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APPLICATION OF THE OPTIMIZED MODIFIED STRONG IMPLICIT PROCEDURE TO NONLINEAR PROBLEMS

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This article applies a recently developed iterative method to solve the system of equations obtained from the discretization of nonlinear, two-dimensional field problems. This method is the modified strong implicit procedure with an adaptive optimization algorithm applied to its iteration parameter, which eliminates the trial-and-error method usually necessary to determine its optimum value. Four nonlinear problems are used to compare the new method to the original MSIP. The results show that, for nonlinear problems, the optimized MSI procedure is faster than the original MSI procedure, even when the latter is used with the best value of its iteration parameter.

INTRODUCTION

The finite-difference or finite-element discretization of two-dimensional field problems leads to large, sparse systems of algebraic equations that have to be solved by iterative methods. Among the existing iterative methods [1], the modified strong implicit procedure (MSIP), developed by Schneider and Zedan [2], is usually considered the one with best convergence behavior.

Like other methods, the MSIP has an iteration parameter that has to be chosen in advance. The convergence characteristics of the iterative methods are strongly influenced by the value (or values) chosen for the iteration parameter, which usually shows an optimum value (or a sequence of optimum values during iteration) for each problem. Although the MSIP is the least sensitive to the value of its iteration parameter, its optimization can accelerate the convergence appreciably. Since the search of the best value for the iteration parameter has to be done by a trial-and-error procedure, its is not worthwhile unless the problem has to be solved several times. Besides, for nonlinear problems, its optimum value may vary during problem solution. This explains why some implementations of the MSI procedure hold the iteration parameter constant for every problem [3].

Recently, Lage [4] developed an adaptive optimization algorithm to search for the best value of the iteration parameter during problem solution using the MSIP.

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NOMENCLATURE

$\mathbf{A}$	coefficient matrix	$\|\| \ \|\|$	Euclidean norm of a vector in an n-dimensional space
$\mathbf{B}$	auxiliary matrix	α	iteration parameter
$\mathbf{b}$	right-hand-side vector	$\boldsymbol{\delta}$	difference vector
c_p	specific heat at constant pressure	ϵ	tolerance in $F(\alpha)$ estimation
f	convergence rate	ϵ_α	tolerance in α values for matrix decomposition
F	asymptotic convergence rate of the residual norm	ϵ_r	relative tolerance
g	convergence rate of arithmetic means	ϵ_a	absolute tolerance
k	thermal conductivity	ρ	density
$\mathbf{L}$	lower triangular matrix		
n	number of iterations		**Subscripts**
N	number of iterations in the smoothing procedure	n	iteration counter
Q	heat source		
$\mathbf{R}$	residual vector		**Superscripts**
t	time coordinate	n	iteration counter
T	temperature	N	number of iterations in the smoothing procedure
$\mathbf{U}$	upper triangular matrix		
$\mathbf{x}$	vector of unknowns		
x, y	Cartesian coordinates		

His results for the solution of five linear heat transfer problems show that the optimized MSI procedure (OMSIP) is almost as fast as the original MSI procedure with its best iteration parameter. For a nonoptimal value of the iteration parameter, the OMSIP is faster than the MSIP in almost all the cases analyzed.

The present work applies the optimized MSI procedure to four nonlinear, two-dimensional heat transfer problems. Two of them are steady-state problems and the other two are the corresponding time-dependent problems. The results are compared to those obtained by using the original MSI procedure. This comparison demonstrates the advantages of the application of the MSI procedure with adaptive optimization over the standard MSI procedure for nonlinear field problems.

THE STANDARD MSI PROCEDURE

The MSI procedure developed by Schneider and Zedan [2] is outlined in this section. Further details can be found in the original work. The discretization of the two-dimensional field problem leads to the system of algebraic linear (or linearized) equations

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b} \tag{1}$$

where the coefficient matrix $\mathbf{A}$ is pentadiagonal or nine-diagonal. The MSI procedure consists of the definition of an auxiliary matrix $\mathbf{B}$, which is chosen in order that the modified coefficient matrix $\mathbf{A} + \mathbf{B}$ has an LU factorization where the upper and lower triangular matrices keep the sparse structure of $\mathbf{A}$. The definition of $\mathbf{B}$ includes a partial cancellation factor, α, which tries to minimize the difference

between the modified and original systems of equations. This is the iteration parameter of the MSI procedure. It should be noted that the LU decomposition of the modified matrix is calculated by a very fast algorithm. Once α is chosen, $\mathbf{B}$ is determined and the following iterative procedure is applied:

$$(\mathbf{A} + \mathbf{B}) \cdot \mathbf{x}^{n+1} = (\mathbf{A} + \mathbf{B}) \cdot \mathbf{x}^n - (\mathbf{A} \cdot \mathbf{x}^n - \mathbf{b}) \tag{2}$$

