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TITLE: COMPARISON OF METHODS FOR SOLVING NONLINEAR FINITE-ELEMENT EQUATIONS IN HEAT TRANSFER

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COMPARISON OF METHODS FOR SOLVING NONLINEAR FINITE-ELEMENT EQUATIONS IN HEAT TRANSFER

by

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ABSTRACT

We have derived two new techniques for solving the finite-element heat-transfer equations with highly nonlinear boundary conditions and material properties. When compared with the more commonly employed successive substitution and Newton-Raphson procedures, the new methods speed convergence rates and simultaneously increase the radius of convergence. We have observed reductions in computation time in excess of 80% when the new techniques are employed. The first method accelerates the standard Newton-Raphson approach when the degree of the nonlinearity is known (for example, radiation boundary conditions or a prescribed temperature dependence in the thermal conductivity). The second technique employs feedback to regulate the solution algorithm during execution. Comparisons of these techniques are given for several practical examples.

I. INTRODUCTION

We have derived two new algorithms for solving heat-transfer equations with nonlinear material properties and boundary conditions. The first technique accelerates the Newton-Raphson algorithm and the second technique employs feedback to regulate the modified method of successive substitution. The highly nonlinear finite-element equations for a heat-generating solid with radiation heat loss at the surface are used to present the two new convergence algorithms and to compare them to the more commonly employed Newton-Raphson

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technique and modified method of successive substitution. We have observed significant improvements in total computing time, ease of use, and radius of convergence.

This work is part of a continuing effort at the Los Alamos National Laboratory to develop finite-element modeling capabilities in problems with thermal, fluid, and structural interactions [1,2,3].* The numerical techniques presented here are being tested and have shown themselves to be useful in dealing with nonlinearities that result from thermal conductivities, heat generation rates, heat-transfer coefficients, and other combinations of variable dependent material properties and boundary conditions. The problem involving radiation at solid surfaces is, however, one of the more difficult nonlinear convergence problems encountered in our work, and adequately illustrates the relative advantages and disadvantages of the various techniques.

Section II presents the finite-element formulation, and Sections III and IV describe the convergence algorithms and the example problems used in this study. In the final sections, the results of various numerical experiments are given, and we suggest conditions under which the modified versions appear to be superior to our original algorithms.

II. FINITE-ELEMENT FORMULATION FOR A CONDUCTING SOLID

The steady-state energy equation for a nondeforming solid is

$$\frac{\partial}{\partial x_i}\left(\lambda_Y \frac{\partial T}{\partial x_i}\right) + Q = 0, \tag{1}$$

*Numbers in brackets designate references at end of paper.

where λ_γ is the thermal conductivity (γ = i with no summation implied), Q is the volumetric heat generation, T is the temperature, and x_i is the coordinate variable in the ith direction. The Einstein summation convention is assumed in Eq. (1) and will be used throughout this paper.

The method of weighted residuals with the Galerkin approximation is applied to Eq. (1) to give

$$\int_V N_i \left\{ \frac{\partial}{\partial x_j} \left(\lambda_\gamma \frac{\partial T}{\partial x_j} \right) + Q \right\} dV = 0, \tag{2}$$

where N_i is the ith element interpolation function. To include the radiation boundary condition, the Green-Gauss theorem is applied to the first term in Eq. (2) to give

$$\int_V N_i \frac{\partial}{\partial x_j} \left(\lambda_\gamma \frac{\partial T}{\partial x_j} \right) dV = \int_S N_i \lambda_\gamma \frac{\partial T}{\partial x_j} n_j dS - \int_V \lambda_\gamma \frac{\partial N_i}{\partial x_j} \frac{\partial T}{\partial x_j} dV, \tag{3}$$

where n_j is the jth component of the unit normal of S. The heat transfer at the surface is described by

$$\lambda_\gamma \frac{\partial T}{\partial x_j} n_j = - \sigma \varepsilon (T^4 - T_o^4), \tag{4}$$

where σ is the Stefan-Boltzmann constant, ε is the emissivity of the surface, and T_o is the temperature of the surroundings. In this development, we assume that there is no radiation between surfaces that constitute S.

If Eqs. (3) and (4) are substituted into Eq. (2) and we use $T = N_k T_k$, then Eq. (2) becomes the finite-element equation

$$\left[\int_V \lambda_Y \frac{\partial N_i}{\partial x_j}\frac{\partial N_k}{\partial x_j}\,dV + \int_S N_i N_k \sigma\epsilon T^3 dS\right] T_k = \int_V N_i Q dV + \int_S N_i \sigma\epsilon T_o^4 dS. \qquad (5)$$

This set of equations has the form

$$A_{ik}(T)\, T_k = B_i(T). \qquad (6)$$

Equation (5) was programmed into a finite-element code that uses 8-node isoparametric elements, Gaussian quadrature, and serendipity shape functions. Additional details about the finite-element formulation may be found elsewhere [2,3].

III. NUMERICAL SOLUTION TECHNIQUES

Finding solutions for sets of nonlinear equations is one of the long-standing and as yet unresolved problems in numerical analysis. Regardless of which convergence algorithm is employed, one encounters practical systems that require user intervention with physical insight to converge to an answer.

