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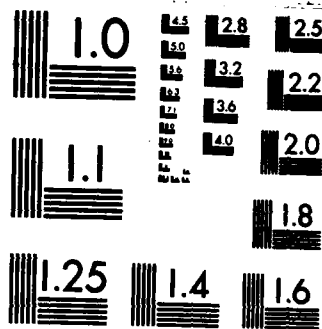
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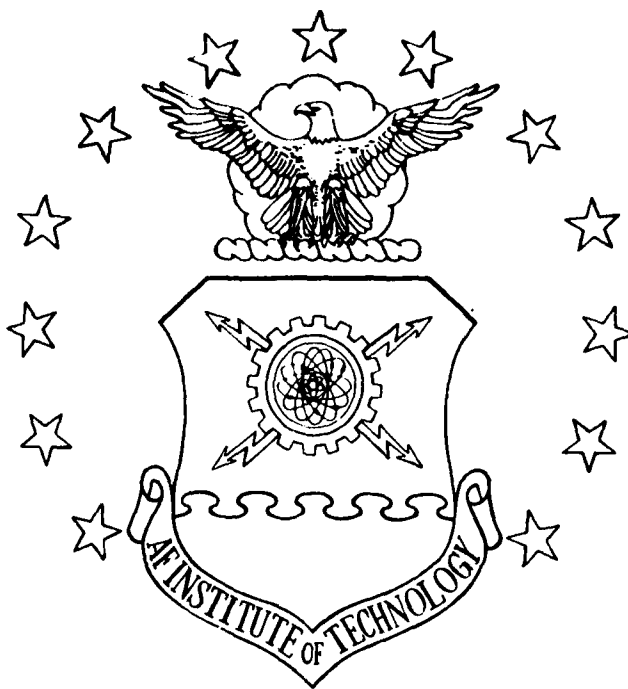
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 IMPLICIT METHOD AND A COMPARISON OF METHODS  
 FOR THE SOLUTION OF THE TWO DIMENSIONAL  
 HEAT DIFFUSION EQUATION

THESIS

Roger F. Kropf  
 Captain, USAF

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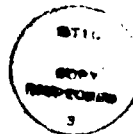
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IMPLICIT METHOD AND A COMPARISON OF METHODS  
FOR THE SOLUTION OF THE TWO DIMENSIONAL  
HEAT DIFFUSION EQUATION

THESIS

Presented to the Faculty of the School of Engineering  
of the Air Force Institute of Technology

Air University

In Partial Fulfillment of the  
Requirements for the Degree of  
Master of Science

Roger F. Kropf, B.A.

Captain, USAF

January 1985

Approved for public release; distribution unlimited

## Preface

This thesis began as an attempt to duplicate the suspect results of a previous thesis by Chivers (3). It quickly evolved into a study with particular emphasis on oscillations of the alternating direction implicit method of Peaceman and Rachford. A literature review has shown that this subject has not been addressed previously in the literature. Chiver's thesis covers much of the textbook material on finite differences and may be of interest to some readers for a review of some basics.

I am deeply indebted to Dr. Bernard Kaplan for his guidance and assistance throughout this study. He proposed that the ADI may have oscillatory solutions and provided the foundation on which this thesis is based.

I would like to express my thanks to Dr. N. Pagano of AFWAL/MLBC for sponsoring this study and to Sheryl Michel for her excellent typing.

Finally, I am most appreciative of my wife, Valerie, as well as Jennifer, Peter, Paul, and Amanda, for their love, encouragement, and great patience.

