a simple polynomial in ω due to the presence of ρ in (29). Nevertheless, we can obtain R in the form (11) if ρ is expanded in a second-order accurate truncated Taylor series. The result is

$$\rho^{n+1} = \rho^n + \delta\rho_1\omega + \delta\rho_2\omega^2 + \mathrm{O}[(\omega\delta\phi_x)^3, (\omega\delta\phi_y)^3]\,, \tag{33}$$

where $\delta\rho_1$ and $\delta\rho_2$ are given by

$$\delta\rho_1^n = \left[-\frac{\rho}{a^2}(\phi_x\delta\phi_x + \phi_y\delta\phi_y)\right]\Big|_n\,, \tag{34}$$

$$\delta\rho_2^n = \left[\frac{\rho}{a^2}\left\{\tfrac{1}{2}\left[(2-\gamma)\frac{\phi_x}{a^2} - 1\right](\delta\phi_x)^2 + \left[(2-\gamma)\frac{(\phi_x\phi_y)}{a^2}\right]\delta\phi_x\delta\phi_y + \tfrac{1}{2}\left[(2-\gamma)\frac{\phi_y}{a^2} - 1\right](\delta\phi_y)^2\right\}\right]\Big|_n\,. \tag{35}$$

Substituting (33) into (29) and using (30)–(32) we obtain

$$R^{n+1} = a_0 + a_1\omega + a_2\omega^2 + a_3\omega^3\,. \tag{36}$$

Thus the RP is of order 3 and the MP is of order $2(3) - 1 = 5$.

4. Results

To test the nonlinear minimal residual acceleration scheme, Burgers' equation was numerically solved on the interval $-\frac{1}{2} \leq x \leq 0$, with $\nu = 0.07$, $\phi(-\frac{1}{2}) = 1$ and $\phi(0) = 0$. A spatially second-order-accurate finite difference discretization of (17) coupled with a temporally first-order-accurate Euler one-step explicit time-consistent integration scheme was formulated and is given by

$$\delta\phi^n = \Delta t\left\{-\frac{[(\phi_{i+1}^n)^2 - (\phi_{i-1}^n)^2]}{(4\Delta x)} + \nu\frac{(\phi_{i-1}^n - 2\phi_i^n + \phi_{i-1}^n)}{(\Delta x^2)}\right\}. \tag{37}$$

The linear explicit stability criterion, $\nu\,\Delta t/\Delta x^2 \leq 0.5$ was used here to determine Δt which was held fixed throughout the calculation. The initial guess for $\phi(x)$ was a linear interpolation between the given values at the endpoints. Starting with this initial guess, the solution was iterated for 800 time steps as shown in Fig. 1 (dashed line).

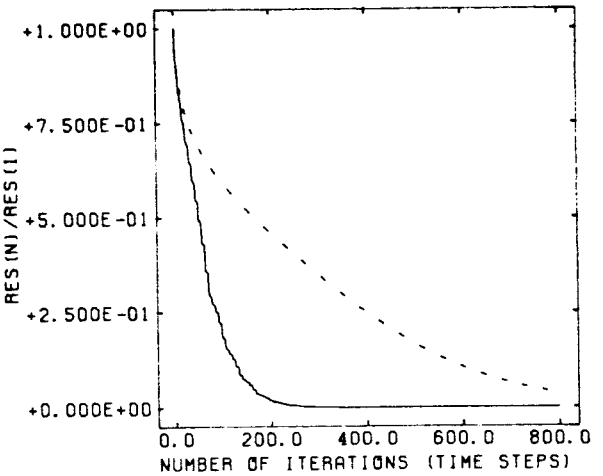

Fig. 1. Convergence history of explicit time-dependent solution of Burgers' equation: non-accelerated (---); accelerated using fixed stategy (——).

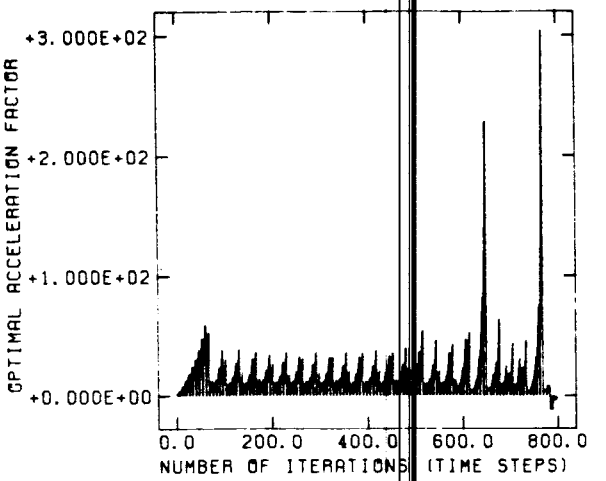

Fig. 2. Optimal acceleration factor ω_{opt} versus number of iterations for explicit time-dependent solution of Burgers' equation using fixed strategy.