The basic difficulty is illustrated by Eq. (6), a linearized form of the energy equation. We have to know the values of the coefficient matrix $(A_{ij}(T_k))$ and the "known" vector $(B_i(T_k))$ to solve for T_k. Unfortunately, one must know the answer, T_k, to calculate $A_{ij}(T_k)$ and $B_i(T_k)$.

To circumvent this problem, a number of iterative techniques have been developed. We make no attempt to cover the breadth of this field, but rather focus on those techniques that offer some special advantage to heat transfer analysis.

Heat-transfer equations and the associated boundary conditions are continuous and differentiable with respect to the independent variables. In addition, the derivatives are often easily evaluated from algebraic expressions so the bulk of the computing time is not spent in their evaluation.

Broyden [4] notes that systems in which the above-mentioned criteria hold are not recommended as candidates for solution by the various quasi-Newton techniques. As will be discussed in the following sections, we found that modified Newton-Raphson concepts and direct successive substitution (the Picard iteration process) have rather weak convergence characteristics. Consequently, the paper focuses attention on the four methods that we found solve the heat transfer equations with highly nonlinear boundary conditions, both rapidly and with a minimum of user intervention.

In this section, we present two widely used numerical techniques for solving Eq. (6): the Modified Successive Substitution (MSS) and the Newton-Raphson (NR). In comparison, we present the two newly developed techniques: the Regulated Successive Substitution (RSS) and the Accelerated Newton-Raphson (ANR).

A. Modified Successive Substitution (MSS)

Direct successive substitution (DSS) is perhaps the most straightforward of the algorithms and may be written symbolically from Eq. (6) as

$$A_{ik}(T_k^n)\ T_k^{n+1} = B_i(T_k^n), \tag{7}$$

where T_k^n = the estimate of temperature solution at the kth node on the nth iteration and T_k^{n+1} = updated estimate of the solution temperature at node k. Solutions obtained with DSS oscillate around the true solution and, in many highly nonlinear problems, they tend to diverge. To dampen the oscillations and extend the radius of convergence, the MSS method is used. In MSS, Eq. (7) is solved with A_{ik} and B_i evaluated at T_k^{n+1}, where

$$T_k'^n = \alpha\left|T_k^n\right| + (1-\alpha)\left|T_k^{n-1}\right|, \tag{8}$$

and α is a constant between zero and one. If $\alpha = 1$, the method reduces to DSS; for nonzero values of α, relaxation occurs and the temperature oscillations inherent in the DSS method are dampened.

B. Regulated Successive Substitution (RSS)

Although significant reductions in computational time and increases in the radius of convergence may be achieved by the MSS method, each problem must have the value of α optimized by the user. In the RSS method, the value of α is optimized by the code during execution. The following steps determine the value of α.

1. The value of α is initialized to one.
2. Then Eq. (8) is solved for T_k^{n+1} (for the first iteration, $T_k^{'0}$ contains the initial starting temperatures at the nodes).
3. Equation (7) is solved for $T_k^{'n+1}$.
4. A residual error is calculated by

$$\nu^{n+1} = \left[\sum_m (T_m^{'n+1} - T_m^{'n})^2\right]^{1/2} \tag{9}$$

and

$$R^{n+1} = \left[\sum_m (T_m^{'n+1})^2\right]^{1/2} . \tag{10}$$

If

$$\nu^{n+1} > \nu^n, \tag{11}$$

or if

$$\nu^{n+1} > \frac{1}{3} R^{n+1}, \tag{12}$$

then α is reduced from the current value by 0.1. The steps are then repeated, starting with step 2.

Equation (11) checks to see if the RSS method is diverging with the current value of α_i. If the equation is true, then the reduction in α will dampen the oscillation sufficiently to allow the method to converge in most cases.

Equation (12) was added to the test in Eq. (11) because in many problems a large, but slowly decreasing, oscillation is established and Eq. (11) may be satisfied, even though the temperatures predicted are still far from the solution. The test in Eq. (12) typically will allow the RSS method to compute an α that is close to the optimal value. After examining many systems, it was found that values of α below 0.3 did not aid in the speed of convergence, so α is constrained to be between 0.3 and one.

C. Newton-Raphson (NR)

In the NR method, the following equation is solved in place of Eq. (6).

$$J_{im}(T_j^n)\ (T_m^{n+1} - T_m^n) = -F_i(T_j^n), \tag{13}$$

where the Jacobian, J_{im}, is defined by

$$J_{im}(T_j^n) = A_{im}(T_j^n) + \left(\frac{\partial A_{ik}(T_j^n)}{\partial T_m^n}\right) T_k - \frac{\partial B_i}{\partial T_m^n} \tag{14}$$

and

$$F_i(T_j^n) = A_{ik}(T_j^n)\ T_k^n - B_i(T_j^n). \tag{15}$$

Complete derivations of the Newton-Raphson technique (also known as Newton's method) may be found in many standard references [5,6]. Among the standard convergence techniques, the NR method is almost unique in that it has a sound

theoretical basis and for many problems its convergence is rapid. Although, the NR method has much to commend it, systems exist for which the unmodified NR method fails to converge. Conditions for convergence are well known (see for example [7]), but they rely on the initial estimate to be sufficiently close to the solution. To determine this initial estimate *a priori* is usually difficult and time consuming, if not impossible. In addition, our experience supports earlier reports [8] of occasional offset when the α_{ij} is compared to analytical solutions.* This problem is unique among the methods we studied, and the small offset (<0.2% in our work and <5% in Ref. [8]) from the analytical solutions is related to the nonoscillating behavior of the unmodified NR algorithm.