Roger F. Kropf

Table of Contents

|   | <u>Page</u> |
|---|-------------|
| Preface . . . . .   | ii          |
| List of Figures . . . . .                                   | iv          |
| Notation and Abbreviations . . . . .                        | vi          |
| Abstract . . . . .  | vii         |
| I. Introduction . . . . .                                   | 1           |
| Background . . . . .  | 1           |
| The Two Dimensional Heat Diffusion Equation . . . . .       | 1           |
| Problem Statement . . . . .                                 | 2           |
| Scope . . . . .   | 2           |
| General Approach . . . . .                                  | 3           |
| Sequence of Presentation . . . . .                          | 3           |
| Computer . . . . .  | 4           |
| II. Finite Difference Methods . . . . .                     | 5           |
| Finite Difference Equations . . . . .                       | 5           |
| Heat Diffusion Equation in Finite Difference Form . . . . . | 6           |
| Systems of Equations . . . . .                              | 8           |
| III. Stability and Properties . . . . .                     | 10          |
| Stability . . . . .   | 10          |
| Stability for Difference Methods in Two Dimension . . . . . | 11          |
| Accuracy of Methods . . . . .                               | 15          |
| Computer Time . . . . .                                     | 16          |
| IV. Results . . . . .                                       | 18          |
| Problem Description . . . . .                               | 18          |
| Results of Accuracy Comparisons . . . . .                   | 21          |
| Oscillatory Solutions . . . . .                             | 28          |
| Computer Time Required . . . . .                            | 48          |
| Chiver's Thesis . . . . .                                   | 52          |
| V. Conclusions and Recommendations . . . . .                | 56          |
| Conclusions . . . . .                                       | 56          |
| Recommendations . . . . .                                   | 57          |
| Bibliography . . . . .                                      | 58          |
| Vita . . . . .  | 60          |

## List of Figures

| <u>Figure</u>  | <u>Page</u> |
|--|-------------|
| 1. Stability Curves for One and Two Dimensions . . . . .   | 14          |
| 2. Error vs Time Step Problem #1 Time=1.0 h=0.1 . . . . .  | 22          |
| 3. Error vs Time Step Problem #1 Time=1.0 h=0.05 . . . . .   | 23          |
| 4. Error vs Time Step Problem #2 Time=0.1 h=0.1 . . . . .  | 24          |
| 5. Error vs Time Step Problem #2 Time=0.1 h=0.05 . . . . .   | 25          |
| 6. Error vs Time Step Problem #2 Time=0.4 h=0.1 . . . . .  | 26          |
| 7. Error vs Time Step Problem #2 Time=0.4 h=0.05 . . . . .   | 27          |
| 8. Numerical Solutions Problem #1<br>Time=5.0 $\Delta t=0.1$ h=0.1 r=10.0 . . . . .                                      | 30          |
| 9. Error Progression With Time Problem #1<br>$\Delta t=0.1$ h=0.1 r=10.0 . . . . .                                       | 31          |
| 10. ADI and Analytical Solutions Problem #2<br>$\Delta t=0.1$ h=0.1 r=10.0 . . . . .                                     | 32          |
| 11. Error Progression With Time ADI Problem #2<br>$\Delta t=0.1$ h=0.1 r=10.0 . . . . .                                  | 33          |
| 12. ADI and Analytical Solutions Problem #2<br>$\Delta t=0.025$ h=0.1 r=2.5 . . . . .                                    | 35          |
| 13. Error Progression With Time ADI Problem #2<br>$\Delta t=0.025$ h=0.1 r=2.5 . . . . .                                 | 36          |
| 14. ADI Solutions Problem #2 h=0.1 Maximum Error vs Time For<br>Various Values of r in the Oscillatory Region . . . . .  | 37          |
| 15. ADI Solutions Problem #2 h=0.05 Maximum Error vs Time<br>For Various Values of r in the Oscillatory Region . . . . . | 38          |
| 16. Numerical Solutions Problem #2<br>Time=0.1 $\Delta t=0.025$ h=0.1 r=2.5 . . . . .                                    | 40          |
| 17. Error Progression With Time Problem #2<br>$\Delta t=0.025$ h=0.1 r=2.5 . . . . .                                     | 41          |
| 18. Numerical Solutions Problem #2<br>Time=0.4 $\Delta t=0.1$ h=0.1 r=10.0 . . . . .                                     | 42          |
| 19. Error Progression With Time Problem #2<br>$\Delta t=0.1$ h=0.1 r=10.0 . . . . .                                      | 43          |

