MODIFIED STRONG IMPLICIT PROCEDURE WITH ADAPTIVE OPTIMIZATION OF ITS ITERATION PARAMETER

P. L. C. Lage

Programa de Engenharia Química, Coordenação dos Programas de Pos-graduação de Engenharia (COPPE), Universidade Federal do Rio de Janeiro, Ilha do Fundão, CEP 21.945-970, Rio de Janeiro, RI. Brazil

This article develops an algorithm to estimate the asymptotic rates of convergence of the residual vector norm of a system of equations when it is solved by the modified strong implicit procedure (MSIP). This algorithm is used to develop an adaptive optimization procedure in order to improve MSIP performance during problem solution. This eliminates the trial-and-error method usually necessary to determine the optimum value of the iteration parameter. Five problems are used to test the new algorithm. The results show that the optimized MSIP can be many times faster than the original procedure for a nonoptimal value of its iteration parameter.

INTRODUCTION

The numerical solution of field problems using finite-difference or finite-element procedures leads to systems of algebraic equations that have a sparse structure. In the case of two-dimensional problems, a pentadiagonal or nine-diagonal coefficient matrix is obtained, depending on the use of a five-point or nine-point discretization scheme, respectively. Since the number of equations in these systems is large, direct methods of solution are usually too costly to be used, and then iterative methods of solution should be chosen.

Several iterative methods are available throughout the literature [1]. Among them, the most commonly used are the point successive overrelaxation method (SOR); the line successive overrelaxation method (LSOR); the alternating direction implicit method (ADI), originally developed by Peaceman and Rachford [2]; the strong implicit procedure (SIP), developed by Stone [3], and the modified strong implicit procedure (MSIP), developed by Schneider and Zedan [4]. The implicitness of the solution method increases in the order of presentation given above, and this is responsible for the better convergence characteristics of the latter methods. All of these methods have an iteration parameter that can be a relaxation factor (SOR, LSOR, and ADI) or a partial cancellation factor (SIP and MSIP). The convergence characteristics of each of these methods are strongly influenced by the value (or

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Address correspondence to Professor Paulo L. C. Lage, Programa de Engenharia Química, COPPE, Universidade Federal do Rio de Janeiro, Ilha do Fundão, Caixa Postal 68502, CEP 21.945-970 Rio de Janeiro, RJ, Brazil. E-mail: paulo@peq.coppe.ufij.br

NOMENCLATURE

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values) chosen for the iteration parameter, which usually shows an optimum value (or sequence of values during iteration) for each problem. The modified strong implicit procedure is the least sensitive to its iteration parameter, even though its optimization can cause an order-of-magnitude reduction in computer time for some problems. Moreover, the optimum value of the MSIP iteration parameter is relatively insensitive to problem parameters. Those advantages over the original strong implicit method have been pointed out by Schneider and Zedan [4] and are the basis for some implementations of the modified strong implicit procedure where the iteration parameter is held constant for every problem [5].

Due to these features, the modified strong implicit procedure is usually considered the best method available for the solution of discretized two-dimensional field problems. However, the optimum value of its iteration parameter has to be obtained by a trial-and-error method for each problem. This involves the solution of the problem for several values of the iteration parameter, which is costly and becomes prohibitive if the solution is needed for only a few groups of problem parameters values.

The present work develops a method for the adaptive optimization of the iteration parameter in the modified strong implicit procedure, eliminating the trial-and-error optimization method. The method is based on the fact that, for each value of the iteration parameter, an asymptotic convergence rate of the residual vector norm can be determined. In a chosen closed interval for the iteration parameter, inside [0, 1], there is a minimum for the asymptotic convergence rate, which corresponds to the optimum value for the iteration parameter. The adaptive optimization of the iteration parameter consists in the following steps:

An estimate of the asymptotic covergence rate for the current value of the iteration parameter;

An interpolation/extrapolation procedure, based on the previously obtained asymptotic convergence rates, for choosing a new value for the iteration parameter closer to its optimum value.