Two common modifications of the NR method address a third problem and try to reduce the time required to evaluate the Jacobian, J_{im}. This evaluation time severely penalizes the NR technique because, even though the NR may take fewer iterations, the large numbers of computations required per iteration can cause the overall computation time to be larger than that of its competitors. The Modified Newton-Raphson technique uses the initial values of J_{im} throughout the calculation or only updates it every few iterations. The quasi-Newton methods avoid the complete evaluation of the Jacobian matrix by making corrections to the approximate inverse of J_{im} from values contained in the vector function F_i [4]. Our experience has been that both of the above-described techniques are of little use in heat transfer problems that have highly nonlinear boundary conditions or material properties. We found that algorithms in which the derivatives were not updated regularly diverged rapidly because the surfaces change so rapidly in the problems. A second

*Offset is defined here as the difference between the temperature an algorithm converges to and the value predicted by the analytical solution.

reason for not using these approximate Jacobian techniques is that the derivatives in heat transfer applications can often be evaluated directly from known relations (radiation) or from the slope of a spline of the data (thermal conductivities and specific heats) with accuracy and little computational effort.

D. Accelerated Newton-Raphson (ANR)

To overcome some of the disadvantages associated with the NR method and to accelerate the convergence, the ANR was developed. This technique is particularly useful when strong nonlinearities of known algebraic form are encountered in either material properties or boundary conditions. A step-size adjustment that the algorithm uses is continuously modified during execution.

The alteration in step size is realized by systematic adjustments in the partial derivatives that are added to A_{im} in Eq. (14) to form the Jacobian. In systems where the nonlinearity is stronger than linear (for example, radiative boundary conditions or heat generation by Arrhenius' law-dependent chemical reactions), the size of the derivatives is reduced. In systems where there is an inverse temperature dependence (for example, thermal conductivity of some materials), the derivatives in the Jacobian are increased.

This algorithm may be illustrated in one dimension with the example of numerically determining a zero for the equation

$$f(x) = (x-4)^4 - 16. \tag{16}$$

According to the NR method,

$$x^{n+1} = x^n - f(x)/f'(x), \tag{17}$$

where $f'(x) = df(x)/dx = 4(x-4)^3$.

With a starting point of $x^0 = 2000$, the NR algorithm takes 28 iterations to reach the root to four significant figures at $x = 6$. In the ANR method the power or order of the derivatives is reduced by a factor, β,

$$f'(x) = 4(x-4)^{3-\beta}, \tag{18}$$

where $\beta \geq 0$.

The reduced derivative is then substituted in Eq. (16) and the NR iteration procedure repeated. For $\beta = 0.175$ and $x^0 = 2000$, only 12 iterations are required (~60% reduction in computation time).*

The above example demonstrates many of the essential features of our experience with this technique in multidimensions. As with the one-dimensional problem, the derivatives are reduced or increased by a constant factor, β, for positive or negative order nonlinearities, respectively. If $|\beta|$ is too large,** severe system oscillations will occur; but if a user-optimized $|\beta|$ is used, significant (up to 80%) reductions in computation time may be realized. When the iterates are close to the solution, ANR and NR do not exhibit significantly different convergence rates; but far from the solution, the ANR converges much more rapidly.

IV. EXAMPLE PROBLEMS

We selected steady-state, one-dimensional problems to best illustrate the differences between the convergence algorithms and because of the availability of exact solutions. Both problems involve radiation from a thin slab that is

* Note that the number of iterations taken to converge to the root at $x = 6$ using the ANR method ($\beta = 0.175$) on this one-dimensional problem is invariant at 12 iterations as the initial guess, x^0, is varied over two orders of magnitude ($10 \leq x^0 \leq 2200$).

** Optimal β values are in the range $-0.10 \leq \beta \leq 0.25$ when the order, m, of the nonlinearity is physically realistic ($-2 \leq m \leq 4$).

being heated by a constant volumetric heat generation rate. In the first problem, the slab is suspended between two walls held at a constant temperature (T_o). The slab is allowed to radiate with a view factor of unity to the walls (also at T_o). Heat is lost through conduction out the ends of the slab and by radiation. The analytical solution to this problem is given by Ref. [9].

The second problem allows no heat conduction from the edges of the slab, so all of the heat is removed by radiation. Increased difficulty in convergence is observed when this problem is compared with the first problem because the nonlinear transport modes dominate. The steady-state solution in the slab is easily shown to be

$$T = \left(\frac{Q \delta}{2\sigma\epsilon} + T_o^4 \right)^{1/4}, \tag{19}$$

where δ is the thickness of the slab, σ is the Stefan-Boltzmann constant, ϵ is the emissivity of the slab, and T_o is the temperature of the surroundings.

Both slabs were modeled with a single row of finite elements. Details concerning the values of the physical constants and initial conditions used may be found in Figs. 1 and 2. We represented the half slabs with both 2- and 10-element rows. All the solution techniques were able to reproduce the analytical solution at the nodes with less than 1% deviation. The solution accuracy and convergence behavior were insensitive to the number of elements, so the case studies reported here were performed with two elements modeling the half-width of the slab.