List of Figures (Continued)

| <u>Figure</u>   | <u>Page</u> |
|---|-------------|
| 20. Numerical Solutions Problem #2<br>Time=0.1 $\Delta t=0.0125$ $h=0.05$ $r=5.0$ . . . . .                                 | 44          |
| 21. Error Progression With Time Problem #2<br>$\Delta t=0.0125$ $h=0.05$ $r=5.0$ . . . . .                                  | 45          |
| 22. CN Solutions Problem #2 $h=0.1$ Maximum Error vs Time For<br>Various Values of $r$ in the Oscillatory Region . . . . .  | 46          |
| 23. CN Solutions Problem #2 $h=0.05$ Maximum Error vs Time For<br>Various Values of $r$ in the Oscillatory Region . . . . . | 47          |
| 24. CPU Time Used to Solve Problem #2<br>2000 Time Steps of $\Delta t=0.0005$ $h=0.1$ Time=1.0 . . . . .                    | 49          |
| 25. CPU Time Used to Solve Problem #2<br>200 Time Steps of $\Delta t=0.005$ $h=0.05$ Time=1.0 . . . . .                     | 50          |
| 26. CPU Time Used to Solve Problem #2<br>20 Time Steps of $\Delta t=0.0001$ $h=0.025$ Time=0.002 . . . . .                  | 51          |
| 27. CPU Time Used to Solve Problem #2 to an Accuracy of<br>Maximum Error Less Than 1.0 Degree Time=0.4 $h=0.1$ . . . . .    | 53          |
| 28. CPU Time Used to Solve Problem #2 to an Accuracy of<br>Maximum Error Less Than 1.0 Degree Time=0.4 $h=0.05$ . . . . .   | 54          |

## Notation and Abbreviations

$\Delta x = \Delta y = h =$  mesh spacing, the increment of space between nodal points.

$t =$  time (seconds)

$\Delta t =$  time increment

$\alpha =$  thermal diffusivity, here always = 1.0

$r = \alpha \Delta t / \Delta x^2 = \alpha \Delta t / \Delta y^2 = \alpha \Delta t / h^2$

$T(i,j,n) =$  Temperature (degrees) at the  $i$ th,  $j$ th nodal point at the  $n$ th time step, =  $T(i\Delta x, j\Delta y, n\Delta t) = T(x,y,t)$

ADI = Peaceman-Rachford alternating direction implicit method

CN = Crank-Nicolson implicit method

IM = Fully implicit method

EX = Fully explicit method

A = matrix notation for the matrix A

b = vector notation for the vector b

## Abstract

The two dimensional heat diffusion equation with Dirichlet boundary conditions was solved using the fully explicit, fully implicit, Crank-Nicolson implicit, and Peaceman-Rachford alternating direction implicit (ADI) methods. Comparisons of accuracy and time requirements were made.

The possibility that the ADI method has stable oscillatory solutions with large time steps was investigated.

Results of computations revealed that the ADI has stable oscillations for large time steps, in some cases producing large enough errors to render the solution unusable. Time steps greater than twice the square of the mesh spacing divided by the thermal diffusivity must be used with care.

For small time steps, the Crank-Nicolson and ADI methods were the most accurate, and the ADI was the fastest method. The fully implicit method was the most accurate at large time steps, but the ADI, with a smaller time step to reduce the oscillatory error, was still the fastest method to reach a solution with the desired degree of accuracy.

*Additional keywords: theses; numerical analysis;  
finite difference theory; conduction (heat transfer);  
partial differential equations; stability*

## I. Introduction

### Background

The heat diffusion equation is encountered in many areas of engineering, including nuclear engineering. Since only the simplest problems have analytical solutions, numerical techniques utilizing computers are commonly used to solve the practical problems encountered in engineering. Finite difference methods are the most basic and widespread techniques for obtaining solutions to the heat diffusion equation.