In the following sections, the MSIP with adaptive optimization of is iteration parameter will be explained in detail. Its results will be compared to those of the standard MSIP for five heat transfer test problems. This comparison demonstrates the advantages of the application of the MSIP with adaptive optimization over the standard MSIP.

THE STANDARD MSIP

The MSIP developed by Schneider and Zedan [4] will be outlined in this section. Further details can be found in the original work. The discretization of the two-dimensional field problem will lead to the system of algebric linear (or linearized) equations

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

where the coefficient matrix A is pentadiagonal or nine-diagonal. The MSIP consists of the definition of an auxiliary matrix B, which is chosen in order that the modified coefficient matrix A + B has an LU factorization where the upper and lower triangular matrices keep the sparse structure of A. The definition of 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 MSIP. It should be noted that the LU decomposition of the modified matrix is calculated by a very fast algorithm. Once α is chosen, B is determined and the following iterative procedure is applied:

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

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

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

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 MSIP, it is necessary to define a measure of the convergence characteristics of the MSIP for a given value of its iteration parameter. It has been found that there usually exists an asymptotic

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convergence rate for the norm of the residual vector, which is defined as

$$F(\alpha) = \lim_{n \to \infty} f_n \quad \text{where} \quad f_n = \frac{\|\mathbf{R}^n\|}{\|\mathbf{R}^{n-1}\|}$$
 (4)

Sometimes, this limiting process does not converge because some oscillatory behavior occurs. Thus, it is necessary to generalize the definition of the asymptotic convergence rate to be the limit obtained for the sequence of arithmetic means, that is,

$$F(\alpha) = \lim_{n \to \infty} g_n \quad \text{where} \quad g_n = \frac{1}{n} \sum_{k=1}^n f_k$$
 (5)

Although mathematically correct, the implementation of Eq. (5) shows that 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:

$$F(\alpha) \cong \lim_{n \to \infty} g_n^N$$
 where $g_n^N = \frac{1}{N} \sum_{k=n+1-N}^n f_k$ (6)

The value of N depends on the degree of smoothness needed for a specific problem, but a value between 4 and 8 has been proved to be enough for all the cases analyzed. Thus, the first step in the algorithm for the adaptive optimization of α , which is the estimation of the asymptotic rate of convergence, has been carried out through the following procedure:

- . Choose an α value and decompose the modified matrix.
- 2. Iterate to obtain new values of the unknowns, that is, solve Eq. (3)
- 3. Determine f_n .
- l. Check for divergence $(f_n > 1)$ after the second iteration, stopping the iteration process (for the current α value) if it is found.
- 5. After N+1 iterations, check if

$$|g_n^N - g_{n-1}^N| < \varepsilon \Leftrightarrow |f_n + f_{n-N}| < N\varepsilon \tag{7}$$

6. If the assertion of Eq. (7) is true, let that smoothed converged value be the estimate for $F(\alpha)$.

THE ADAPTIVE OPTIMIZATION PROCEDURE

Once estimates of the asymptotic convergence rate become available for some values of the iteration parameter, an algorithm can be used to determine a better value for the iteration parameter for the next LU decomposition. This algorithm must have the following characteristics.

It should try to determine the α value that gives the minimum of $F(\alpha)$; that is, it is an optimization procedure.

It should use only the latest information for $F(\alpha)$ in order to compensate estimation errors in past $F(\alpha)$ values and coefficient matrix updates in the case of nonlinear problems, that is, it is an adaptive algorithm.

It should be fast enough in order not to cause excessive overhead in the computational implementation of the method.

Thus, a simple second-order curve fitting for $F(\alpha)$ was chosen for the adaptive optimization of α . This method satisfies the characteristics cited above because it is fast, uses only the last three values of $F(\alpha)$, and allows the determination of a minimum for $F(\alpha)$. Therefore, the adaptive optimization is carried out by the following procedure.