Since $\mathbf{A} + \mathbf{B} = \mathbf{L} \cdot \mathbf{U}$ and defining the difference vector $\boldsymbol{\delta}^{n+1} = \mathbf{x}^{n+1} - \mathbf{x}^n$ and the residual vector $\mathbf{R}^n = \mathbf{b} - \mathbf{A} \cdot \mathbf{x}^n$, the iteration step consists of the solution of

$$(\mathbf{L} \cdot \mathbf{U}) \cdot \boldsymbol{\delta}^{n+1} = \mathbf{R}^n \tag{3}$$

which is obtained by a two-step process consisting of a forward substitution followed by a backward substitution.

MSIP ASYMPTOTIC RATES OF CONVERGENCE

In order to optimize the iteration parameter of the MSI procedure, it is necessary to define a measure of the convergence characteristics of the MSI procedure for a given value of its iteration parameter. It has been found [4] that there exists an asymptotic convergence rate for the sequence of the arithmetic means of the norm of the residual vector,

$$F(\alpha) = \lim_{n \to \infty} g_n \tag{4}$$

where

$$g_n = \frac{1}{n} \sum_{k=1}^{n} f_k \tag{5}$$

and

$$f_k = \frac{\|\mathbf{R}^k\|}{\|\mathbf{R}^{k-1}\|} \tag{6}$$

Since the sequence of arithmetic means converges too slowly to be used in an adaptive optimization procedure, a faster estimate of the asymptotic convergence rate has been obtained through a smoothed value of f_n after a few iterations:

$$F(\alpha) \cong \lim_{n \to \infty} g_n^N \quad \text{where} \quad g_n^N = \frac{1}{N} \sum_{k=n+1-N}^{n} f_k \tag{7}$$

where $N = 4$ has shown to be a good choice [4]. The procedure for the estimation of the asymptotic rate of convergence is explained elsewhere [4].

ADAPTIVE OPTIMIZATION PROCEDURE

Once estimates of the asymptotic convergence rate become available for some values of the iteration parameter, an algorithm should be used to determine a better value for the iteration parameter for the next LU decomposition. The details of this algorithm are found in [4]. It has been found in the present work that, for nonlinear problems, the algorithm performs better if the tolerances for $F(\alpha)$ determination (ϵ) and for accepting a new α value (ϵ_α) are increased from 0.001 to 0.01. The interval for searching the best a value is still [0.01, 0.99].

DESCRIPTION OF TEST PROBLEMS

In order to test the OMSIP for nonlinear problems, test problems 1 and 4 of [4] (originally presented by Stone [5] and by Schneider and Zedan [2], respectively) are modified by adding a temperature-dependent thermal conductivity to give our present steady-state nonlinear problems 1 and 2, respectively. Then, the corresponding transient problems are also solved. For the sake of completeness, these test problems are described below.

The basic equation to be solved is the heat transfer equation in Cartesian coordinates in a two-dimensional domain with a medium that might have temperature-dependent thermal conductivity, given by

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) + Q \qquad (8)$$

which is discretized using the control-volume technique. The above equation is assumed to be in a dimensionless form.

Steady-state problem 1. The domain is a square with side length 1 that is completely insulated. Point heat sources are located at (0.1, 0.1), (0.1, 0.9), (0.767, 0.133), (0.467, 0.5), and (0.9, 0.9), with strengths 1.0, 0.5, 0.6, −1.83, and −0.27, respectively. Also,

$$k(T) = \exp(-0.23T) \qquad (9)$$

which corresponds to a dimensionless iron conductivity between 200 and 1,000 K. The initial guess for the temperature field is the uniform field with zero temperature ($T = 0$).