Note that our criteria for convergence of the solution algorithms were based on the difference in the temperature field between successive iterations. The normalized square root of the summation of the temperature differences between iterations squared, $\xi^{n+1} = v^{n+1}/R^{n+1}$, was chosen. The solution was taken to be converged when the inequality

$$\xi^{n+1} \leq 1 \times 10^{-4} \tag{20}$$

was satisfied. The extremely small allowable error was for the benefit of this study only; in many engineering applications the tolerance could be several orders of magnitude larger.

A comparison of point convergence rates for the solution techniques is given in Figs. 3 and 4, where the temperature at the center of the bar is plotted as a function of the iteration number. The average step size is plotted as a function of computation time in Figs. 5 and 6. Exact values of the computation times and number of iterations are listed in Table I.

V. DISCUSSION

We selected the radiation boundary condition for the example problems not only because it represents one of the most severe physical nonlinearities, but also because its convergence properties are representative of many of the nonlinear transport problems in our experience.

In these example problems, the methods requiring user intervention, MSS and ANR, converged in the fewest iterations, with the RSS and NR methods taking significantly more steps. Observing the number of iterations, however, only tells part of the story because each iteration in the NR and ANR methods takes approximately four times the amount of computational time that is required for a successive substitution step.

TABLE I

COMPARISON OF CONVERGENCE PARAMETERS FOR VARIOUS ALGORITHMS

Numerical Method	Example 1 Radiation and Conduction		Example 2 Radiation	
	Computation Time (s)	Number of Iterations	Computation Time (s)	Number of Iterations
Newton Raphson	9.53	24	18.27	46
Accelerated Newton Raphson	6.00	15	4.34	11
Regulated Successive Substitution	2.72	29	2.22	24
Modified Successive Substitution	1.61	15	1.00	8

The MSS method required only 50 and 33% of the computational effort used in the RSS method to converge to the analytical solutions in Problems 1 and 2, respectively. Note that the search for the optimal α requires at least three trial runs, and that nonoptimal α's in MSS or RSS without feedback can lead to wild oscillations or even divergence of the solution.

A comparison of ANR and NR also shows significant improvements for the user-optimized method. The method involving user intervention, ANR, converged in only 60 and 24% of the time required by the NR in Problems 1 and 2, respectively. The selection of the optimal value of $\beta = 0.15$ was not as sensitive as the selection of an optimal α. A value of $\beta = 0.15$ appears to be a reasonable starting point for problems involving radiation boundary conditions.

The larger amount of heat transferred in Problem 2 by radiation helps illustrate that the most interesting contrast between the methods is found when the heat transfer is dominated by nonlinear transport modes. For problems with only slightly nonlinear properties or boundary conditions, all of the algorithms converge satisfactorily. In contrasting Example 1 with Example 2, we see that the presence of the linear conduction makes convergence easier.

The primary difficulty with the additional nonlinear nature of the equations in the pure radiation example is that the radius of convergence for all four methods is greatly reduced over that in the combined radiation-conduction example. In each method, the result of a direct successive substitution step was used as the initial solution vector. The choice of this particular solution as an initial vector is rather arbitrary, though it appears to us to be a logical and generally available solution from which to begin an iterative procedure. A second procedure that was used to increase the radius of convergence was to limit the step size (900 K in these examples) at any node. In

some of the problems addressed, these limitations might fractionally slow the convergence rate, but this potential disadvantage is outweighed in our experience by enhanced stability and increased radius of convergence. In addition, we have found that the above steps are more convenient to implement and require less user intervention than more traditional procedures such as an initial solution vector based on physical insight or increasing the number of elements in the model.

VI. RECOMMENDATIONS

As one might expect, the performance of the various convergence procedures depends on the problem, and there is no *a priori* way to predict the optimum convergence technique. We do not wish to imply that all nonlinearities or geometries encountered in heat transfer analysis will behave in a manner analogous to that observed in the examples given in this paper. For example, in certain models with complex geometry and strong nonlinearities (such as volumetric heat generation or radiation boundary conditions), we have observed that the methods based on successive substitution have very small radii of convergence. In these cases, the techniques derived from the Newton-Raphson procedure are preferred.

Appreciating the individual nature of each nonlinear problem encountered in practice, we have designed our computational scheme to include all four methods. We suggest that the RSS procedure be employed first. A principal advantage is that employing the RSS method many times determines the applicability of the successive substitution based methods to the problem without user intervention. Also, in our experience, if the modified successive substitution works, it works rapidly. For example, in Problems 1 and 2, we observed that even though RSS required 80 to 120% more computation time than

the optimized MSS, it required no user intervention and it was still much faster than the NR method. If the initial RSS trial is successful and one wishes to examine a number of separate cases with minor property or geometry changes, then an optimum α for the MSS method is obtained from RSS.

The NR algorithm should be employed if the RSS and MSS methods fail to converge. If the absolute value of the order of the nonlinearity is ≥ 2, significant savings in computation time may result from the accelerated convergence provided by the ANR method.

VII. CONCLUSIONS

The focal point of this study was the convergence properties of several solution algorithms for nonlinear finite-element equations used in heat transfer. We developed two new modifications of existing methods that speed the rate of convergence of the Newton-Raphson algorithm and employ feedback to control a modified method of successive substitution. The modifications required to implement the new convergence procedures are simple, and the savings in computational time and user interfacing are significant.