- 1. For the given initial value of α , α_1 , decompose the modified matrix and iterate until an estimate of $F(\alpha_1)$ can be made.
- 2. Choose another α value, α_2 , using the heuristic procedure $\alpha_2 = 1 (1 \alpha_1)/2$. Then if $\alpha_2 > 0.9$, let $\alpha_2 = \alpha_1 0.02$. Decompose the modified matrix and iterate until $F(\alpha_2)$ is estimated.
- 3. Using the values of $F(\alpha_1)$ and $F(\alpha_2)$, obtain, by a linear extrapolation, the α_3 value, using the heuristic condition $F(\alpha_3) = 0.98 \min[F(\alpha_1), F(\alpha_2)] 0.02$. Decompose the modified matrix and iterate until $F(\alpha_3)$ is estimated.
- 4. Using the last three estimates for $F(\alpha)$, fit a second-degree polynomial in terms of α and determine $F_{\min} = \min[F(\alpha_k), F(\alpha_{k-1}), F(\alpha_{k-2})]$ and the corresponding α_{\min} .
- 5. Find the new α value, α_{k+1} , as follows:

If the polynomial fit has a minimum inside the interval of interpolation, choose α_{k+1} as the minimum point.

Otherwise, if there are real roots for $F(\alpha) = 0.98 F_{\min} - 0.02$, choose the one nearest to α_{\min} as the α_{k+1} value.

If there is no real root, choose the point of minimum outside the interval of interpolation as the α_{k+1} value (note that the extreme point must be a minimum when $F(\alpha) = 0.98F_{\min} - 0.02$ has no real roots).

- 6. Check whether α_{k+1} is inside the interval of allowable α values, $[\alpha^0, \alpha^1]$. If it is greater than α^1 , let $\alpha_{k+1} = (\alpha_k + \alpha^1)/2$; if it is less than α^0 , let $\alpha_{k+1} = (\alpha_k + \alpha^0)/2$.
- 7. If $|\alpha_{k+1} \alpha_k| > \varepsilon_{\alpha}$, perform the LU decomposition of the modified matrix and iterate until $F(\alpha_{k+1})$ is estimated; otherwise continue to iterate with the current α_k value.
- Return to step (4) if the desired convergence criterion is not met.

If, by any chance, two of the three α values are equal in step 4, a linear extrapolation is used, as described in step 3. The heuristic criterion used for extrapolation simply tries to increase the convergence rate, decreasing the value of $F(\alpha)$. In the present implementation, the following values have been chosen: $\alpha^0 = 0.01$, $\alpha^1 = 0.99$, and $\varepsilon = \varepsilon_\alpha = 0.001$.

DESCRIPTION OF TEST PROBLEMS

In order to test the new procedure, five heat transfer problems have been selected from the existing literature. Stone [3] gives four two-dimensional heat transfer problems in a square insulated domain with point heat sources and sinks. His first three problems, in a grid with 31×31 nodes, are our current Test Problems 1, 2, and 3, in the same order. Schneider and Zedan [4] give three heat transfer problems. One of them is a one-dimensional problem in a square grid with two insulated boundaries, which will also be used. Our final test problem, numbered 4, is the last heat transfer problem presented by Schneider and Zedan [4], which is a problem in a rectangular domain with boundary conditions of mixed kinds. Since Schneider and Zedan [4] verify that, for the MSIP, the optimum value of α is insensitive to problem parameters, we will not analyze the behavior for different meshes. For the sake of completeness, the five test problems used in this work are described below.

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

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial T}{\partial y} \right) = -Q \tag{8}$$

This equation is considered here to be in a dimensionless form. The problems are characterized by their source terms, boundary conditions, and anisotropic thermal conductivity field. The hear transfer equation is discretized using the control-volume technique.

One-Dimensional Test Problem. The domain is a square with side length 1, there are no heat sources, the two horizontal sides (y = 0, 1) are insulated, the two vertical sides have prescribed temperature levels, T = 0 at x = 0 and T = 1 at x = 1, and $k_x = k_y = 1$.

Test Problem 1. The domain is also a square with side length 1, but it is completely insulated. There are point heat sources 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, $k_x = k_y = 1$.