Steady-state problem 2. The domain is $0 < x < 2$, $0 < y < 1$. The two vertical sides at $x = 0, 2$ are insulated. The side at $y = 0$ is insulated for $1 < x < 2$ and receives a uniform heat flux $q_y = 1$ for $0 < x < 1$. The upper boundary at $y = 1$ is subjected to a boundary condition of the third kind, with a convective heat transfer coefficient of 5, losing heat to an ambient at zero temperature. The thermal conductivity is given by Eq. (9) and the initial guess is the uniform field with zero temperature ($T = 0$).

Transient problems 1 and 2. These are the transient problems of the above steady-state problems for an initial uniform field with zero temperature and for $\rho c_p = 1$. The fully implicit scheme is used in the control-volume discretization.

These test problems have been solved in a fixed 30 × 30 mesh (identical to the one used by Stone [5]). For the transient problems, the time interval in the finite-difference discretization was varied, for each problem, in order to give 10, 20, and 100 time points during the transient solution. The time necessary to practically reach steady state was found to be $t = 2$ for the first problem and $t = 8$ for the second one.

During the solution of all problems, the following convergence criterion was used:

$$\frac{|T^{(n)} - T^{(n-1)}|}{\epsilon_r |T^{(n)}| + \epsilon_a} < 1 \qquad (10)$$

for every point in the field, where $\epsilon_r = 10^{-4}$ and $\epsilon_a = 10^{-6}$. Since these problems are nonlinear, the coefficient matrices of the discretized system of equations have to be updated during the solution of the steady-state problems or during a time-step fully implicit integration of the transient problems. The iteration scheme applied to both cases, using either the MSIP or the OMSIP, is given in Figure 1. In this figure, the iterative method (MSIP or OMSIP) is applied until the convergence criterion given by Eq. (10) is met internally. Then, the temperature field is checked against the temperature field at the beginning of the iteration. If the convergence criterion given by Eq. (10) is not met, new iteration is started; otherwise the steady-state problems are considered to be solved and, for the transient problems, a new time-step integration is then started. The only difference in the iterative scheme is that the OMSIP reevaluates the coefficient matrix each time it chooses a new α value.

RESULTS

Since the OMSI procedure is based on evaluation of the asymptotic rate of convergence, our first aim is to verify its behavior during the solution of a nonlinear problem. For a nonlinear problem, a unique $F(\alpha)$ curve does not exist because its coefficient matrix changes during solution. However, if the linearity is not too severe, one should expect that most of the (α, F) values obtained during problem solution belong approximately to a single curve. For all the problems analyzed, this fact has been verified, as can be seen in Figures 2, 3, 4, and 5, for the steady problems 1 and 2 and the transient problems 1 and 2, respectively. These

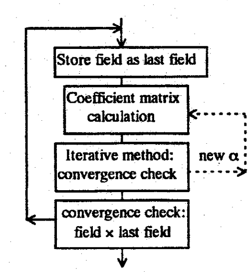

Figure 1. Iterative scheme for nonlinear problem solution (the path with dashed line occurs only when using the OMSI procedure).

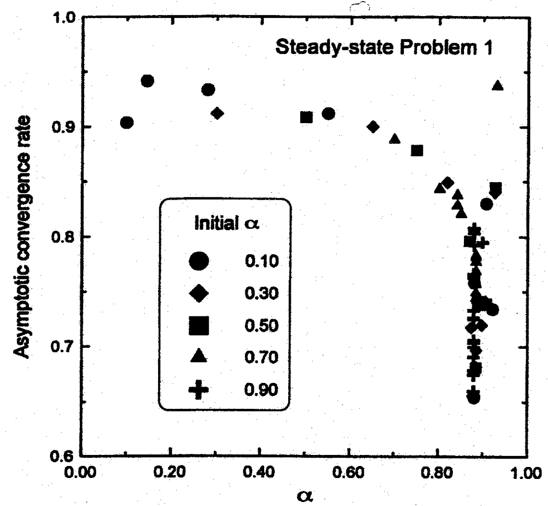

Figure 2. Asymptotic convergence rate for steady-state problem 1.

figures show the $F(\alpha)$ values obtained during problem solution with the OMSIP for several initial α values. From these figures, it is clear that there is considerable data scatter due to two factors: (1) the problem nonlinearity and (2) the large tolerance used in $F(\alpha)$ estimation. The same α data are plotted against the total number of iterations [the number of times Eq. (3) is solved] in Figures 6, 7, 8, and

