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Generalized nonlinear minimal residual (GNLMR) method for iterative algorithms

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Abstract: Most iterative methods for solving steady-state problems can be shown to be equivalent to solving time-dependent problems of either parabolic or hyperbolic type. The relaxation factor used in accelerating an iterative method to obtain the converged solution plays the same role as the time step size used in advancing the transient solution to the steady state solution for a time-dependent problem. With this transformation, one can expose the mechanism of the acceleration schemes. In the presented study, this time-dependent approach together with the single-iteration, multi-step algorithm are applied to generalize the nonlinear minimal residual (NLMR) method for iterative solutions of linear and nonlinear problems. Most importantly, both theoretical studies and numerical experiments confirm the monotone convergence behavior of the generalized NLMR method. With the multi-step algorithm, it is found that both the rate and the smoothness of convergence of the NLMR method can be improved even further. Several interesting problems that originated from this method are also discussed.

1. Introduction

The time-dependent technique proposed by Moretti and Abbett [1] in the mid-1960's was the first successful method to solve problems governed by equations of mixed type. The steady-state solution was obtained by starting with the unsteady equation, and marching the solution along the time coordinate until convergence was achieved. Nowadays, the time-dependent method is widely used in computational fluid dynamics for the solution of the steady-state Euler and Navier–Stokes equations [2,3,4].

It is interesting to note that most iterative methods for the solution of steady-state problems can be shown to be equivalent to methods for solving time-dependent problems of either parabolic or hyperbolic type [5,6]. The relaxation factor used in accelerating an iterative method to obtain the converged solution plays the same role as the time step size in advancing the transient solution to the steady-state solution for a time-dependent problem. This approach offers several advantages.

For example, the mechanism of an acceleration scheme can be unveiled and an optimal value of relaxation factor (optimal time step size) could be analytically determined. If accurate time evolution is required for an unsteady problem, the time step size should be small to guarantee both the stability and the accuracy of the solution. Consequently, very often a compromise must

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be made between the computer time requirements and the accuracy of the solution of such computation provided the method is stable. Since the limitation on the time step size can be analytically determined using the GNLMR method, a satisfactory compromise can be achieved. If transient behavior is of no interest to us, it is convenient to interpret the physical time as the artificial time or to reformulate the governing equations in terms of certain artificial time. Then the GNLMR method can be applied to determine the optimal value of the time step size (optimal relaxation factor) to minimize the time steps (number of iterations) for obtaining the steady-state converged solution.

The NLMR method developed by Kennon [7], actually can be considered as a time-dependent method with variable time step size. The NLMR method is based on the sequential minimization of the global residual. A relaxation factor is introduced to minimize the L_2 norm of the residual at each iteration. This iteration-dependent optimal relaxation factor drives the iterative solutions to convergence. In order to obtain a smooth convergence history, several options are available to this acceleration procedure. For instance, each three regular smoothing iterations are followed by two accelerated iterations [7]. Marchuk [6] has proved that under certain conditions, the variational optimization process will produce the highest convergence rate for iterative method, and the norm of the residual will form a monotone decreasing sequence with iteration. Marchuk [6] also pointed out that the convergence speed of the minimum residual method can be even further improved by using single-iteration, two-step minimum residual method.

The main objective of the present study is to extend Marchuk's idea to generalize the NLMR method using the time-dependent approach and the single-iteration, multi-step algorithm. The applications of the GNLMR method are demonstrated by two numerical examples: one-dimensional Burgers' equation and the two-dimensional heat conduction equation. Several interesting problems originating from this method such as integration by sampling, the concept of grid-dependent relaxation factor, and the determination of the global minimum are also discussed.

2. Theoretical aspects

2.1. Optimization of the Euler scheme for linear problems

Let us first consider a well-posed linear initial value problem

$$\partial\phi/\partial\tau = L\phi - F \quad \text{in } \Omega, \tag{1}$$

$$\phi = \phi_B \quad \text{on } \partial\Omega, \tag{2}$$

$$\phi = \phi_0 \quad \text{at } \tau = \tau_0. \tag{3}$$

Applying the Euler one-step, time-consistent, explicit scheme, the finite difference equation of (1) can be written as:

$$\phi^{t+1} = \phi^t + \Delta\tau(l\phi^t - f) \tag{4}$$

where l denotes the scheme-dependent difference analog of L, f is the discrete analog of F, and t denotes the time level.

Most linear stability analyses of the scheme represented by equation (4) do not consider the effects of boundary conditions, thus resulting in overly restrictive and even incorrect conclusions. For example, Thompson, et al. [10], proved that the cell Reynolds number restriction for

convection-diffusion problems derived from linear stability analysis is a commonly accepted misconception. Moreover, the numerical experiments performed by Kennon and Dulikravich [7,8,9], using the NLMR method showed that the usual Courant–Friedrichs–Lewy (CFL) number limitation for both linear and nonlinear problems can be significantly exceeded. It should be pointed out that, although Thompson et al. clarified the misconception of cell Reynolds number limitation for *linear* convection-diffusion problems, their results did not give the best value of time step size for accelerating the scheme. The NLMR method provided a simple analytic way to determine the optimal acceleration factors for both linear and nonlinear problems. However, the elementary time steps used for obtaining the corrections still follow the CFL number limitation concluded from the linear analysis.

Assuming that coding of a numerical scheme will not cause too much difficulty, stability, convergence speed (computer time) and accuracy of the solution are three major factors to be compromised in optimizing the numerical scheme. We now present an easy and analytic formulation which allows us to make this compromise effectively.

Let the exact solution of $l\phi - f = 0$ be denoted as ϕ^*. Define

$$\xi^t = \phi^t - \phi^*, \tag{5}$$

$$r^t = l\phi^t - f \tag{6}$$

as the error and residual vectors at time level t, respectively. Hence, the time evolution of both error and residual vectors satisfy the following equations:

$$r^t = l\xi^t, \tag{7}$$

$$r^{t+1} = r^t + \Delta\tau(lr^t), \tag{8}$$

$$\xi^{t+1} = \xi^t + \Delta\tau(l\xi^t). \tag{9}$$

The residual and the error norms at time step $t+1$ can be expressed as

$$\| r^{t+1} \|^2 = \| r^t \|^2 + 2\,\Delta\tau(r^t,\, lr^t) + (\Delta\tau)^2 \| lr^t \|^2, \tag{10}$$

$$\| \xi^{t+1} \|^2 = \| \xi^t \|^2 + 2\,\Delta\tau(\xi^t,\, l\xi^t) + (\Delta\tau)^2 \| l\xi^t \|^2. \tag{11}$$

Define the rate of convergence Γ and rate of damping Λ by

$$\Gamma = -\log(\| r^{t+1} \| / \| r^t \|), \tag{12}$$

$$\Lambda = -\log(\| \xi^{t+1} \| / \| \xi^t \|). \tag{13}$$

The convergence and stability of scheme (4) requires that both Γ and Λ are greater than zero. However, the Lax equivalence theorem [11] states that *for linear initial value problems*, stability is the sufficient and necessary condition for convergence. Thus, the limitation on $\Delta\tau$ can be obtained by solving the inequalities

$$\Delta\tau > 0 \quad \text{and} \quad \| r^{t+1} \|^2 < \| r^t \|^2. \tag{14}$$

The solution of the above inequalities can easily be obtained as

$$0 < \Delta\tau < -2(r^t,\, lr^t) / \| lr^t \|^2. \tag{15}$$

It should be noted that equation (15) addresses only stability and not the accuracy of the solution. Nevertheless, if time-accurate solution is required (with a specified accuracy), equation (15) provides the free choice of $\Delta\tau$ to meet both stability and the desired accuracy condition. On

the other hand, if time evolution is not important, $\Delta\tau$ can be chosen as large as possible to minimize the number of time steps for obtaining the steady state solution. The optimal value of $\Delta\tau$ can be determined by maximizing the convergence rate Γ and the result is

$$(\Delta\tau)_{\text{opt}} = -(r^t, lr^t)/\| lr^t \|^2 \tag{16}$$

Thus, for steady state solution of equation (1), the optimized scheme

$$\phi^{t+1} = \phi^t + (\Delta\tau)_{\text{opt}}(l\phi^t - f) \tag{17}$$

will produce the highest rate of convergence. The monotone convergence behavior of the optimized scheme can be best illustrated pictorially by Figs. 9 and 10. As for the stopping criteria, the L_2 norm or L_∞ norm of the residual at new time level are commonly used in determining if the steady state solution is obtained. However, by examining equations (8) and (10), it is interesting to note that $\Delta\tau$ will approach zero as the converged solution is achieved. This provides us with a new criteria for stopping the iterative process.