Test Problem 2. The problem is basically the same as Test Problem 1, but with $k_y = 0.01, k_x = 1.$

Test Problem 3. This problem is also basically the same as Test Problem 1, but with a different thermal conductivity field, given as $k_x = k_y = 1$, except in the following regions: 0.467 < x < 1 and 0 < y < 0.533, where $k_y = 100$, $k_x = 1$; 0.167 < x < 0.4 and 0.167 < y < 0.4, where $k_y = 1$, $k_x = 100$; and 0.4 < x < 0.633 and 0.7 < y < 0.933, where $k_x = k_y = 10^{-6}$ (being practically a barrier for heat flow).

Test Problem 4. 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 h = 5, losing heat to an ambient at zero temperature. Also, $k_x = k_y = 1$.

All these test problems have been solved in a fixed mesh with 31×31 control volumes (similar to the one used by Stone [3]) and for initial guesses of zero for all problem variables. Since all these problems are linear, the coefficient matrix of the discretized system of equation is calculated only once.

ASYMPTOTIC CONVERGENCE RATES OF MSIP

Although it may sometimes present an oscillatory behavior, the sequence of f_n reaches the asymptotic rate for each α value in Figure 1b in less than 20 and 8, for three values of α . It is clear that the sequence of arithmetic means convergence rate of the residual norm achieves an asymptotic rate very quickly characteristics of all test problems have proven to be very similar, and only the problem solution. A numerical study of the convergence rates of all test problems The cornerstone of the optimization procedure is the existence of asymptotic convergence rates for the MSIP and the ability of their estimation during the rate of convergence has to be estimated quickly, a sequence of smoothed f_n values rate quickly (20-30 iterations), with no oscillatory behavior. Since the asymptotic reaches the asymptotic convergence rate much more slowly than the original series $10^{-1}-10^{-2}$. Figure 1b shows the convergence rates f_n , g_n , and g_n^N , with N=4, 6, usually within 20-30 iterations, where the residual norm is still in the range MSIP for several values of the iteration parameter. It can be seen that the results for the Test Problem 1 are shown in Figure 1. Figure 1a shows the norm of has been carried out in order to determine their behavior. The convergence rate (g_n^N) was chosen for its estimation, as described previously. iterations. The sequence of g_n^N , for each value of N, also reaches the asymptotic the residual vector, $\|\mathbf{R}^n\|$, during the iterative solution of the problem using the

The proposed procedure for the estimation of the asymptotic convergence rate has to be verified. Figures 2a and 2b show the asymptotic convergence rate, $F(\alpha)$, as obtained by MSIP simulations for Test Problems 1 and 2, respectively. These figures also show the estimated values of $F(\alpha)$ using Eq. (6) with N=4, 6, and 8, for the optimized MSIP (OMSIP) runs for Test Problems 1 and 2, with an initial α value of 0.10. The predictions of $F(\alpha)$ are fairly good, except near the point of minimum, where the estimated asymptotic convergence rate is usually smaller than $F(\alpha)$. This error, however, does not affect appreciably the optimization of α , because the point of minimum of $F(\alpha)$ is estimated with a small error. Besides, as we shall see later, the sequence of different α values during an OMSIP run may lead to a faster convergence than the MSIP run with the best α value. Similar results have been obtained for the other test problems. From Figures 2a and 2b, it is clear that there is no difference among the $F(\alpha)$ predictions for the three values of N for these problems. Since a small N value implies a larger number of α values, and thus LU decompositions, during the OMSIP run, the

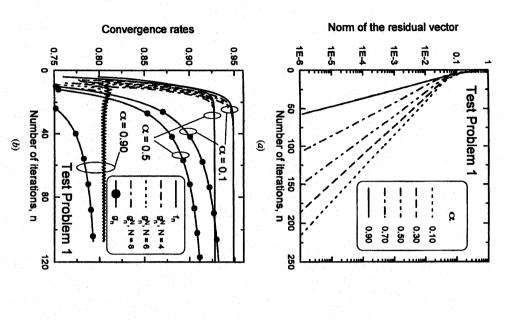


Figure 1. Asymptotic convergence rate of the MSIP: (a) norm of residual vector during iteration; (b) behavior of several convergence rates during iteration.

choice of the N value is then a compromise between the need of estimated $F(\alpha)$ values to perform the optimization and the overhead necessary for the extra LU decompositions.