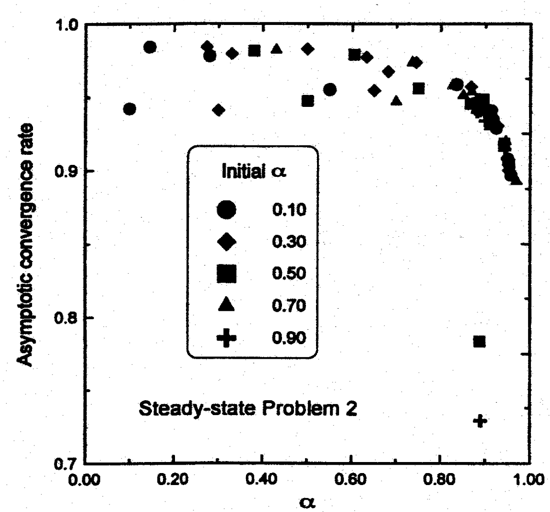

Figure 3. Asymptotic convergence rate for steady-state problem 2.

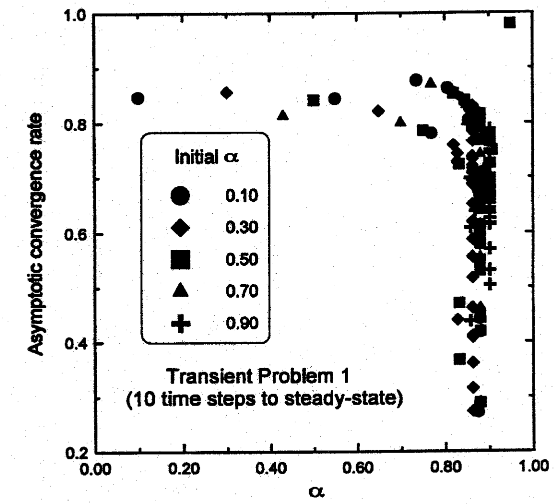

Figure 4. Asymptotic convergence rate for transient problem 1.

9, for the steady problems 1 and 2 and the transient problems 1 and 2, respectively. It should be noted that only the first 200 iterations are shown in Figures 8 and 9 for the solutions of the transient problems. From these figures, it is clear that the optimization algorithm is able to bring the α value close to its optimum for both problems, even though some oscillations occur, most of them during the first

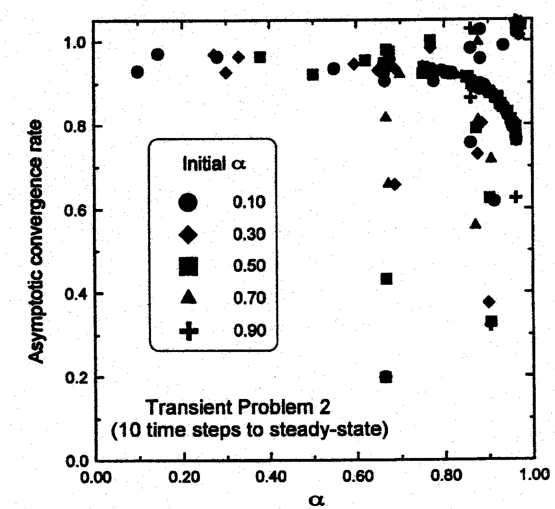

Figure 5. Asymptotic convergence rate for transient problem 2.

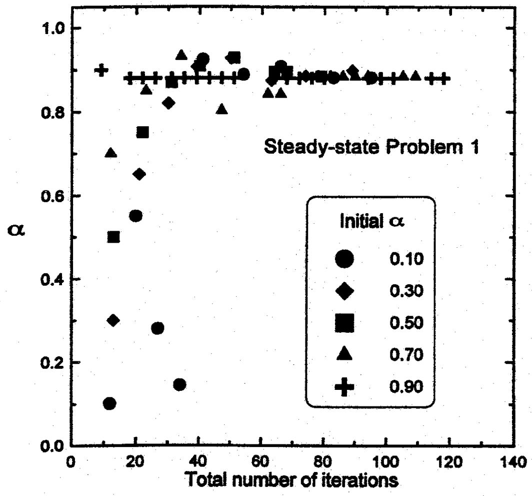

Figure 6. Behavior of the iteration parameter during solution of steady-state problem 1.