The problems of a semi-infinite slab with volumetric heating cooled by radiation plus conduction and radiation alone were presented as test problems for these algorithms. We observed that the accelerated Newton-Raphson procedure was capable of converging to the analytical solution in less than one-quarter of the time needed by the Newton-Raphson method. The methods based on successive substitution converged more rapidly than the Newton-Raphson methods in these example problems. The feedback mechanism in the regulated successive substitution (RSS) method allowed it to converge without user intervention by self-adjustment of the relaxation parameter. The RSS method took longer than modified successive substitution, but it was more rapid than either of the

Newton-Raphson methods. The need to use any or all of the algorithms in actual engineering applications is addressed and a procedure for testing new nonlinear models is outlined.

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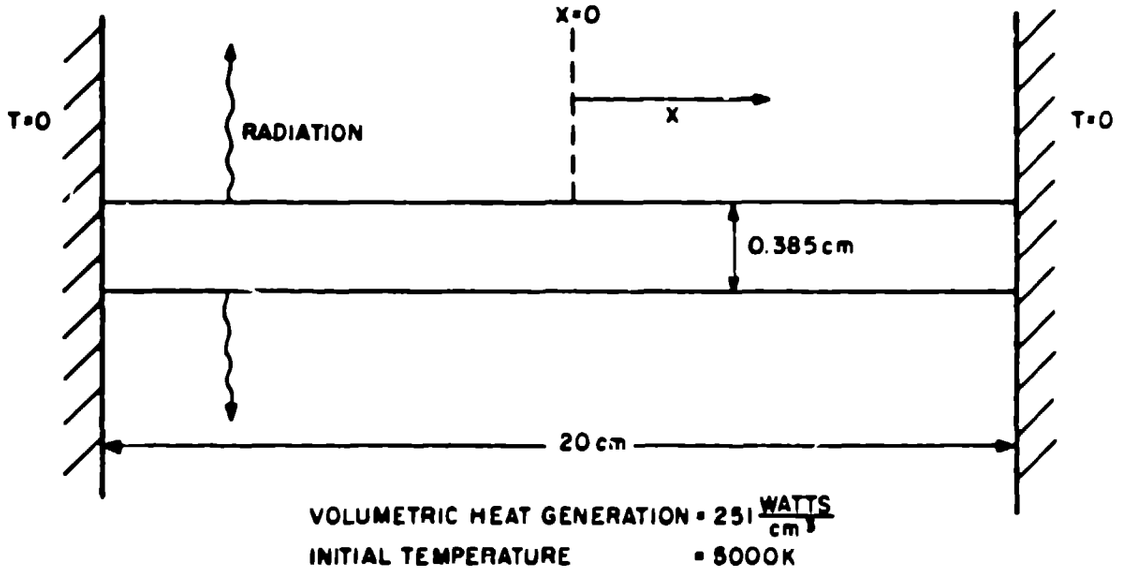

Fig. 1. Problem definition for a semi-infinite slab with internal heat generation. Heat transfers from the slab by conduction to the wall and radiation. Note that $\lambda_x = 0.275$ cal/s K and $\lambda_y = \lambda_z = 30$ cal/s-cm K.

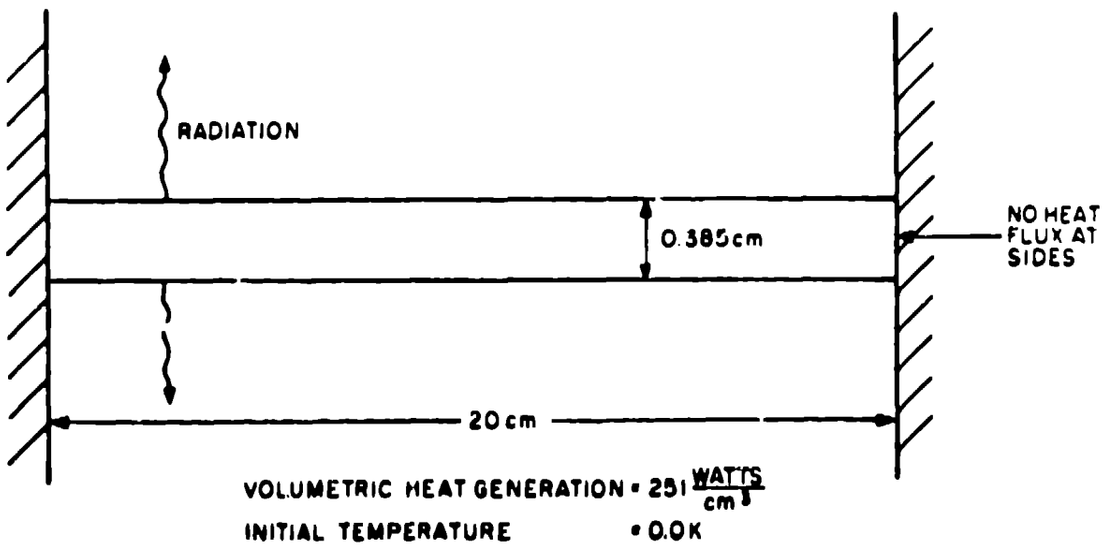

Fig. 2. The geometry, boundary conditions, and initial temperature conditions for a semi-infinite slab with internal heat generation. Radiation is the only thermal transport mode. In this problem, $\lambda_x = \lambda_y = \lambda_z = 30$ cal/s-cm K.