APPLICATION OF THE OPTIMIZED MSIP

The optimized MSIP (OMSIP) has been applied for the five test problems described previously, using different initial values of α and for N=4, 6, and 8. It should be noted that the particular choice of initial guesses for the variables does

not affect the procedure appreciably because, when the first estimation of $F(\alpha)$ is made, the norm of the residual vector has already reached a reasonably small value (around 10^{-2}), that is, the problem variables are partially converged.

Figure 3 shows the convergence characteristics of the MSIP and OMSIP applied to Test Problem 1. These results are typical for all the cases analyzed. Figure 3a shows the reduction of the residual vector norm during the problem solution for N=4 and for initial $\alpha=0.10,0.50$, and 0.90. The value of α remains constant during the iterations for the MSIP. For this problem, the minimum value of $F(\alpha)$ is for $\alpha=0.90$. The abscissa is the number of iterations, that is, the

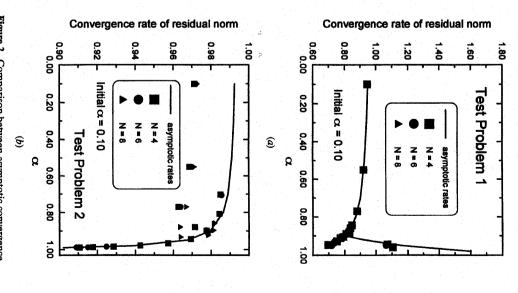
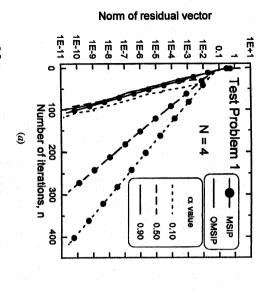
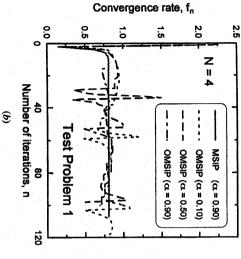


Figure 2. Comparison between asymptotic convergence rate and its estimated value by the proposed algorithm for: (a) Test Problem 1; (b) Test Problem 2.





OMSIP for Test Problem 1: (a) norm of residual vector Figure 3. Comparison between the MSIP and the during iteration; (b) convergence rate during iteration.

should be noted that the OMSIP can achieve a given convergence in a smaller clear that the OMSIP dramatically increases the convergence rate when the of the MSIP with its optimum α value (0.90, in this case). For the worst case convergence rate of the OMSIP tends quickly to the asymptotic convergence rate number of iterations than the MSIP with its optimum α value. This is shown in totic convergence rate of the MSIP for a residual vector norm value of 10⁻³. It ($\alpha = 0.10$), the OMSIP reaches a convergence rate close to the optimum asympiteration parameter is far from its optimum value. For all initial α values, the number of times the system given by Eq. (3) has been solved. From this figure, it is

ADAPTIVE OPTIMIZATION OF MSIP

using the OMSIP for the same cases presented in Figure 3a. The convergence rate 10^{-4} , and for the solution with initial $\alpha = 0.90$, when the residual norm is below 10^{-2} . Figure 3b shows the convergence rates for the solution of Test Problem 1 Figure 3a for the solution with initial $\alpha = 0.50$, when the residual norm is below exactly because of its adaptive characteristics and the errors in the $F(\alpha)$ predicasymptotic rate of the MSIP, even though it cannot reach this asymptotic rate be seen that the OMSIP keeps the convergence rate close to the optimum behavior of the MSIP for the best α value (0.90) is also shown in Figure 3b. It can

of iterations for a given tolerance in the residual norm is presented for the two Test Problem 1, is not uncommon, as can be seen from Table 1, where the number The convergence of the OMSIP in fewer iterations, as shown in Figure 3a for