Although numerous schemes appear in the literature, the standard finite difference methods used in solving the heat diffusion equation remain the fully explicit (EX), fully implicit (IM), Crank-Nicolson implicit (CN), and the Peaceman-Rachford alternating direction implicit (ADI) methods. The employment of these methods requires an understanding of their behavior under different conditions, since large errors may sometimes occur.

### The Two Dimensional Heat Diffusion Equation

The heat diffusion equation in two dimensions is a parabolic partial differential equation of the form

$$\frac{\partial T(x,y,t)}{\partial t} = \alpha \left[ \frac{\partial^2 T(x,y,t)}{\partial x^2} + \frac{\partial^2 T(x,y,t)}{\partial y^2} \right] \quad (1)$$

where  $T$  is the temperature and  $\alpha$  is the thermal diffusivity. This equation describes the diffusion of heat in a solid in which the heat diffusion is independent of the  $z$  direction (4:12).

To solve a problem, the initial and boundary conditions must be specified. The three standard types of boundary conditions are the Dirichlet, which specifies the value of  $T$  at the boundaries, the Neumann, which specifies the value of the derivative of  $T$  at the boundaries, and the mixed, which combines the Dirichlet and Neumann (4:21).

### Problem Statement

The problem investigated in this thesis is to compare the accuracy and time required for the fully explicit, fully implicit, Crank-Nicolson, and Peaceman-Rachford alternating direction implicit methods of solution of the two dimensional heat diffusion equation. Further, the possibility is investigated that the ADI method has stable oscillations under certain conditions, similar to the stable oscillations known to exist in the Crank-Nicolson method (7:284;8:57). Finally, it should be noted that this thesis is a follow-on to a previous thesis by Chivers. His results, that the ADI and CN methods had unstable oscillations (3:35), do not agree with theory and his error, if any, needed to be found.

### Scope

This study was restricted to the two dimensional heat diffusion equation over a unit square. The mesh was set up such that  $\Delta x = \Delta y = h$ , only Dirichlet boundary conditions were used, and the thermal diffusivity was 1.0.

## General Approach

Initially, a previous thesis by Chivers (3) was reviewed to try to find any errors in his approach, and a literature review was conducted. After these, the coefficient method was used to determine the stability of the ADI method in two dimensions. Computer programs for the four finite difference methods were then written to solve the two dimensional heat diffusion equation with Dirichlet boundary conditions.

Two problems with known analytical solutions, allowing comparison, were studied. The first problem solved was the same one Chivers used, since it was desired to either duplicate his results or determine his error. A second problem was then selected to give more insight into the behavior of the finite difference methods with a practical engineering problem. This problem was solved, after which the oscillations of the ADI method were investigated in more detail.

## Sequence of Presentation

Chapter 2 presents general finite difference equations along with the specific formulations of the four methods. Systems of equations, resulting in the replacement of the heat equation with finite differences, are also discussed.

An analysis of stability of the four methods, using the coefficient method, is presented in Chapter 3. Also discussed in this chapter are the expected characteristics of the finite difference methods, such as accuracy and time required.

Chapter 4 presents results of the computer solutions to the heat diffusion equation using the four different methods. Conclusions and recommendations are given in Chapter 5.

is often the slowest method (9:27). The ADI may be fastest as a result of the tridiagonal form of its matrix (5:111), and the more grid points involved, the more advantage it has over the CN and IM methods, as discussed in Chapter 2. Whether the IM method has an advantage over the ADI for larger  $\Delta t$  may depend on the size of the error created by any oscillations of the ADI method. If forced to use a smaller  $\Delta t$  due to oscillations, the method could conceivably take longer than the IM method. This is investigated in the next chapter.

where

$I$  = the number of interior nodal points in  $x$

$J$  = the number of interior nodal points in  $y$

$T_a(i,j,n)$  = the analytical solution at the  $i$ th,  $j$ th grid point at the  $n$ th time step

$T(i,j,n)$  = the computed solution at the  $i$ th,  $j$ th grid point at the  $n$ th time step

This uses the standard definition of root mean squared average (1:506) and varies slightly from the one used by Towler and Yang (14:1023) in that  $IJ$  is under the square root. Note that since Dirichlet boundary conditions are used, the boundary nodal points are not included in the average (14:1023).