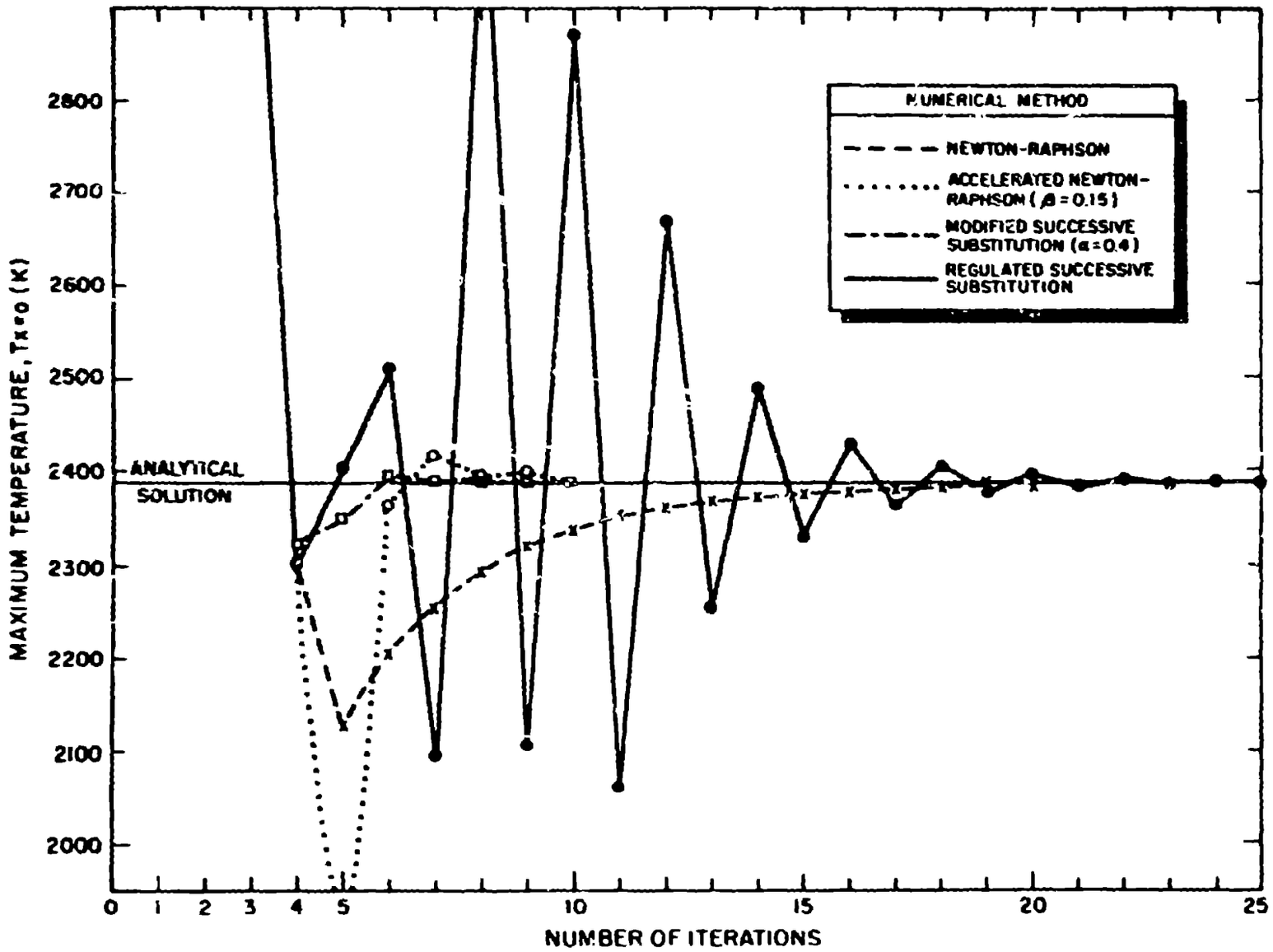

Fig. 3. The temperature ($T_{X=0}$) at the center of the bar computed by various methods as a function of the number of iterations in the radiation-conduction problem.