iterations. Carefully comparing the data on these figures, we find out that the points out of the $F(\alpha)$ curves of Figures 2 and 4 are exactly those obtained for the first iterations as shown in Figures 6 and 8. Thus, the points out of the $F(\alpha)$ curves for test problem 1 are due mainly to the change in the coefficient matrix during problem solution, even though there exists some error in the evaluation of the asymptotic convergence rates as shown below. This error is much larger for the

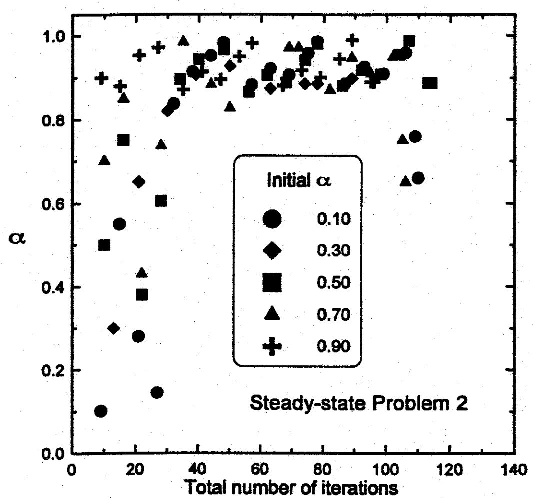

Figure 7. Behavior of the iteration parameter during solution of steady-state problem 2.

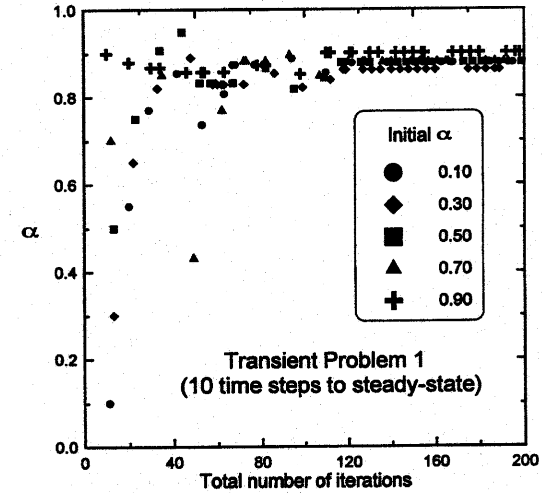

Figure 8. Behavior of the iteration parameter during solution of transient problem 1.

steady-state or transient solution of test problem 2, as can be seen from the large data scatter in Figures 7 and 9.

Figure 10 shows the behavior of f_n during solution of steady-state problem 1 using the MSI and OMSI procedures, for an initial α value of 0.5. It is clear that the asymptotic rate is reached for the first two calls of the MSI procedure. Those determined by the OMSI procedure have some error, due to the increase in the ϵ

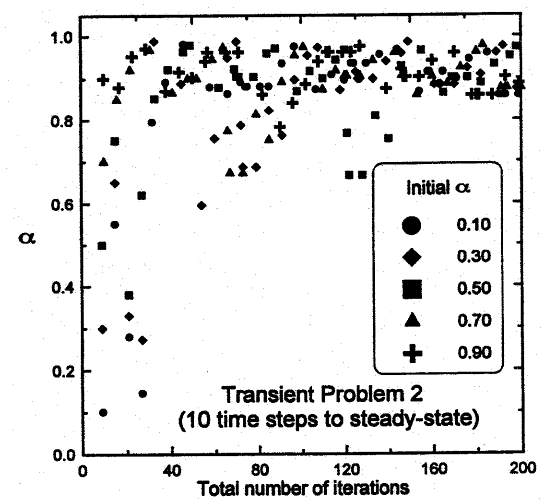

Figure 9. Behavior of the iteration parameter during solution of transient problem 2.