Next, the new acceleration method was applied using $\delta\phi$ from (37) to find the optimum value of the acceleration factor ω. The accelerated convergence history is shown in Fig. 1 (solid line). In practice, it was found that a fixed strategy of setting $\omega = 1$ for five iterations and then $\omega = \omega_{opt}$ for two iterations produced the best results. Fig. 1 clearly shows that for this nonlinear problem, the linear explicit stability limit on Δt can be far exceeded. Fig. 2 shows that at one point in the calculations, the effective time step ($\omega_{opt}\Delta t$) was over 300 times that given by the linear explicit stability limit. Two adaptive strategies for determining how many non-accelerated ($\omega = 1$) iterations to use between each accelerated ($\omega = \omega_{opt}$) iteration were tried. These two strategies are defined as

$$\omega = \begin{cases} 1 & \text{for } \dfrac{\partial}{\partial n}(\omega_{opt}) > 1\,, \\ \omega_{opt} & \text{for } \dfrac{\partial}{\partial n}(\omega_{opt}) < 1\,, \end{cases} \tag{38}$$

and

$$\omega = \begin{cases} 1 & \text{for } \dfrac{\partial^2}{\partial n^2}(\omega_{opt}) > 0\,, \\ \omega_{opt} & \text{for } \dfrac{\partial^2}{\partial n^2}(\omega_{opt}) < 0\,. \end{cases} \tag{39}$$

The first strategy is based on the concept of letting ω_{opt} build up until an additional iteration with $\omega = 1$ does not increase ω_{opt} by more than one. This strategy gave very large drops in the residual but only at a few points in the global iteration (Fig. 3 (solid line)). The second strategy is based on maximizing the rate of change of ω_{opt} (Fig. 4 (solid line)). This strategy gave results comparable to the previously discussed fixed stategy.

To test the new minimal residual technique on a linear two-dimensional problem, (22) was solved on a unit square using both a time-dependent integration scheme and successive overrelaxation. The two solution schemes are given by

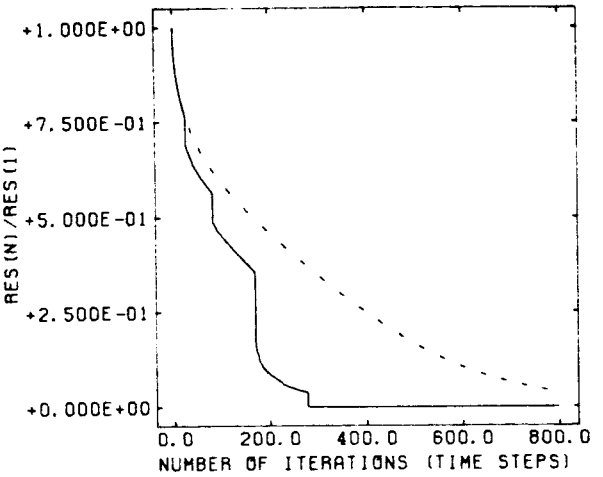

Fig. 3. Convergence history of explicit time-dependent solution of Burgers' equation: non-accelerated (---); accelerated using first adaptive strategy (——).

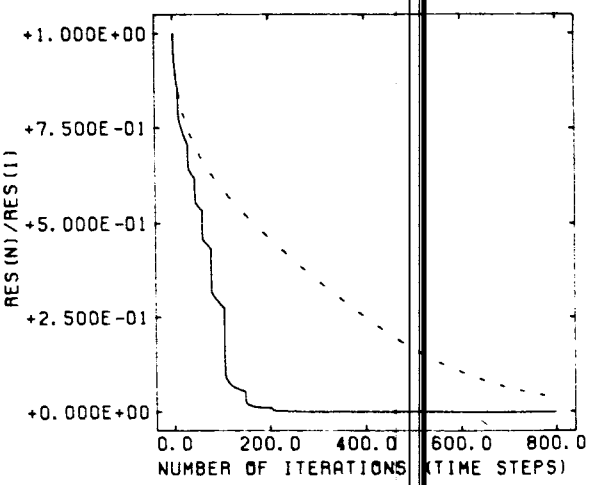

Fig. 4. Convergence history of explicit time-dependent solution of Burger's equation: non-accelerated (---); accelerated using second adaptive strategy (——).