2.2. Multi-step minimum residual method for linear problems

The method described in the previous section can be used to optimize the single-iteration, one-step scheme. However, the speed of convergence of scheme (17) can be improved even further by multi-step algorithm.

Assume that M steps are used to iterate at each time level. Using the Einstein summation convention where repeated subscripts are summed, the multi-step algorithm for equation (1) is then defined as follows:

$$\phi^{t+1} = \phi^t + \omega_m \delta_m, \quad m = 1 \sim M \tag{18}$$

where

$$\begin{aligned} \delta_1 &= l\phi^t - f, \\ \delta_m &= l^{m-1}(\delta_1), \quad m > 1 \end{aligned} \tag{19}$$

are the residual vectors at step m, and ω_m are the relaxation factors to be determined by minimizing the L_2 norm of the residual at time level $(t+1)$. If the previous definitions of error vector and residual vector are used, the following equations can easily be verified:

$$r^t = l\xi^t, \tag{20}$$

$$r^{t+1} = r^t + \omega_m l\delta_m, \tag{21}$$

$$\xi^{t+1} = \xi^t + \omega_m \delta_m. \tag{22}$$

The L_2 norm of the residual at time level $t+1$ can be expressed as

$$\| r^{t+1} \|^2 = \| r^t \|^2 + 2\omega_m (r^t, l\delta_m) + (l\delta_m, l\delta_n)\omega_m\omega_n, \quad m, n = 1 \sim M. \tag{23}$$

In order to get the highest rate of convergence, clearly, ω_m are the solutions of the following system of linear equations:

$$\partial\Gamma/\partial\omega_m = 0 \quad \text{or} \quad (r^t, l\delta_m) + (l\delta_m, l\delta_n)\omega_n = 0. \tag{24}$$

Multiplying (24) by ω_m, it follows that

$$(r^t, l\delta_m)\omega_m + (l\delta_m, l\delta_n)\omega_m\omega_n = 0. \tag{25}$$

Subtracting (25) from (23) and using (24) results in

$$\| r^{t+1} \|^2 - \| r^t \|^2 = (r^t, l\delta_m)\omega_m = -(l\delta_m, l\delta_n)\omega_m\omega_n$$
$$= -\int_\Omega (\omega_m l\delta_m)^2 \, d\Omega < 0 \tag{26}$$

Thus, the residual norms for the multi-step minimum residual method also shows a monotone convergence behavior which guarantees the stability of the iterative scheme and produces the highest rate of its convergence.

2.3. Optimization of the Euler scheme for nonlinear problems

For clarity, we consider two-dimensional problems and equations in conservative form only. The extension to the multi-dimensional problems and nonconservative equations is then straightforward.

The conservative form of the governing equations for most engineering problems can be written as

$$\partial\phi/\partial\tau = L_\nu N^\nu(\phi, \phi_x, \phi_y) - F, \tag{27}$$

where

$$L_1 = \partial/\partial x, \qquad L_2 = \partial/\partial y \tag{28}$$

and N^ν is the nonlinear differential operator in x_ν coordinates. Using the Euler one-step, time-consistent, explicit scheme, the finite difference form of equation (27) can be written as:

$$\phi^{t+1} = \phi^t + \Delta\tau\left[l_\nu N^\nu(\phi^t, \phi_x^t, \phi_y^t) - f\right] \tag{29}$$

or

$$\phi^{t+1} = \phi^t + \Delta\tau r^t \tag{30}$$

where

$$r^t = l_\nu N^\nu(\phi^t, \phi_x^t, \phi_y^t) - f \tag{31}$$

is defined as the residual at time level t.

Therefore, the residual at time level $t+1$ can be expressed as

$$r^{t+1} = l_\nu N^\nu(\phi^{t+1}, \phi_x^{t+1}, \phi_y^{t+1}) - f. \tag{32}$$

After expanding the nonlinear operator N^ν into Taylor series, it follows that

$$r^{t+1} = l_\nu\{N^\nu(\phi^t, \phi_x^t, \phi_y^t) + \left[(\partial N^\nu/\partial\phi^t)r^t + (\partial N^\nu/\partial\phi_x^t)(r^t)_x + (\partial N^\nu/\partial\phi_y^t)(r^t)_y\right]\Delta\tau + O(\Delta\tau^2)\} - f. \tag{33}$$

In summary,

$$r^{t+1} = r^t + a_m(\Delta\tau)^m \tag{34}$$

where

$$a_1 = l_\nu\left[(\partial N^\nu/\partial\phi^t)r^t + (\partial N^\nu/\partial\phi_x^t)(r^t)_x + (\partial N^\nu/\partial\phi_y^t)(r^t)_y\right] \tag{35}$$

and the coefficients of higher-order terms a_2, a_3, a_4,... can be determined by direct Taylor series expansion. Equation (34) indicates that the residual at time level $t+1$ is a polynomial (hereinafter called residual polynomial [7] or RP) of the time step size. The total number of terms in the residual polynomial (34) depends on the degree of nonlinearity of the operator N^ν.

If N^ν is a polynomial in its arguments then the Taylor series truncates and becomes exact. Thus, the L_2 norm of the residual at time level $t+1$ can be expressed as

$$\| r^{t+1} \|^2 = \| r^t \|^2 + 2(r^t, a_m)(\Delta\tau)^m + (a_m, a_n)(\Delta\tau)^m(\Delta\tau)^n, \quad m, n \geqslant 1 \tag{36}$$

Equation (36) implies that the residual norm at time step $t+1$ is a positive polynomial (hereinafter called minimizing polynomial [7] or MP) of the time step size (to be determined). Thus, the stability of scheme (29) will be guaranteed provided that $\Delta\tau$ is chosen as the optimizer of the minimizing polynomial (36) such that $\| r^{t+1} \|$ is an infimum (global minimum). However, the determination of the optimizer needs special numerical techniques [14]. The rate of convergence depends on the relative difficulty in finding the optimizer. To reduce this difficulty, the linearized operator of N^ν may be applied. If N^ν is truncated to the first order of $\Delta\tau$ (linearized operator), the approximate residual vector is

$$(r^{t+1'}) = r^t + a_1 \Delta\tau. \tag{37}$$

Then, the approximate MP is

$$\| r^{t+1'} \|^2 = \| r^2 \|^2 + 2(a_1, r^t)\ \Delta\tau + (a_1, a_1)(\Delta\tau)^2. \tag{38}$$

The optimizer of the above equation can be easily found. It should be noted that (36) and (38) have the same, but negative slope at $\Delta\tau = 0$. Figures 3 and 4 give the best illustration for the effects of the linearization on the convergence rate.