Table 1. Comparison of solution methods in terms of the number of iterations

0.94	0.92	0.90	0.50	0.10		0.90	0.87	0.50	0.10		0.99	0.98	0.90	0.50	0.10		0.91	0.90	0.85	0.80	0.50	0.10		0.91	0.90	0.89	0.50	0.10		α		
154	1200	172	518	724	Test Proble	Diverge	146	338	471	Test Problem	180"	291	852	1,904	2,278	Test Problem	149	107"	131	160	292	417	Test Problem	119	105"	113	347	500	One-dimensional 1	MSIP		
116	117	121	132	140	Test Problem 4 (tolerance of the residual norm = 10^{-12})	137	132"	199	158	Test Problem 3 (tolerance of the residual norm = 2.1×10^{-10})	201"	219	247	262	264	Test Problem 2 (tolerance of the residual norm = 2.1×10^{-10})	103	100	96 <i>a</i>	99	98	118	Test Problem 1 (tolerance of the residual norm = 2.1×10^{-12})	97	96	94"	110	119	One-dimensional test problem (tolerance of the residual norm = 10^{-12})	N=4		
125°	126	128	140	149	residual norm = 10^{-1}	131"	132	148	168	sidual norm = 2.1×10^{-3}	203"	221	253	250	251	sidual norm = 2.1×10^{-3}	100	104	100	96"	110	120	sidual norm = 2.1×10^{-3}	97	97"	97	116	121	e of the residual norm	N=6	OMSIP	
128	120	1174	148		[2]	136°	139	156	168	0-10)		225				0^{-10})		107	105	102	118		0^{-12})	99"	101	101	121		$=10^{-12}$)	N=8		

^a Smallest number of iterations in the corresponding method

solution procedures for different α values and for all test problems. For all test problems except Test Problem 2, and for all N values used in the present analysis, the OMSIP with its best α value converges in fewer iterations than the MSIP using its best α value. This is not true for Test Problem 2 because its point of minimum of $F(\alpha)$ in the $[\alpha^0, \alpha^1]$ interval is the chosen α^1 value (0.99). Actually, the minimum of $F(\alpha)$ is somewhere inside the interval (0.99, 1], which makes the adaptive optimization worse. However, this minimum is quite sharp, which makes the OMSIP better than the MSIP for any α value below 0.98 (see Table 1).

Since the extra LU decompositions of the modified matrix have some computational cost, it is not quite fair to compare the MSIP and OMSIP by the number of iterations needed to achieve a given convergence. Therefore, the computer time spent by each method to solve each one of the test problems for a given accuracy must be compared. The I/O operations used to monitor the intermediate results are eliminated to avoid any effect in the actual computation time needed for each calculation. All the results shown above have been obtained by using strict convergence criteria for the residual norm. Although this is desirable to test the optimization procedure fully, it is unrealistic for the usual solution of field problems. Therefore, a series of calculations using the MSIP and the OMSIP is also made for all test problems using the following convergence criterion for every point in the field:

$$\frac{|T^{(n)} - T^{(n-1)}|}{\varepsilon_r |T^{(n)}| + \varepsilon_a} < 1 \tag{9}$$

where $\varepsilon_r = 10^{-4}$ and $\varepsilon_a = 10^{-6}$.

Figures 4-7 show the relative time necessary to satisfy the prescribed convergence criterion as a function of α , for each one of the two-dimensional test

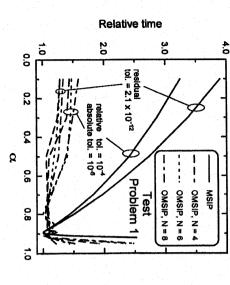
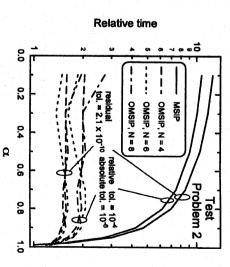


Figure 4. Comparison between the MSIP and the OMSIP: Relative time spent in computations for the Test Problem 1.



rigure 5. Comparison between the MSIP and the OMSIP: Relative time spent in computations for the Test Problem 2.