Besides using an average error, the maximum error at any nodal point is a useful tool, since a small average does not insure accuracy at all the points. A determination of the maximum error shows whether the solution has accuracy over the entire grid, which is important for most engineering applications.

### Computer Time

For a set number of time steps, the EX method should be fastest, and the CN and IM slowest. This is because the EX solves for the temperature directly at each nodal point. The ADI, as previously noted, solves a system of equations with a tridiagonal matrix, so that it is faster per time step than the IM and CN methods.

For actually solving a problem, the stability restriction on the EX method forces many times steps with a small  $\Delta t$  so that the EX method

### Accuracy of Methods

The accuracy of these methods due to truncation error of the Taylor series approximations are of the order  $\Delta t^2 + h^2$  for the ADI and CN methods, and of the order  $\Delta t + h^2$  for the EX and IM methods (11:212;13:42,90). Generally, the numerical solutions are more accurate than these estimates. Since not all the errors have the same sign, they tend to partially cancel (13:57).

Other errors are introduced besides truncation error. Oscillatory solutions of the CN method - and as proposed here of the ADI - for some values of  $r$  may add significant error. Oscillatory behavior of the EX method for  $r > 1/4$  results in gross error. Round off error by the computer may increase when a large number of arithmetic operations are required, as when solving a system of simultaneous equations.

Finally, it should be noted it is widely known that the CN method is more accurate than the IM method at small time steps, while the IM method is more accurate than the CN method for large time steps (9:27-28).

### Measuring Accuracy

The accuracy of the solutions was found by computing the root mean square (RMS) average error of all the grid points and by finding the maximum error at any of the grid points. These errors were computed using the analytical and computed solutions at each nodal point. This follows the convention suggested by Towler and Yang (14:1023-1024). The RMS error is computed as

$$E_{RMS} = \sum_{j=1}^J \sum_{i=1}^I \left\{ \frac{(T_a(i,j,n) - T(i,j,n))^2}{IJ} \right\}^{1/2}$$