$$\delta\phi^n = r[\phi^n_{i+1,j} + \phi^n_{i-1,j} + \phi^n_{i,j+1} + \phi^n_{i,j-1} - 4\phi^n_{i,j}], \tag{40}$$

$$\delta\phi^n = 0.25[\phi^{n+1}_{i-1,j} + \phi^n_{i+1,j} + \phi^n_{i,j+1} + \phi^{n+1}_{i,j-1} - 4\phi^n_{i,j}], \tag{41}$$

where $r \equiv \Delta t/\Delta x^2 \leqslant 0.25$ and $\Delta x = \Delta y$. Initial and boundary conditions on $\phi(x, y; t)$ were

$$\begin{aligned} &\phi(x, y; 0) = 1, \\ &\phi(0, y; t) = 1.5, \qquad \phi(1, y; t) = 0, \\ &\phi(x, 0; t) = 0, \qquad \phi(x, 1; t) = 0. \end{aligned} \tag{42}$$

Fig. 5 shows the convergence history of the fixed strategy accelerated (solid line) and

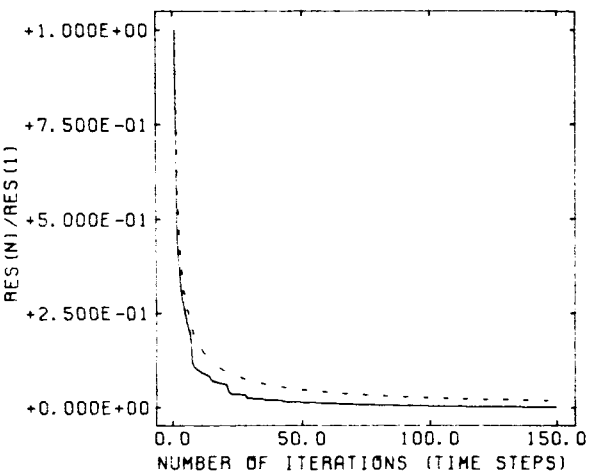

Fig. 5. Convergence history of explicit time-dependent solution of two-dimensional heat equation: non-accelerated (---); accelerated using fixed strategy (——).

non-accelerated (dotted line) time-dependent explicit integration scheme. Again we see that the explicit stability limit can be exceeded.

Young [8] analytically found an optimum value for ω that minimizes the spectral radius of the successive overrelaxation iteration matrix as the number of iterations tends to infinity. In other words, the asymptotic rate of convergence is maximized. Setting $\omega = \omega_{Young}$ gives the convergence history shown in Fig. 6 (dotted line). Using the new acceleration method, ($\omega = \omega_{opt}$) we get the result shown in Fig. 6 (solid line). This result appears to demonstrate that we can maximize the average rate of convergence [9] as in so-called semi-iterative methods involving Chebyshev polynomials. Moreover, a result shown by Varga [9] that the average rate of convergence approaches the asymptotic convergence rate as $n \to \infty$ is confirmed by this numerical experiment.

Finally, the nonlinear minimal residual acceleration method was applied to the solution of the full potential equation (27). An existing computer program developed by Dulikravich [13] that solves the full potential equation for compressible flows through airfoil cascades using the finite area technique and locally type-dependent rotated finite differencing was modified to include the new acceleration method. The original program uses the successive line over-relaxation technique (SLOR) to determine the change in the potential $\delta\phi_{ij}$ at each point of an O-type non-orthogonal boundary conforming computational grid. The modified program uses these computed changes (along with the known solution) to determine ω_{opt} for each iteration sweep.

The modified program was run for a test case of air flow through a nonstaggered cascade of NACA 0012 airfoils at a gap-to-chord ratio of 3.6 and with the upstream Mach number set at 0.6. One hundred SLOR iterations were performed on each of a sequence of two consecutively refined grids. The dotted line of Fig. 7 shows the convergence history of the non-accelerated scheme. After applying the new acceleration method we get the results shown

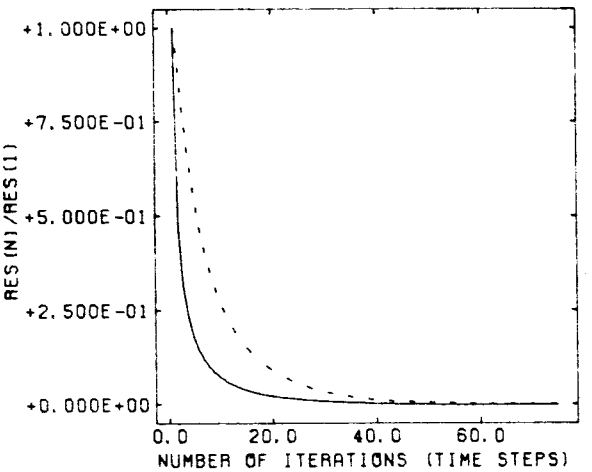

Fig. 6. Convergence history of successive over-relaxation solution of two-dimensional heat equation using: $\omega = \omega_{Young}$ (---); $\omega = \omega_{opt}$ (——).