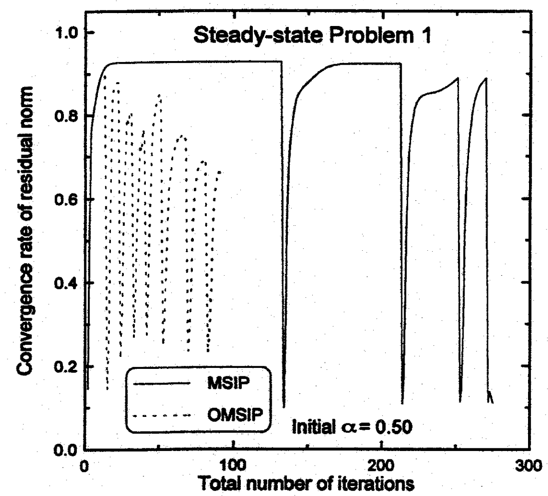

Figure 10. Behavior of the convergence rate during solution of steady-state problem 1.

value used in the algorithm. This can be noted by comparing the first call of both procedures and by verifying that the curves for the OMSIP calls barely flatten before the algorithm interrupts the process to choose a new α value. The corresponding results for steady problem 2 show similar behavior but with a somewhat larger error in $F(\alpha)$ estimation.

A comparison of the two methods is shown in Tables 1, 2, and 3, for the steady-state problems, transient problem 1, and transient problem 2. N_{iter} is the total number of iterations [solutions of Eq. (3)], N_{LU} is the total number of coefficient matrix evaluations followed by its LU decomposition, and t_{rel} is the relative CPU time spent for the problem solution. This relative CPU time is based

Table 1. Comparison between methods for steady-state problems 1 and 2

	MSIP			OMSIP		
α	N_{iter}	N_{LU}	t_{rel}	N_{iter}	N_{LU}	t_{rel}
			Steady-State Problem 1			
0.10	368	7	1.895	107	12	0.641
0.30	327	7	1.702	91	10	0.538
0.50	276	7	1.448	91	9	0.536
0.70	212	7	1.128	120	10	0.678
0.90	185	7	1.000	129	7	0.690
			Steady-State Problem 2			
0.10	743	6	2.965	110	19	0.630
0.30	667	6	2.663	125	21	0.708
0.50	576	6	2.313	114	19	0.640
0.70	448	6	1.820	106	16	0.573
0.90	240	6	1.000	96	16	0.540

Table 2. Comparison between methods for transient problem 1

	MSIP			OMSIP		
α	N_{iter}	N_{LU}	t_{rel}	N_{iter}	N_{LU}	t_{rel}
			Transient problem 1 (100 time steps to steady state)			
0.10	1,741	307	1.363	1066	317	0.997
0.30	1,617	308	1.298	1072	316	1.001
0.50	1,463	308	1.216	1081	316	1.007
0.70	1,268	312	1.118	1089	316	1.010
0.90	1,037	315	1.000	1191	314	1.067
			Transient problem 1 (20 time steps to steady state)			
0.10	1,502	81	1.671	733	85	0.954
0.30	1,354	81	1.527	889	86	1.117
0.50	1,184	82	1.365	741	84	0.960
0.70	953	83	1.141	727	89	0.957
0.90	796	87	1.000	684	90	0.915
			Transient problem 1 (10 time steps to steady state)			
0.10	1,468	48	1.881	622	50	0.920
0.30	1,324	48	1.714	615	50	0.910
0.50	1,147	48	1.504	609	49	0.901
0.70	926	48	1.242	617	48	0.907
0.90	718	49	1.000	629	49	0.917

on the fastest result for the MSIP for each problem, which was obtained by using $\alpha = 0.9$ for all problems.

For the steady-state problems, as can be seen from Table 1, the OMSIP needs less iterations and is faster than the MSIP even for the best α in this table. This direct comparison might not be quite fair because the algorithm of the

Table 3. Comparison between methods for transient problem 2

	MSIP			OMSIP		
α	N_{iter}	N_{LU}	t_{rel}	N_{iter}	N_{LU}	t_{rel}
			Transient problem 2 (100 time steps to steady state)			
0.10	1,909	255	1.570	911	264	0.975
0.30	1,761	257	1.487	933	264	0.986
0.50	1,575	256	1.374	897	264	0.964
0.70	1,330	259	1.235	935	262	0.986
0.90	929	261	1.000	911	263	0.971
			Transient problem 2 (20 time steps to steady state)			
0.10	1,585	72	2.218	522	106	1.026
0.30	1,443	72	2.042	509	104	1.003
0.50	1,269	74	1.835	513	105	1.011
0.70	1,017	73	1.519	500	103	0.989
0.90	604	71	1.000	518	106	1.023
			Transient problem 2 (10 time steps to steady state)			
0.10	1,452	43	2.438	378	71	0.914
0.30	1,321	42	2.235	381	74	0.938
0.50	1,154	42	1.970	387	75	0.948
0.70	923	42	1.617	374	71	0.910
0.90	530	41	1.000	366	67	0.877