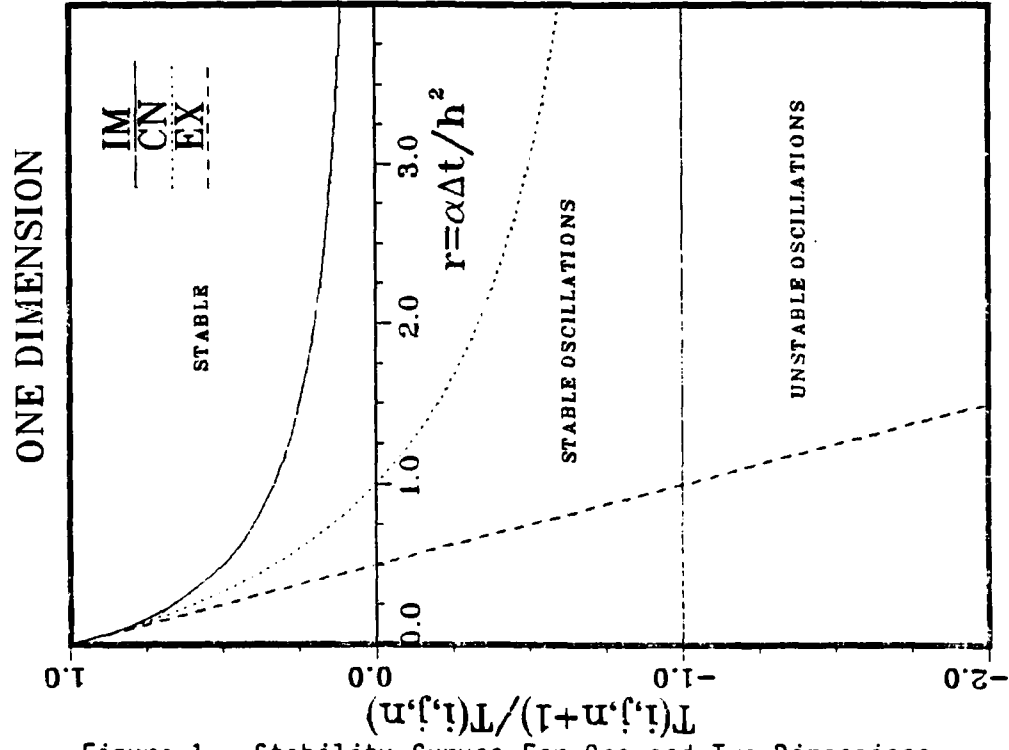
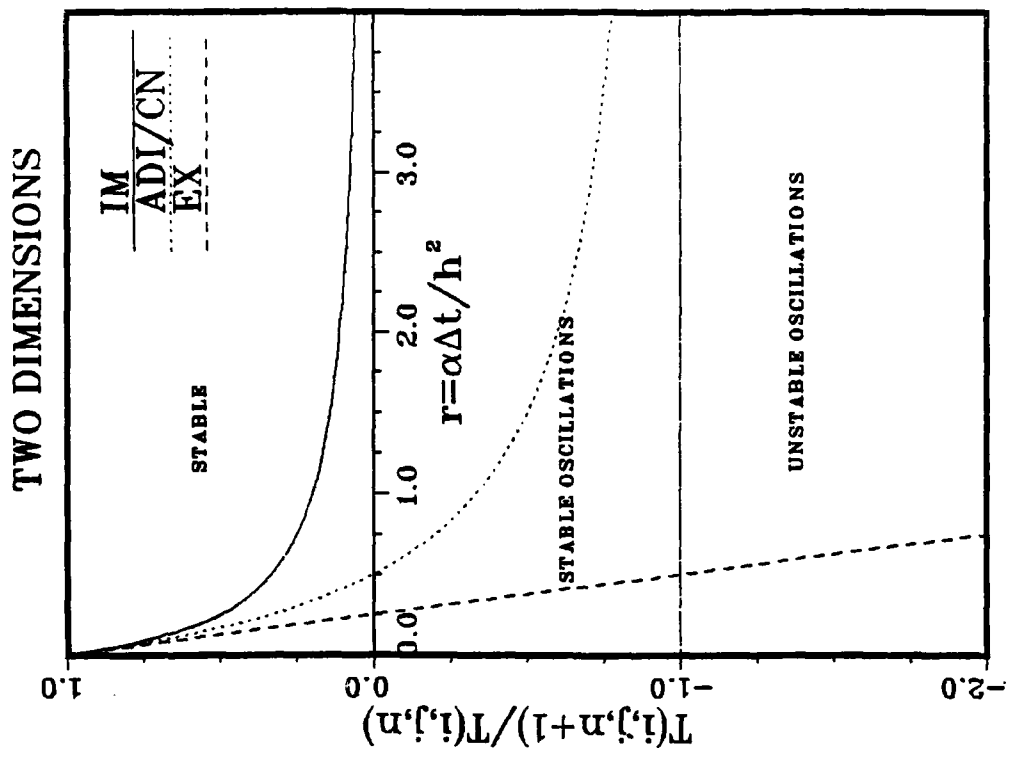


Figure 1. Stability Curves For One and Two Dimensions

This will always be between the values of +1 and -1. Therefore, the CN formulation is always stable, but the solution may oscillate when the temperature ratio is less than zero, which occurs when

$$r > 1/2 \quad (15)$$

Again, this is more restrictive than the one dimensional cases where stable oscillations may occur if  $r > 1$  (9:30). Note that any oscillations will eventually die out since the error is bounded.