problems. The results for the one-dimensional test problem are very similar to those for Test Problem 1 and are not shown. The relative time is the computational time for a given case divided by the computational time spent by the MSIP, using its best α value, to solve the same problem. Results for both convergence criteria, that is, the strict tolerance in the residual norm and that given by Eq. (9), are shown. From these figures, it is clear that, in general, the OMSIP is faster than the MSIP for all range of α values except those very close to the minimum point. The

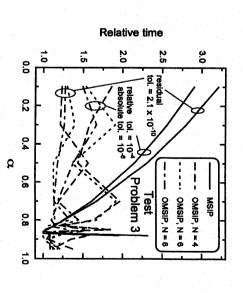


Figure 6. Comparison between the MSIP and the OMSIP: Relative time spent in computations for the Test Problem 3.

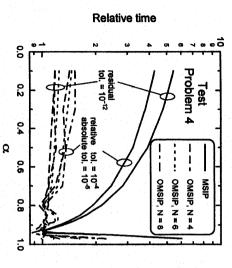


Figure 7. Comparison between the MSIP and the OMSIP: Relative time spent in computations for the Test Problem 4.

only exception is Test Problem 3, where the OMSIP is slower than the MSIP for some cases and for initial $\alpha \in [0.7,0.8]$. For that problem, which is the most difficult among those that have been analyzed, the OMSIP calculation time-oscillates vigorously with the α value. However, the difference between the calculation times is not too large. It can also be seen that the OMSIP is quite insensitive to the initial α value used to start the algorithm. Nevertheless, the OMSIP has an optimum value for the initial α which sometimes gives a smaller calculation time than the MSIP with its best α value (see Figure 7). Finally, these figures show that the computational time spent by the OMSIP to solve a given problem does not depend much on the value of N used in Eqs. (6) and (7). Small values of N are slightly better for simple problems (one-dimensional test problem, Test Problems 1 and 4), while more difficult problems seem to behave better with larger N values (Test Problems 2 and 3).

A comparison can be made between the computational time needed to solve each one of the test problems using the MSIP and OMSIP with their best α values. Of course, we should not expect the OMSIP to perform better than the MSIP, because of the existing overhead of the optimizing algorithm. Although there are some cases where the OMSIP is really faster than the MSIP, the difference in computational time is small, being around 10% (Test Problem 4). In general, the OMSIP is 5-10% slower than the MSIP when both procedures are started with their best values of α . For Test Problem 2, which has a sharp maximum for $F(\alpha)$ outside the search interval, the OMSIP is 20-30% slower than the MSIP. However, it is not fair to compare these algorithms at their best values for a given convergence criterion, because the trial-and-error procedure of finding the best value of the iteration parameter is exactly what the OMSIP is trying to avoid. Therefore, one should use a fixed initial value of the iteration parameter to compare the relative performance of the algorithms. Thus, $\alpha = 0.5$ is

chosen, as used by some implementations of the MSIP [5], to compare the MSIP and the OMSIP. Table 2 shows the relative computation time (time spent by the OMSIP over time spent by the MSIP) for all the cases analyzed. It can be seen that the OMSIP is faster than the MSIP by a factor of 1.47 to 7.09 for those cases. In general, the OMSIP is about twice as fast as the MSIP.

CONCLUSIONS

This article demonstrates numerically the existence of asymptotic rates of convergence of the residual norm of a system of equations when it is solved by the MSIP, developing an algorithm to their estimation. Based on the prediction of the asymptotic rates of convergence, an algorithm for the adaptive optimization of the iteration parameter is developed to improve MSIP performance during problem solution. This eliminates the trial-and-error procedure usually necessary to determine the optimum value of the iteration parameter. Five heat transfer problems are solved by the optimized MSIP, called OMSIP, to verify its performance. From the results shown above, the following conclusions can be drawn.

The OMSIP is about 5-10% slower than the MSIP when both are used with their best values for the iteration parameter. That is, even if one chooses the best values for both procedures, the time that will be spent by the optimization algorithm and extra LU decompositions is almost completely compensated by the reduction in the number of iterations necessary to achieve convergence. The performance of the OMSIP is only slightly dependent on the value of the iteration parameter used to start the algorithm and on the value of N used in the smoothing process necessary to estimate the asymptotic rate of convergence.