2.4. The generalized nonlinear minimum residual (GNLMR) method

The GNLMR method actually is the application of the methods described in the previous sections. Let us consider the problems governed by (27) and assume that M steps are used at each time level t. The multi-step algorithm for nonlinear problems is defined as

$$\phi^{t+1} = \phi^t + \omega_m \delta_m + O(\omega_m^2), \quad m = 1 \sim M \tag{39}$$

where repeated indices are summed. The residual at step m is defined as

$$\delta_1 = l_\nu N^\nu(\phi^t, \phi_x^t, \phi_y^t) - f, \tag{40}$$

$$\delta_m = l_\nu\left[(\partial N^\nu/\partial\phi^t)\delta_{m-1} + (\partial N^\nu/\partial\phi_x^t)(\delta_{m-1})_x + (\partial N^\nu/\partial\phi_y^t)(\delta_{m-1})_y\right]. \tag{41}$$

The coefficients of the higher order terms of ω_m can be obtained by Taylor's series expansion. If only linear terms of ω_m are retained, the residual polynomial (RP) at time step $t+1$ can be expressed by Taylor's series expansion as

$$\begin{aligned} r^{t+1} &= l_\nu N^\nu(\phi^{t+1}, \phi_x^{t+1}, \phi_y^{t+1}) - f \\ &= l_\nu N^\nu\left[\phi^t + \omega_m\delta_m, \phi_x^t + \omega_m(\delta_m)_x, \phi_y^t + \omega_m(\delta_m)_y\right] - f \\ &= r^t + l_\nu\left\{\left[(\partial N^\nu/\partial\phi^t)\delta_m + (\partial N^\nu/\partial\phi_x^t)(\delta_m)_x + (\partial N^\nu/\partial\phi_y^t)(\delta_m)_y\right]\omega_m + O(\omega_m^2)\right\}. \end{aligned} \tag{42}$$

Therefore, the minimizing polynomial (MP) at time step $t+1$ can be determined as

$$\| r^{t+1} \|^2 = \| r^t \|^2 + g(\omega_m) \tag{43}$$

where $g(\omega_m)$ is a polynomial in ω_m. For a highly nonlinear differential equation, g will be a complicated multi-variable polynomial that depends on the number of steps we used and the degree of the nonlinearity of the differential operator N^r. Thus, a fast and accurate method to determine the optimizer of MP is required for the GNLMR method to guarantee the highest rate of convergence. If the linearized operator of N^r is applied to reduce the difficulty of finding the global minimum, the approximate optimizer of (43) can be determined by the method described in section 2.2.

Since the coefficients in the MP are obtained by integrating the residuals over the whole domain, the GNLMR method requires a large amount of computer storage to save the residuals from each step m. This is also the common problem for all the conjugate-gradient-type methods [12]. For the new generation of supercomputers, storage may not cause too much problems [12]. However, if storage restriction does exist, an integration by sampling could be considered. Nevertheless, several problems accompany this idea [13]. Since a statistical sampling procedure can be used to get the random data for integration, the question of error incurred by the sampling should be addressed. If the error caused by sampling approximation can be determined, it should be possible to design an optimal sampling procedure to minimize the error.

The problem of finding the global minimum (infimum) or the global maximum (supremum) for a function of several variables is a basic problem in global optimization theory. In the GNLMR method, the optimal relaxation factors are actually the optimizer of the MP. The relative difficulty to find the optimizer depends on the degree of nonlinearity of the governing differential equations and the number of steps we used for the multi-step algorithm. As pointed out by Ratschek and Rokne [14], interval method is the only one among all the existing methods that always guarantee the location of the global extremum with arbitrary accuracy. Since the interval method is basically iterative, it will require considerable computer time to get the accurate result for a multi-variable polynomial of higher order. The highest rate of convergence of GNLMR method will be guaranteed if the optimizer of MP can be efficiently determined.

Since boundary conditions can be applied exactly in the regions that are neighboring to the boundary, it is obvious that during the process of relaxation, the iterative solutions in those regions are more accurate than the regions that are far away from the boundary. This implies that the relaxation factor should vary from one subregion to another, or even from point to point, since the subregions or points where residuals are large, definitely need more correction.

3. Numerical examples

Two numerical test cases are used to demonstrate the applications of the GNLMR method: one-dimensional Burgers' equation and two-dimensional heat conduction equation. Both test cases were computed using nonaccelerated method where time step size satisfies the CFL limitation. In addition, three accelerated computations were performed with $M = 1, 2, 3$ where M is the number of steps used in the multi-step algorithm. It should be pointed out that, when applying the GNLMR method, it is not necessary to specify the time step size to obtain the residuals at each step. However, in order to compare the relative speed of convergence between

the GNLMR method and the nonaccelerated method, a time step size that satisfies the CFL limitation is used in calculating the residual at each step for both cases. Moreover, the effect of linearization to the rate of convergence is investigated by solving both exact and approximate MPs for $M = 1$ in the case of Burgers' equation. Comparisons are based on the accuracy of the solution and the actual computer time required.

3.1. Burgers' equation

According to the notations defined in the Section 2, the one-dimensional, viscous Burgers' equation can be written as

$$\partial\phi/\partial\tau = L_x N(\phi, \phi_x)$$

where

$$N(\phi, \phi_x) = -\tfrac{1}{2}\phi^2 + \nu\phi_x \tag{44}$$

and ν is the viscosity coefficient. In this example, $\nu = 0.07$ is used. The initial and the boundary conditions are chosen as follows

$$\phi(1, \tau) = 0, \qquad \phi(0, \tau) = 1, \qquad \phi(x, 0) = 1 - x. \tag{45}$$

The FTCS scheme is applied to discretize (44) as

$$\phi^{t+1} = \phi^t + \Delta\tau\left\{-\left[\left(\phi^t_{i+1}\right)^2 - \left(\phi^t_{i-1}\right)^2\right]/4\,\Delta x + \nu\left(\phi^t_{i+1} - 2\phi^t_i + \phi^t_{i-1}\right)/\Delta x^2\right\} \tag{46}$$

where i denotes the ith grid point in the total of 41.

The exact RP for $M = 1$ can be expressed as

$$\mathrm{RP} = r^{t+1} = r^t + a_1\,\Delta\tau + a_2(\Delta\tau)^2 \tag{47}$$

where

$$a_1 = \partial/\partial x\left(-\phi^t r^t + \nu r^t_x\right), \qquad a_2 = -0.5\partial/\partial x(r^t)^2. \tag{48}$$

The optimal value of $\Delta\tau$ is chosen as the optimizer of the exact MP

$$\mathrm{MP} = \|r^{t+1}\|^2 = A_0 + A_1\,\Delta\tau + A_2(\Delta\tau)^2 + A_3(\Delta\tau)^3 + A_4(\Delta\tau)^4 \tag{49}$$

where

$$A_0 = \|r^t\|^2, \qquad A_1 = 2(r^t, a_1) \qquad A_2 = (a_1, a_1) + 2(r^t, a_2),$$
$$A_3 = 2(a_1, a_2), \qquad A_4 = (a_2, a_2). \tag{50}$$

If linearized operator of N and M steps are used, the residual polynomial is truncated up to its first order as

$$\mathrm{RP} = r^{t+1} = r^t + a_m\omega_m$$

where

$$a_m = (\partial/\partial x)\left[-\phi^t\delta_m + \nu(\delta_m)_x\right] \tag{51}$$

and δ_m can be determined from (40)–(41). The minimizing polynomial MP is then

$$\mathrm{MP} = \|r^{t+1}\|^2 = \|r^t\|^2 + 2(r^t, a_m)\omega_m + (a_m, a_n)\omega_m\omega_n.$$

Thus, the optimal relaxation factors ω_m can be easily determined by solving the following system of linear equations.

$$A_{mn}\omega_n = b_m$$

where

$$A_{mn} = (a_m, a_n), \qquad b_m = -(r^t, a_m), \tag{52}$$

and A_{mn} is a symmetric matrix of order M.