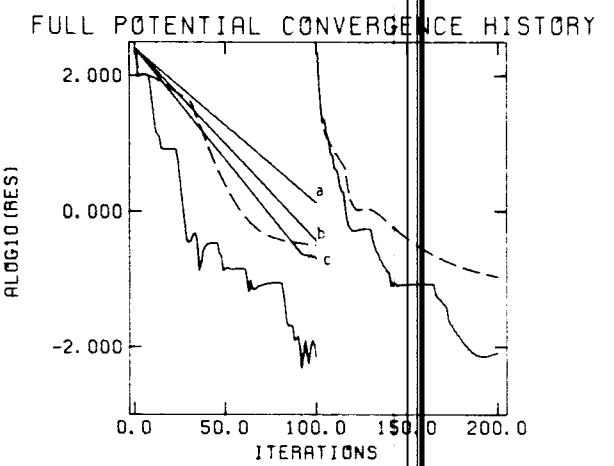

Fig. 7. Convergence history of SLOR solution of full potential equation for a cascade of NACA 0012 airfoils at zero stagger angle, $M_{-\infty} = 0.6$, gap-to-chord ratio 3.6: non-accelerated(---); accelerated using $\omega = \omega_{opt}$ (——). Prescribed convergence rates: (a) $\beta = 0.900$; (b) $\beta = 0.877$; (c) $\beta = 0.856$.

by the solid line. The accelerated scheme produces an order of magnitude larger drop in the residual on both the coarse and the fine grid than the non-accelerated scheme.

5. Convergence rate specification

An important property of the nonlinear minimal residual method is that the value of the global residual, given by the cost function $J(\omega)$ (9) is a simple polynomial of degree $2N$ in ω. Hence, we can determine a priori the value of the global residual at the new iteration level $n+1$. Define the convergence rate β of the accelerated scheme by

$$\beta \equiv J^{n+1}/J^n . \tag{43}$$

Thus

$$\beta = 1 + B_1\omega + B_2\omega^2 + \cdots + B_{2N}\omega^{2N} \tag{44}$$

or

$$(1-\beta) + B_1\omega + B_2\omega^2 + \cdots + B_{2N}\omega^{2N} = 0 . \tag{45}$$

Therefore, we can prescribe a desired convergence rate β, and at each iteration solve (45) for the value of ω compatible with the specified convergence rate β. Note that if β is not too small, that is, if the prescribed value of β does not exceed the maximum possible convergence rate, we get

$$\ln(J^n/J^0) = n(\ln\beta) . \tag{46}$$

Thus the convergence will exhibit exponential decay.

An alternative to prescribing β would be to fix the number of iterations, n, and specify the desired final value of the global residual, J. The value of β that gives the desired result is given by

$$\beta = (J^n/J^0)^{1/n} . \tag{47}$$

Fig. 7 shows the convergence history of the full potential equation solution on a single grid when the convergence rate is specified. Results are shown for three values of β: 0.900, 0.877 and 0.856. When $\beta = 0.856$ we see that the convergence no longer exhibits exponential decay, that is, we have specified a value of β that is too small (the maximum possible convergence rate is exceeded during the last few iterations). Note that we could specify β not as a constant but as some function of the iteration count n. Thus, we could specify that β be small near the beginning of the procedure, and have its value increase with n. The advantages of specifying β are (a) one has complete control over the convergence of the scheme, and (b) the convergence will be smooth.

6. Summary

A new technique for accelerating the convergence of iterative solution methods for linear and nonlinear differential systems have been presented. The method is based on elementary variational calculus and it can be applied to any ordinary or partial differential system that can be solved by an iterative method, in either an exact or semi-exact fashion. Moreover, existing

computer programs can be readily modified to incorporate this acceleration method. For all test cases considered, the method was shown to provide a significant improvement in the convergence rate.

Acknowledgment

The authors would like to express their sincere gratitude to Prof. David M. Young and Prof. J. Tinsley Oden for many helpful discussions. This research was supported by the Department of Aerospace Engineering and Engineering Mechanics at the University of Texas at Austin. Computational work was performed using computing facilities of the Texas Institute of Computational Mechanics (TICOM).

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