For a fixed value of 0.5 for the iteration parameter, the OMSIP is 47-700% faster than the MSIP in the cases analyzed. In the mean, the OMSIP is about twice as fast as the MSIP.

Furthermore, the adaptive characteristic of the optimization algorithm of the OMSIP allows its usage in nonlinear or time-dependent field problems that require iterative solution of linearized systems of equations. It is believed that the OMSIP using the idea of optimization of the iteration parameter during problem solution is a significant contribution to the state of the art of field problem solution.

Table 2. Comparison of computation times of the MSIP and the OMSIP with $\alpha = 0.50$

Time ratio	Conver	gence of the 1	residual norma	Converge	ence given by	Eq. (9)
(OMSIP/MSIP)	N=4	<i>N</i> = 6	N = 8	N = 4	N=6	<i>N</i> = 8
One-dimensional	0.377	0.390	0.398	0.542	0.585	0.609
	0.385	0.432	0.457	0.457	0.581	0.571
2	0.150	0.141	0.155	0.220	0.178	0.219
အ	0.679	0.490	0.513	0.669	0.634	0.642
4	0.284	0.299	0.306	0.417	0.406	0.421

^a See Table 1 for residual norm tolerances used in each test problem.

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REFERENCES

- 1. K. Aziz and A. Settari, Petroleum Reservoir Simulation, Elsevier, New York, chap. 8, 1979.
- 2. D. W. Peaceman and H. H. Rachford, the Numerical Solution of Parabolic and Elliptic Differential Equations, J. Soc. Ind. Appl. Math., vol. 3, pp. 28-41, 1955.
- 3. H. L. Stone, Iterative Solution of Implicit Approximation of Multidimensional Partial Differential Equations, SIAM J. Numer. Anal., vol 5, pp. 530-558, 1968.
- 4. G. E. Schneider and M. Zedan, A Modified Strongly Implicit Procedure for the Numerical Solution of Field Problems, Numerical Heat Transfer, vol. 4, pp. 1-19, 1981.
- S. I. Güçeri, Finite Difference Solution of Field Problems, in C. L. Tucker III (ed.), Fundamentals of Computer Modeling for Polymer Processing, Hanser Publishers, Munich, chap. 5, 1991.

COMPARISON OF EQUATION OF TRANSFER WITH SIMULATIONS ON LARGE ARRAYS OF CYLINDRICAL REFLECTOR ELEMENTS

Bruce J. Palmer

Energy and Environmental Sciences Division, Pacific Northwest Laboratory, Richland, Washington 99352, USA

M. Kevin Drost

Energy Division, Pacific Northwest Laboratory, Richland, Washington 99352, USA

James R. Welty

Department of Mechanical Engineering, Oregon State University, Corvallis, Oregon 97331, USA

The suitability of modeling an array of fixed, discrete surfaces as a homogeneous medium is investigated by comparing a Monte Carlo simulation of the equation of transfer for the homogeneous medium with the results of a Monte Carlo model of the array as discrete elements. The results show that when ordered arrays are considered, the assumptions underlying the equation of transfer are violated, and simulation results differ significantly from the discrete model. The results indicate that great care must be used when assuming that a regular array can be modeled as a homogeneous medium.

INTRODUCTION

Highly ordered arrays of fixed, discrete surfaces are encountered in a number of important applications, including volumetric air heating solar central receivers [1, 2], fibrous insulation [3, 4], and ceramic fabrics. As Howell has observed, when the orientation of an absorbing array element is fixed, the scattering phase function depends on the angle of incidence as well as the angle of reflection [5]. This increases the complexity of the problem. Howell observes that methods for treating this problem are not available.

The usual analytical approach to modeling arrays of fixed, discrete surfaces is to model the array as a homogeneous participating medium that has been parame-

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Address correspondence to Dr. Bruce J. Palmer, Energy and Environmental Sciences Division, Pacific Northwest Laboratory, P.O. Box 999, Richland, WA 99352, USA. E-mail: bj_palmer@pnl.gov

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