Figure 1 shows the exact steady state solution and the numerical solutions after 100 iterations. It is obvious that the GNLMR method gives the most accurate results. The computer time costs of 100 iterations for each case are shown in Fig. 2. It indicates that the GNLMR method needs more computer time per iteration. This depends on the number of steps that were used in the multi-step algorithm and whether a linearized or exact MP was solved. However, if a desired accuracy is specified, the GNLMR method needs fewer iterations to achieve the accuracy requirement as shown in Fig. 3. Therefore, the overall judgement of the efficiency of the GNLMR method should be based on the computer time rather than number of iterations required to obtain a solution with a specified accuracy. Figure 4 does prove the efficiency gained by using the GNLMR method. The variations of the relaxation factors with respect to time (or iteration) show that a sudden change in their magnitudes occurred just before converged solution is reached as shown in Figs. 5, 6 and 7. It is interesting to note that all the relaxation factors reduce to zero as converged solution is obtained. Since the relaxation factor is equivalent to the time step size in our formulations, this phenomena can be interpreted as that the time marching will stop once the steady state solution is obtained. This provides an alternative criteria for stopping the iterative process in the GNLMR method.

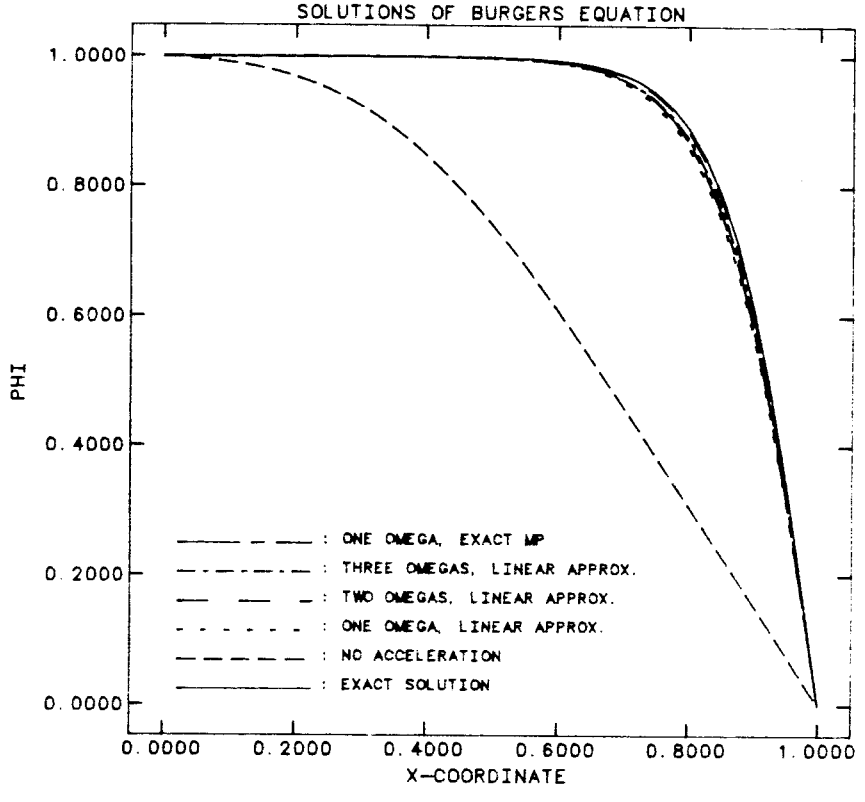

Fig. 1. Exact and numerical solutions of Burgers' equation

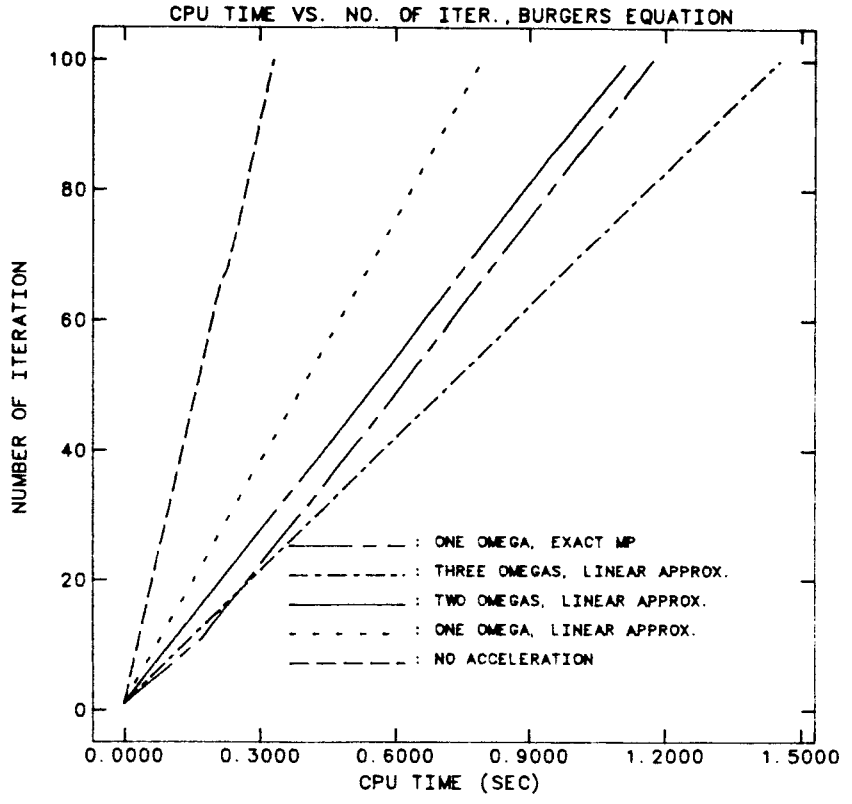

Fig. 2. Number of iterations versus computer time.

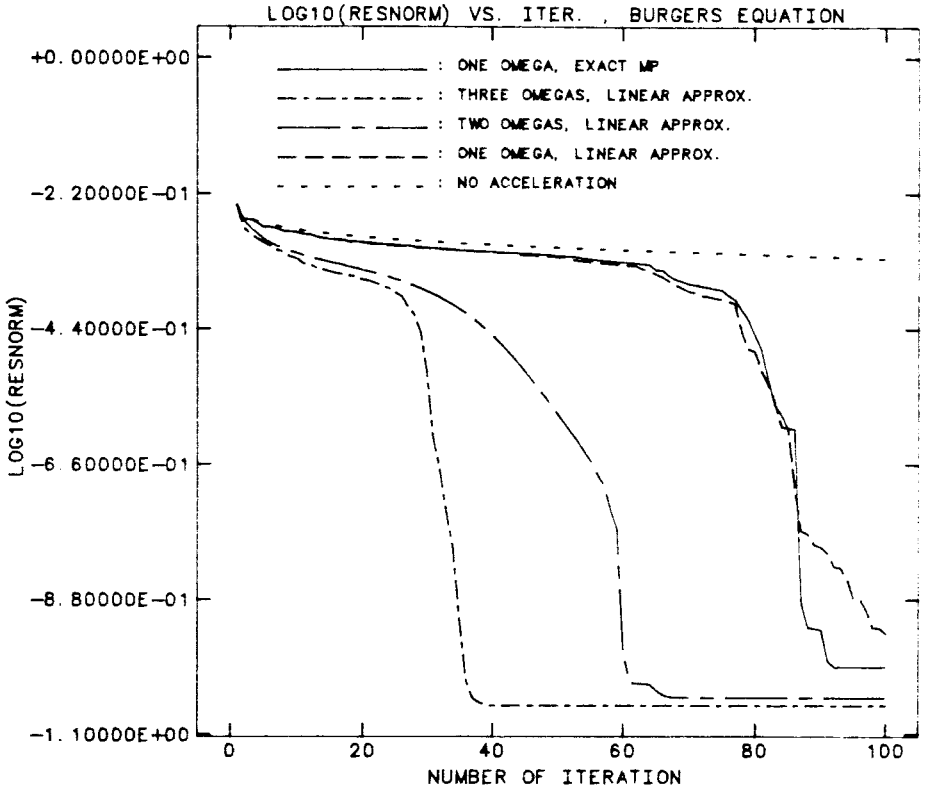

Fig. 3. Residual norm versus number of iterations.