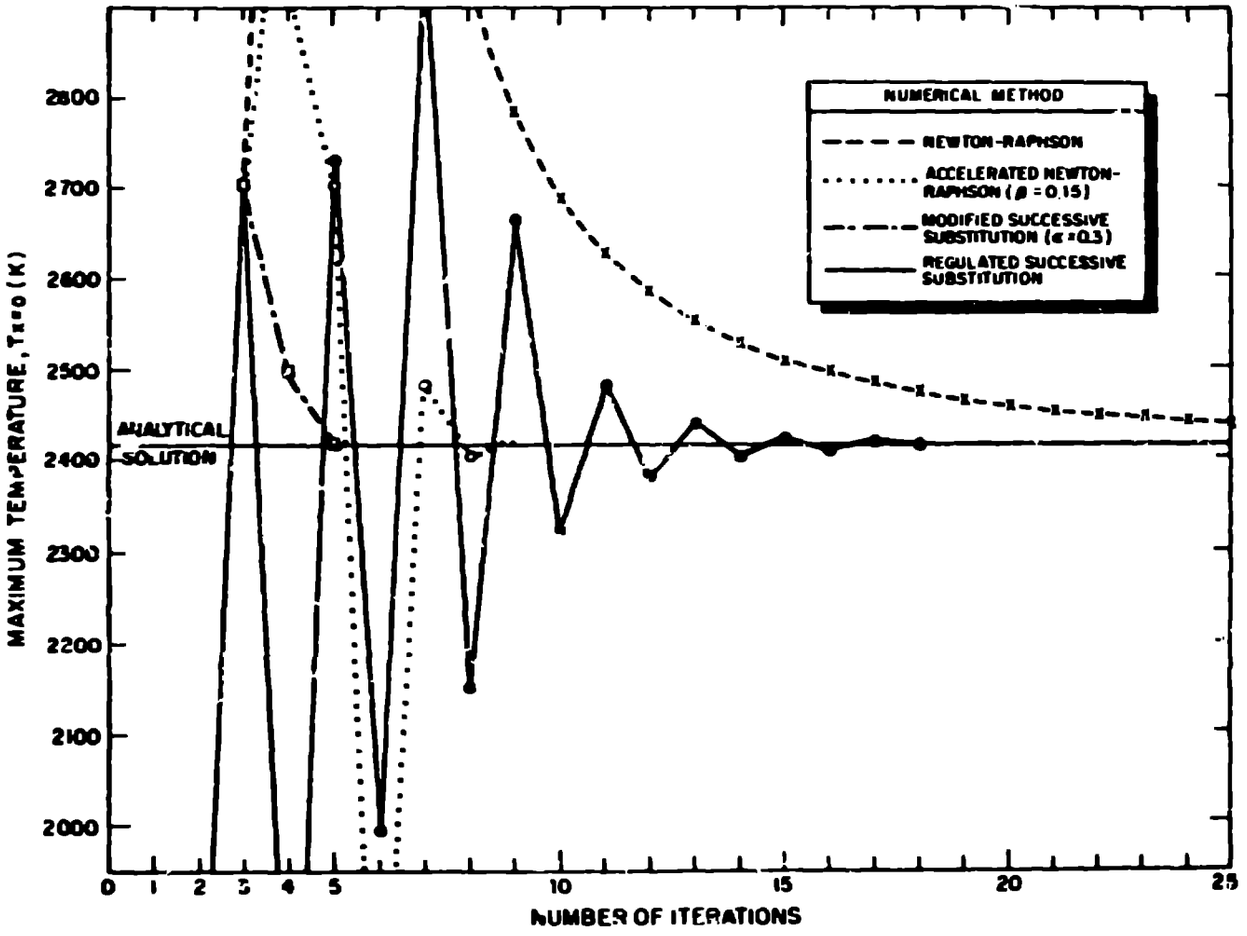

Fig. 4. The temperature ($T_{x=0}$) at the center of the bar computed by various methods as a function of the number of iterations in the radiation problem.