OMSIP evaluates the coefficient matrix more often than the MSI iterative procedure. That is, during problem solution using the OMSIP, time is saved by not requiring high convergence for nonconverged coefficient matrices. For steady-state problem 1 and $\alpha = 0.9$, both methods evaluate the coefficient matrix seven times, but the OMSIP is still superior to the MSIP. In order to minimize the effect of requiring high convergence before the coefficient matrix converges, the iterative procedure given in Figure 1 is modified by starting it with $\epsilon_r = \epsilon_a = 0.05$ and decreasing these values one order of magnitude for every new iteration until the final tolerance values, $\epsilon_r = 5 \times 10^{-5}$ and $\epsilon_a = 5 \times 10^{-7}$, have been reached. Steady-state problem 1 has been solved by both methods using this modified iteration algorithm and $\alpha = 0.9$. Both methods need eight LU decompositions to obtain the solution; the OMSIP needs only 80 iterations, while the MSIP needs 95 iterations. The relative computation time is $t_{rel} = 0.856$. These results show that the OMSIP is 15% faster than the MSIP, requiring 15% fewer iterations to achieve convergence. Since both methods evaluate the coefficient matrix the same number of times and the value of α used in both methods varies only slightly (0.88 to 0.90), the difference in performance must be accounted for by the points chosen by the OMSIP to reevaluate the coefficient matrix.

Thus, the difference in performance between the methods is due to two factors: (1) the optimization of α and (2) the fact that the algorithm used by the OMSIP to choose the points to reevaluate the coefficient matrix is highly effective in reducing the computational time. The reason for this effectiveness is that the coefficient matrix is reevaluated when a new α value is chosen by the algorithm, which happens only when the system is fairly converged. But this is exactly the best point to update the coefficient matrix. Therefore, the comparison of the two methods by the results given in Table 1 is really fair. Thus, we can conclude that the OMSIP, for all α values in Table 1, is 30–45% faster than the fastest MSIP run ($\alpha = 0.9$). For the same initial value of α, the OMSIP can be 4.7 times faster than the MSIP.

For the transient problems, the initial guess for every time integration is not too far from the converged solution for the next time point. This eliminates part of the effect of the choice of points at which to reevaluate the coefficient matrix. Of course, this effect should decrease with the time step, because the initial guess becomes better. Therefore, it is not expected that the OMSIP would be much faster than the MSIP with its best α value, due to the extra computational overhead, especially for small time steps. These trends can be seen in Tables 2 and 3, where the results for transient problems 1 and 2 are shown for three different time steps, corresponding to 10, 20, and 100 time integrations before the systems reach their steady states. Accordingly, the results show that, for 100 time steps, the OMSIP is basically equivalent to the MSIP with its optimum value of iteration parameter; that is, only the optimization of α contributes to the better performance of the OMSIP, which is up to 61% faster than the MSIP for the same initial value of α. As the number of time steps decreases, and so the time step increases, the effect of the choice of points for the coefficient matrix reevaluations becomes appreciable. For 10 time steps the OMSIP is about 10% faster than the MSIP with its best α value. For the same initial α value, the OMSIP is up to 2.6 times faster than the MSIP.

It is worth noting that, in all the cases analyzed, the computational time spent by the OMSI procedure to solve a given problem varies less than 25% for an initial α value between 0.1 and 0.9, being of the order of, or smaller than, the computational time used by the MSI procedure with its optimum value of α.

CONCLUSIONS

The recently developed optimized MSI procedure is applied to nonlinear heat transfer problems in this work. From the results obtained, the following conclusions can be drawn.

1. The OMSI procedure is able to estimate roughly the asymptotic rate of convergence of the residual norm of the system of equations obtained by the discretization of a nonlinear problem.
2. The $F(\alpha)$ curve can be approximately obtained for problems with weak nonlinearity.
3. For steady-state problems, the OMSI algorithm also chooses good points at which to reevaluate the coefficient matrix.
4. For this reason, the OMSIP is shown to be 30–45% faster than the MSIP for the steady-state problems that have been analyzed.
5. For transient problems, the OMSI procedure is still effective in optimizing the α value, with a computational time within $\pm 10\%$ of that used by the MSI procedure with the optimum value of its iteration parameter.

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