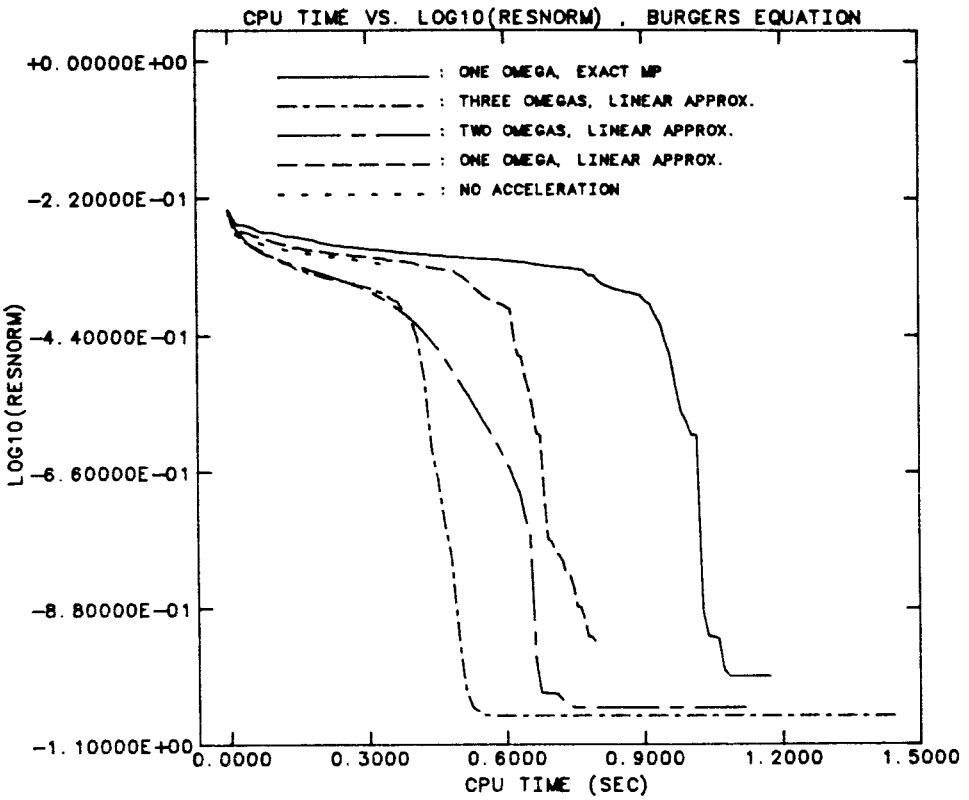

Fig. 4. Residual norm versus computer time.

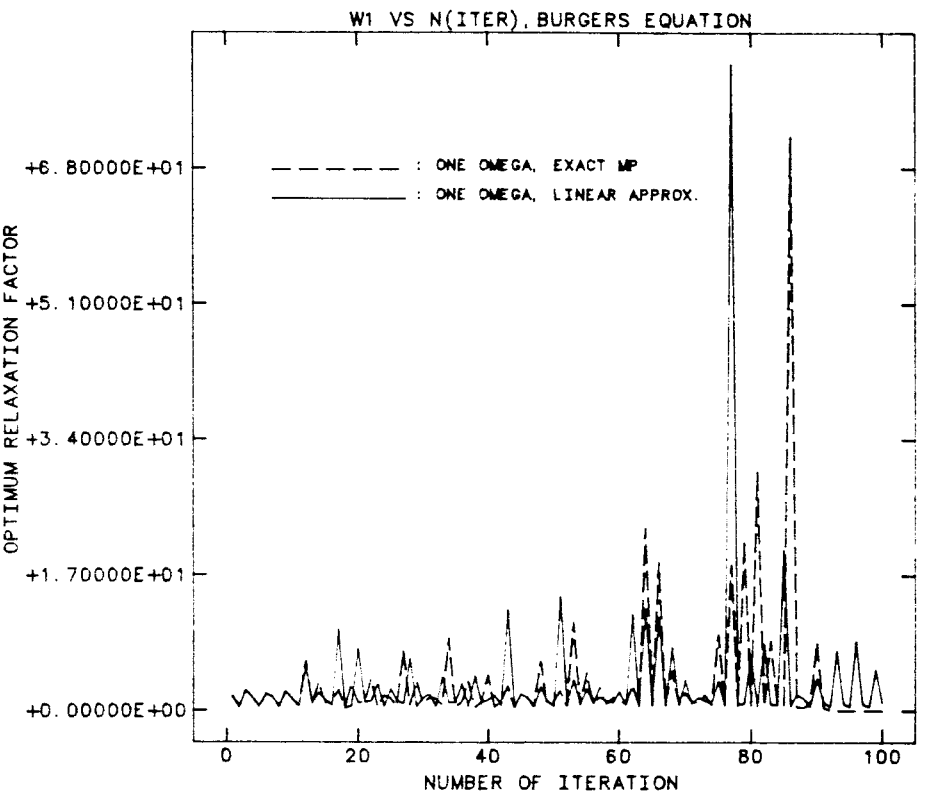

Fig. 5. Optimal relaxation factor versus number of iterations.

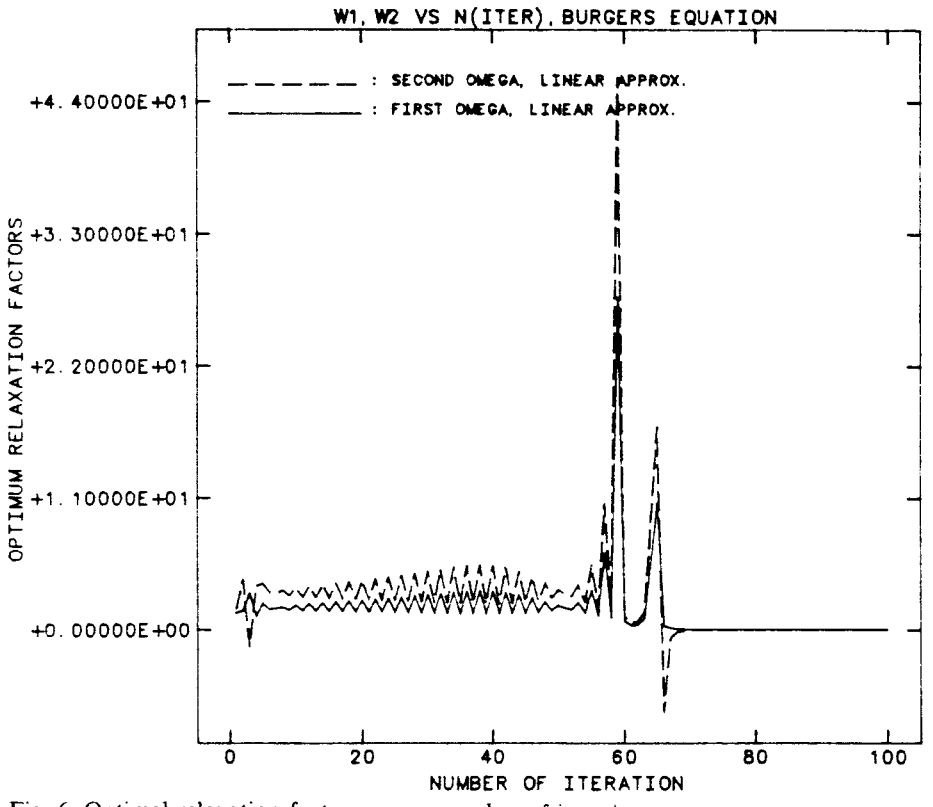

Fig. 6. Optimal relaxation factors versus number of iterations.