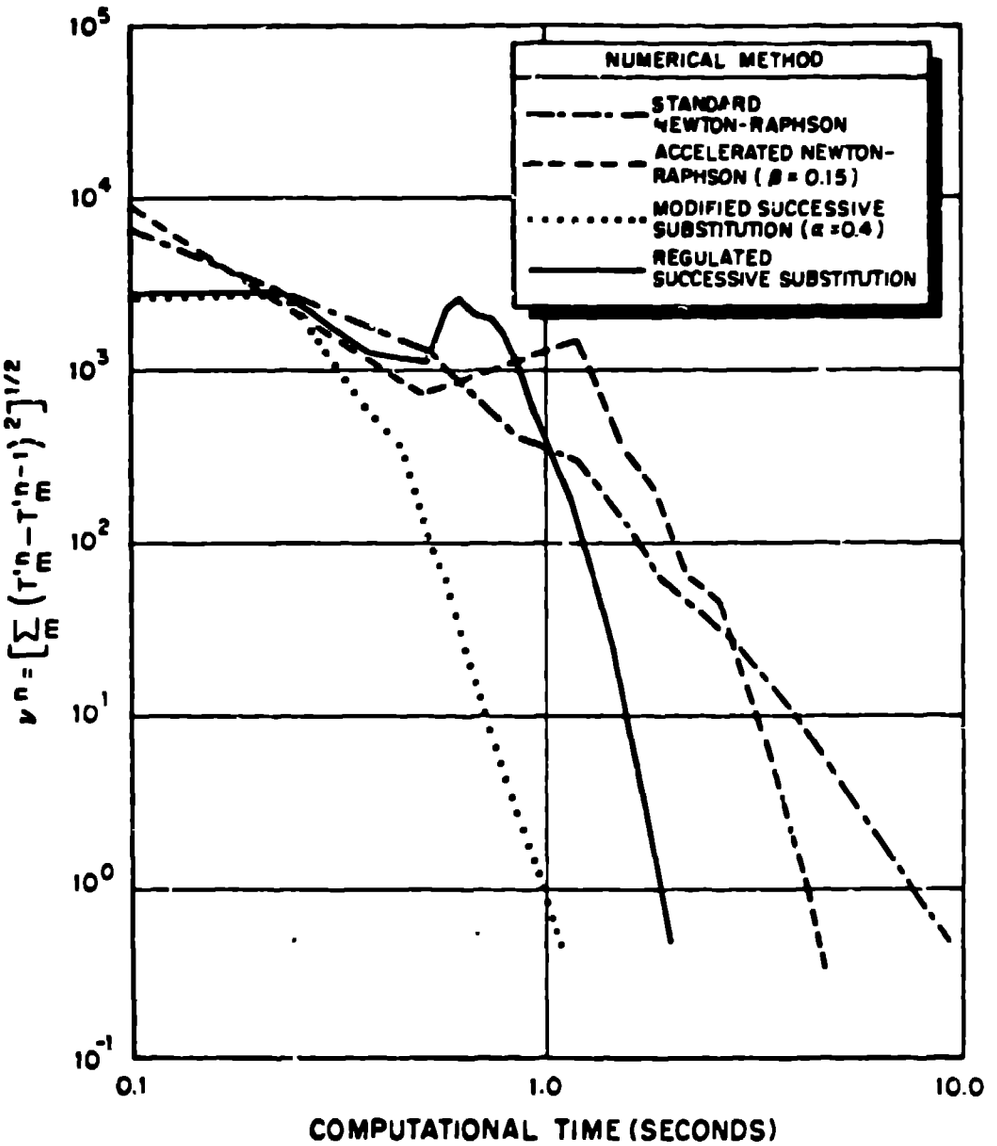

Fig. 5. The error in the radiation-conduction problem as defined by the temperature differences between iterations ($\nu^n = [\sum_m (T_m^n - T_m^{n-1})^2]^{1/2}$) as a function of the elapsed computational time for various numerical algorithms.

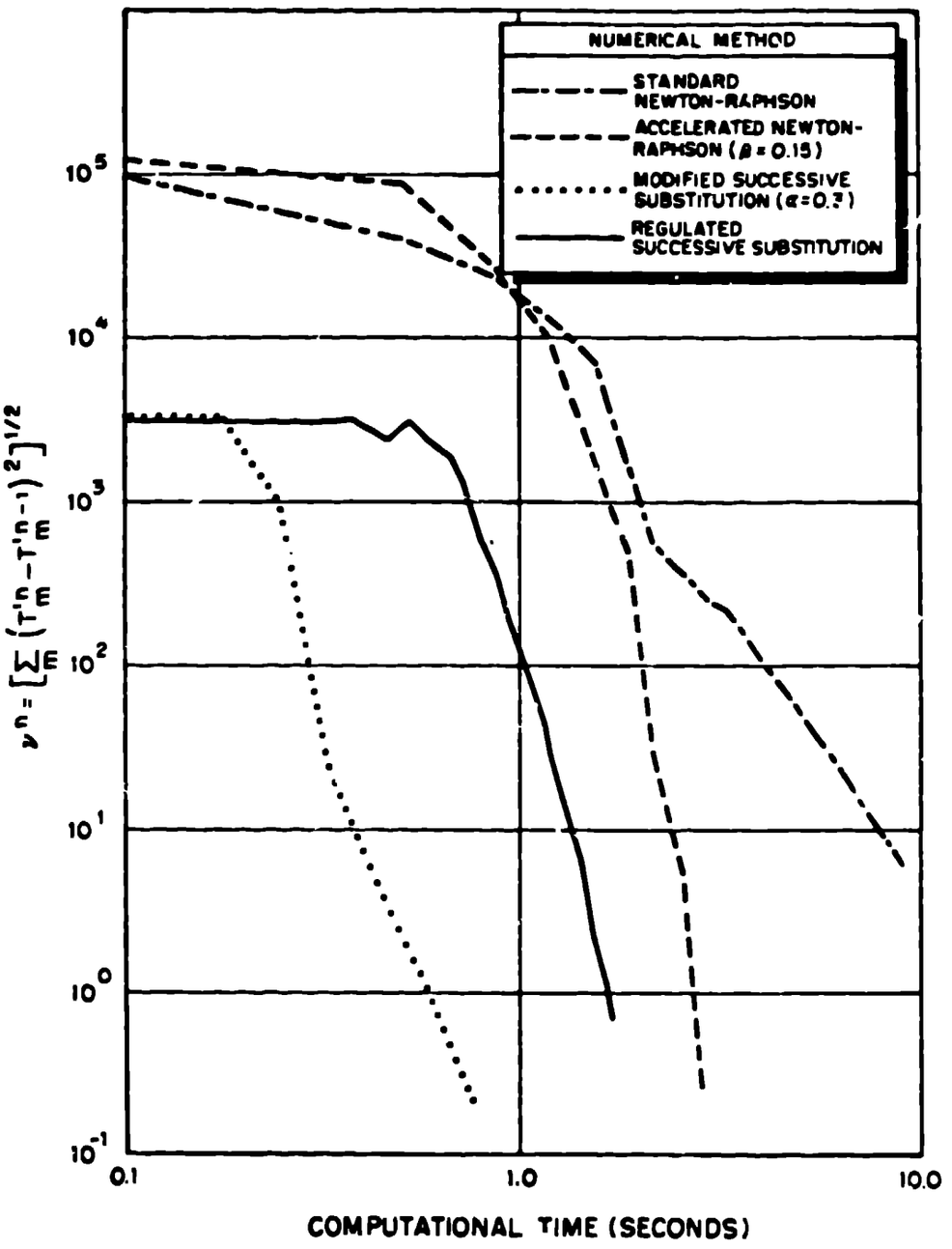

Fig. 6. The error in the radiation problem as defined by the temperature differences between iterations ($\nu^n = [\sum_m (T_m^n - T^{n-1})^2]^{1/2}$) as a function of the elapsed computational time for various numerical algorithms.