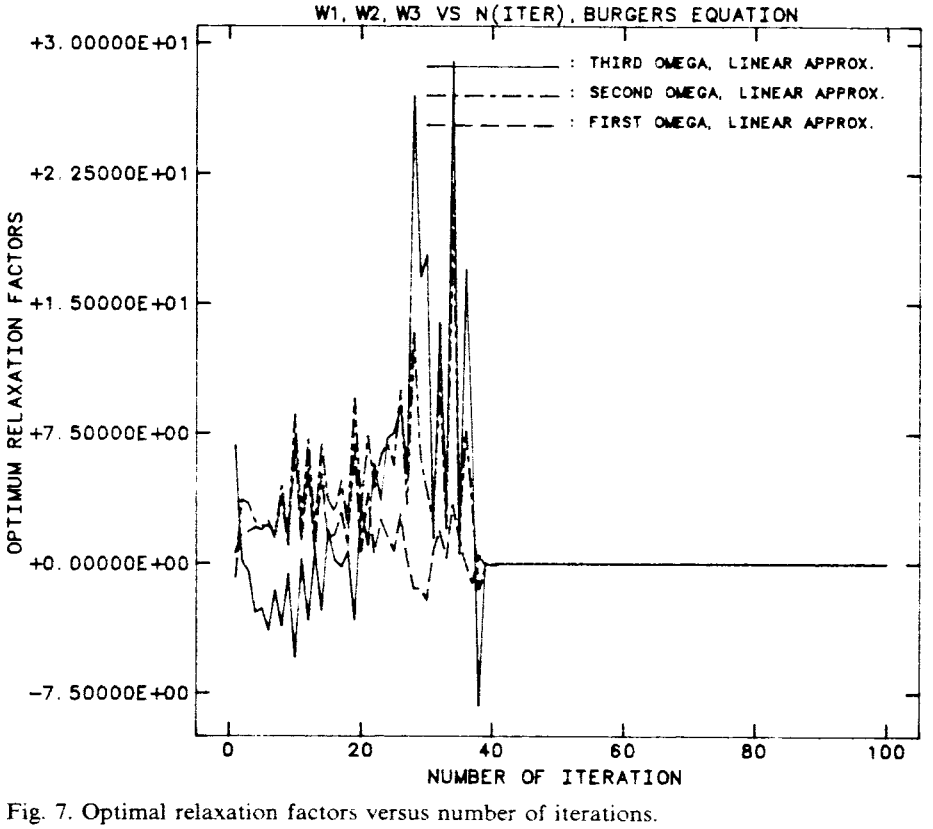

Fig. 7. Optimal relaxation factors versus number of iterations.

It must be mentioned that according to Figs. 3, and 4, both the rate of convergence and smoothness of convergence of the NLMR method can be improved even further by the multi-step algorithm. Moreover, Figs. 3 and 4 show a peculiarity that during the first few tens of iterations solution converges very slowly and then suddenly accelerate to its maximum rate. The converged solution is then reached almost immediately following the maximum rate interval. This behavior is entirely different from linear problems as mentioned by Marchuk [6]. For a positive definite matrix (a linear operator), the convergence rate during the initial iterations is much higher than the asymptotic rate of convergence if the method of minimum residual is applied. Hence, in practice it is not necessary to solve the exact MP for a nonlinear problem; the linearized MP can be used and still guarantee a high rate of convergence as shown in Figs. 2, 3 and 4.

3.2. *The heat conduction equation*

The unsteady heat conduction equation is given by

$$\partial\phi/\partial\tau = L\phi, \qquad L = \alpha\left(\partial^2/\partial x^2 + \partial^2/\partial y^2\right) \tag{53}$$

where α is the thermal diffusivity.
A rectangular uniform grid having 21×21 grid points was used for this example. The initial and boundary conditions are as follows:

$$\begin{aligned} &\phi(x, y, 0) = 100, \qquad \phi(0, y, \tau) = 100 * \cos(2\pi y/H), \qquad \phi(W, y, \tau) = 100, \\ &\phi(x, 0, \tau) = 100, \qquad \phi(x, H, \tau) = 100. \end{aligned} \tag{54}$$

Applying FTCS scheme, (53) discretizes into

$$\phi^{t+1} = \phi^t + \Delta\tau r^t$$

where

$$r^t = \alpha\left[\left(\phi^t_{i+1,j} - 2\phi^t_{i,j} + \phi^t_{i-1,j}\right)/\Delta x^2 + \left(\phi^t_{i,j+1} - 2\phi^t_{i,j} + \phi^t_{i,j-1}\right)/\Delta y^2\right]. \tag{55}$$

Here i, j denote the grid point at $i\,\Delta x$, $j\,\Delta y$). The residual polynomial is given by (21) as

$$r^{t+1} = r^t + \omega_m l\delta_m$$

The minimizing polynomial is given by (23) as

$$\mathrm{MP} = \| r^{t+1} \|^2 = \| r^t \|^2 + 2\left(r^t, l\delta_m\right)\omega_m + \left(l\delta_m, l\delta_n\right)\omega_m\omega_n.$$

The optimal relaxation factors ω_m are the solution of the following linear system of equations.

$$A_{mn}\omega_n = b_m$$

where

$$A_{mn} = \left(l\delta_m, l\delta_n\right), \qquad b_m = -\left(r^t, l\delta_m\right), \tag{56}$$

and A_{mn} is a symmetric matrix of order M.

The numerical results are summarized by Figs. 8 to 13. As indicated in Figure 8. the computer time required per iteration for the GNLMR method is longer than for the nonaccelerated

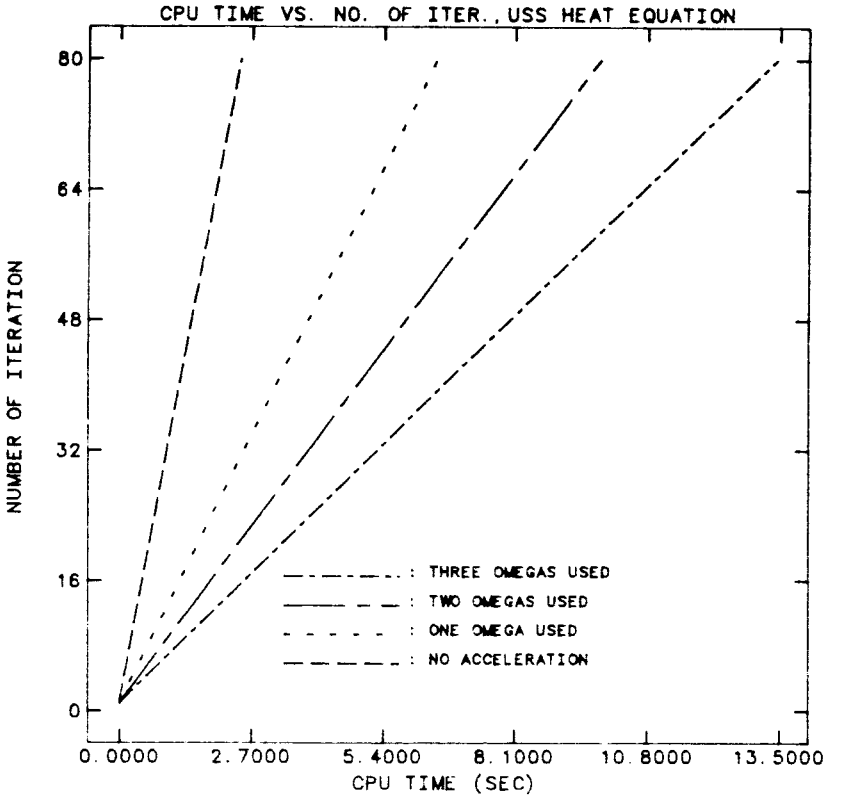

Fig. 8. Number of iterations versus computer time.

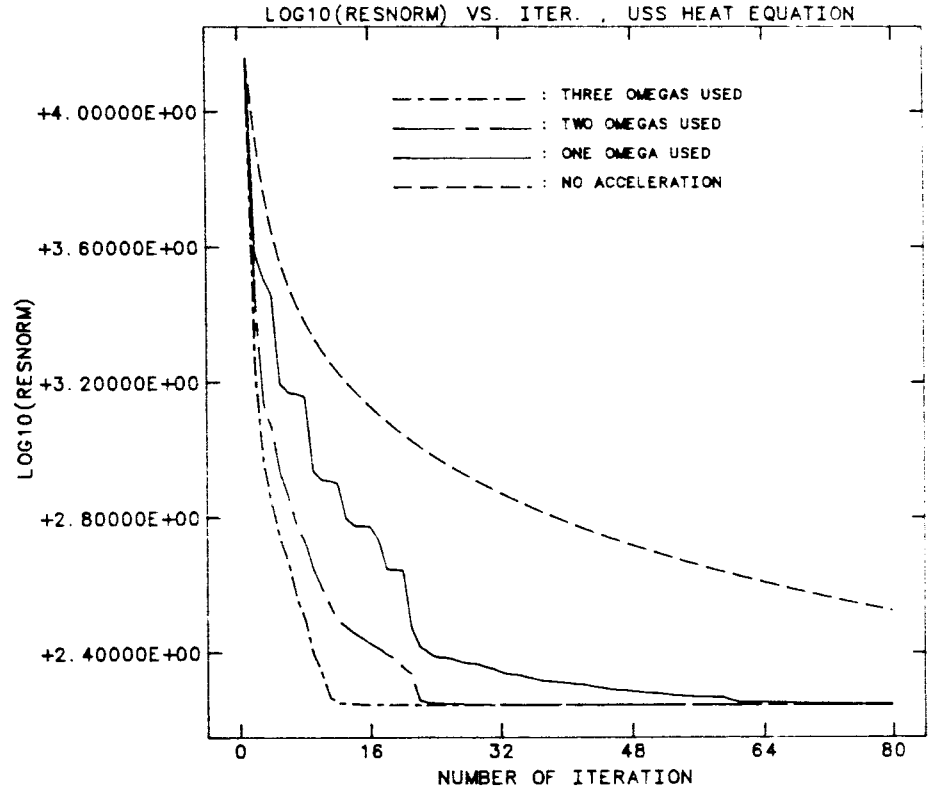

Fig. 9. Residual norm versus number of iterations.

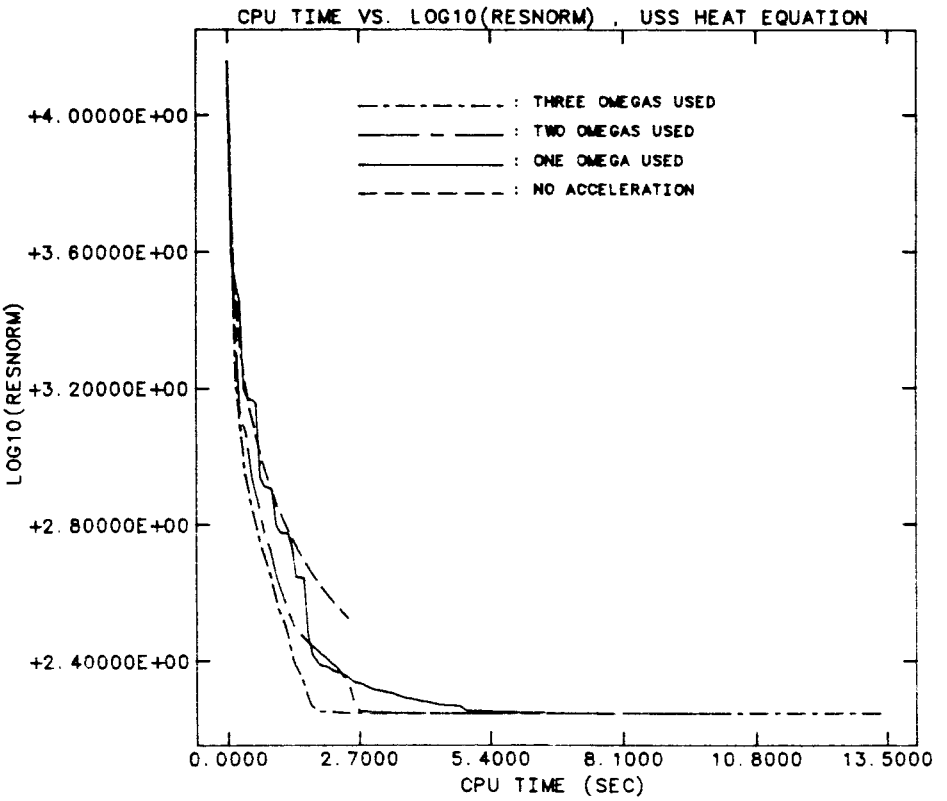

Fig. 10. Residual norm versus computer time.

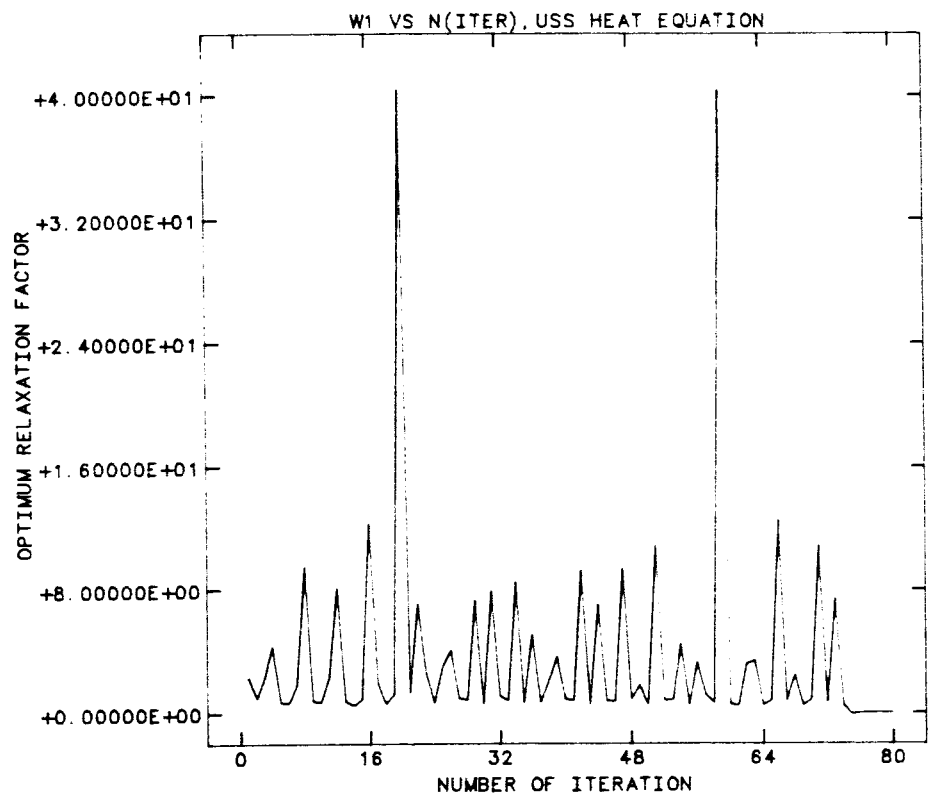

Fig. 11. Optimal relaxation factor versus number of iterations.

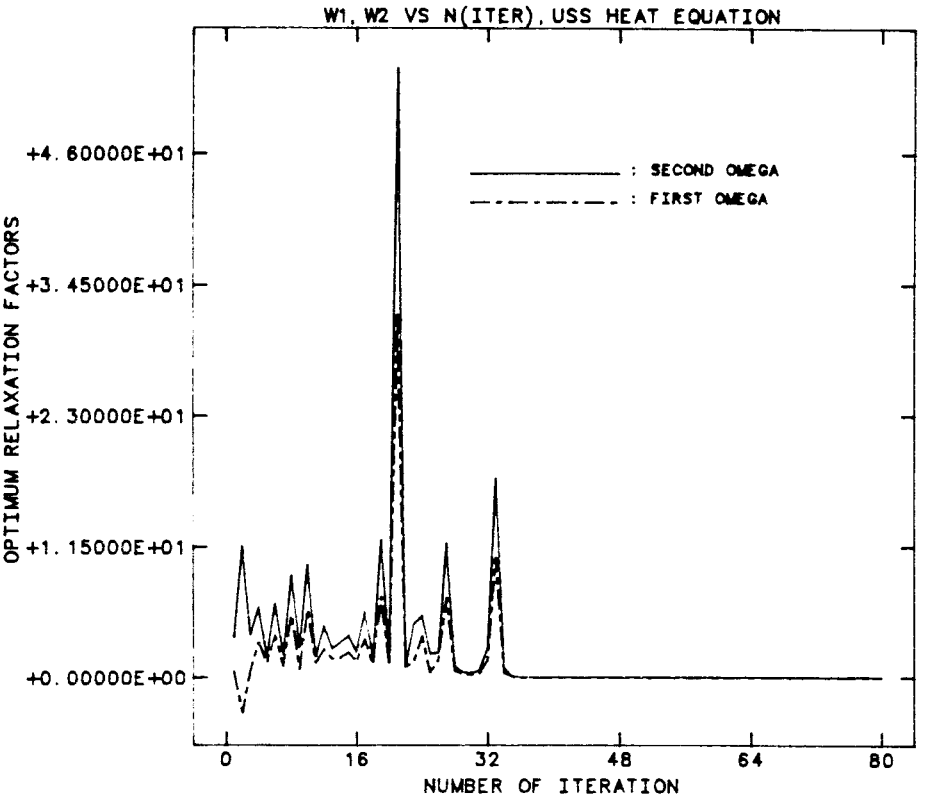

Fig. 12. Optimal relaxation factors versus number of iterations.

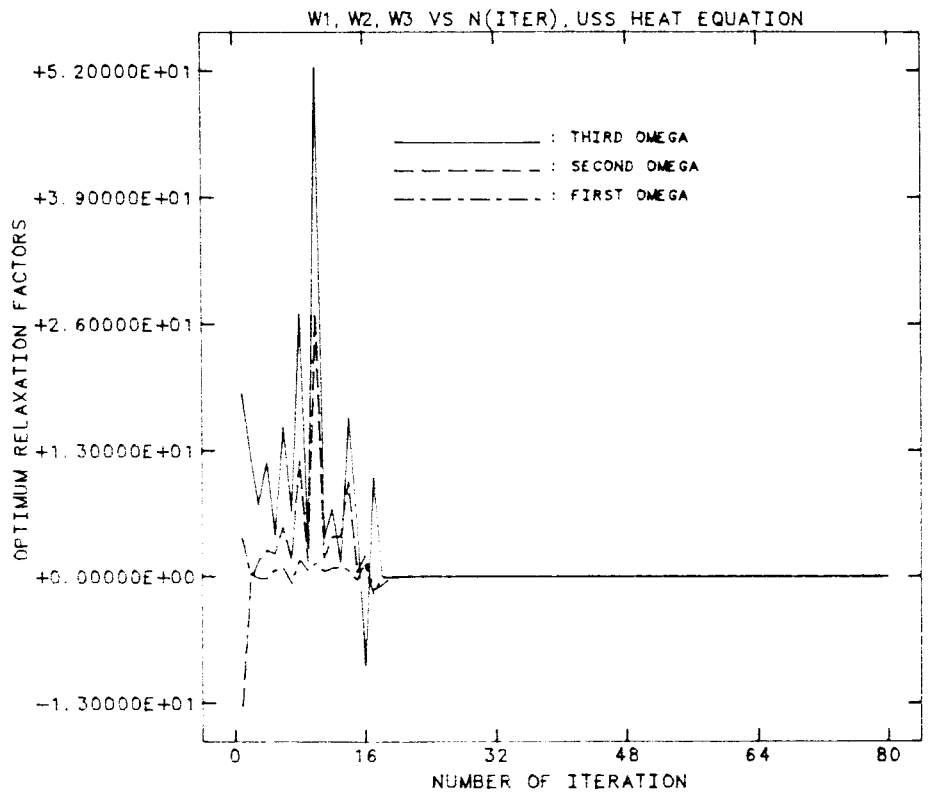

Fig. 13. Optimal relaxation factors versus number of iterations.

method. However, Fig. 9 shows that if the maximum number of iterations is limited to 80, the accuracy that can be obtained by the GNLMR method is better than that of the non-accelerated method. If a fixed computer time is specified, Fig. 10 clearly shows that the GNLMR method will produce the best solution. Figures 11 to 13 show the variations of the optimal relaxation factors versus number of iterations. Figures 9 and 10 confirm that using the multi-step algorithm improves both the smoothness and the rate of convergence for the NLMR method. If the GNLMR method is applied to a linear problem, it is interesting to note that the rate of convergence during the initial few iterations is much higher than the asymptotic rate of convergence as indicated by Figs. 9 and 10.

It should be pointed out that the linear version of the GNLMR method is similar to the generalized minimum residual GMRES method developed by Saad and Schultz [15] to solve nonsymmetric linear systems of equations. This method was recently modified by Wigton et. al. [12] to solve nonlinear problems in gas dynamics using Newton's iteration method. Since Gram–Schmidt orthogonalization procedures are applied to orthogonalize the search directions at each iteration in the GMRES method, this method demands a large number of arithmetic operations and a large computer memory. Moreover, as pointed out by Marchuk [6], the implementation of the orthogonalization algorithm with respect to high-order matrices usually results after a few tens of iterations in a numerical instability because of nonlinearity. This implies that the maximum number of steps which can be used in one iteration for the multi-step algorithm is practically limited to a moderate finite number.

4. Concluding remarks

The GNLMR method and its applications were presented. The accelerating mechanism and the monotone convergence behavior of the GNLMR method has been proved by theoretical studies and the numerical experiments. It was found that both the rate and the smoothness of convergence of the NLMR method can be improved even further by the optimized multi-step algorithm. Both numerical test cases confirmed that all the optimal relaxation factors vanish as converged solution is achieved thus providing a new stopping criteria for the iterative process. The numerical results also proved that linearization of a nonlinear operator in the GNLMR method reduces the problems of determining the optimizer of the MP. This linearization still guarantees a high rate of convergence. Hence, the GNLMR method can be simplified in practical problems when iteratively solving nonlinear partial differential equations.

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