The ADI formula, Eq (5), gives, for a one nodal point grid

$$\frac{T(i,j,n+1)}{T(i,j,n)} = \frac{1 - 2r}{1 + 2r} \quad (16)$$

This is the same stability criteria as for the CN method, Eq (14). Thus the ADI method is always stable but may have oscillatory solutions.

The stability curves of all four methods for the one and two dimensional cases are plotted in Figure 1. Although here,  $\Delta x = \Delta y$ , the above analysis can easily be extended to a grid system where  $\Delta x \neq \Delta y$ . For example, for the ADI and CN method, Eqs (14) and (16) become

$$\frac{T(i,j,n+1)}{T(i,j,n)} = \frac{1 - \Delta t/\Delta x^2 - \Delta t/\Delta y^2}{1 + \Delta t/\Delta x^2 + \Delta t/\Delta y^2}$$

and both mesh spacings will determine the behavior of the method.

The possible ranges of the ratio are

$$0 < T(i,j,n+1)/T(i,j,n) < 1 \quad (7)$$

when

$$r < 1/4 \quad (8)$$

and

$$-1 < T(i,j,n+1)/T(i,j,n) < 0 \quad (9)$$

when

$$1/4 < r < 1/2 \quad (10)$$

and

$$T(i,j,n+1)/T(i,j,n) < -1 \quad (11)$$

when

$$r > 1/2 \quad (12)$$

Note that this is more restrictive than the one dimensional case, where the stability condition for  $T(i,j,n+1)/T(i,j,n) > 0$  is that  $r < 1/2$  (5:108).

The fully implicit formula, Eq (3), yields

$$\frac{T(i,j,n+1)}{T(i,j,n)} = \frac{1}{1+4r} \quad (13)$$

which is always positive and, therefore, always stable.

The CN formulation, Eq (4), yields

$$\frac{T(i,j,n+1)}{T(i,j,n)} = \frac{1-2r}{1+2r} \quad (14)$$

1.  $0 < T(i,j,n+1)/T(i,j,n) < 1$ . Stable solution, the error decreases with time, no oscillations.
2.  $-1 < T(i,j,n+1)/T(i,j,n) < 0$ . Stable oscillations, error and oscillations decrease with time.
3.  $T(i,j,n+1)/T(i,j,n) < -1$ . Unstable oscillations, error is unbounded, growing with time.

Note that the ratio is never greater than 1.

This behavior is easily understood. If the temperature ratio is positive, each time step results in a temperature of the same sign but with smaller magnitude. Thus the temperature steadily decreases with time, and is stable.

If the temperature ratio is negative but greater than -1, each new temperature will have the opposite sign of the previous temperature and a smaller magnitude. Thus the temperature will oscillate between positive and negative values, but will decrease in magnitude as time steps are taken, and so it is stable.

If the temperature ratio is less than -1, each new temperature will have the opposite sign of the preceding temperature and will be larger in magnitude. Thus the temperature will oscillate while its magnitude will grow without bound, causing instability.

#### Stability for Difference Methods in Two Dimensions

In two dimensions, the explicit formula, Eq (2), evaluated for a one nodal point grid, yields

$$\frac{T(i,j,n+1)}{T(i,j,n)} = 1 - 4r \quad (6)$$

### III. Stability and Properties

#### Stability

The concept of stability is sometimes misunderstood. Stability is simply the guarantee that the error does not grow in time, that is, the error is bounded (5:98). Stability of a finite difference formulation does not guarantee accuracy or non-oscillatory behavior of the solution, although any oscillations will die out eventually (9:27). On the other hand, a non-stable formulation will blow up as the number of time intervals increase, that is, the error will grow with time in an unbounded fashion.

A common and easily understood method of considering stability is the coefficient method. Myers and Patankar both present this method, but only for the one dimensional heat diffusion equation (7:281-284; 9:28-30). The method is developed here for two dimensions.

The idea of the coefficient method is to consider a system consisting of only one nodal point, so that the only non-zero temperatures are  $T(i,j,n)$  and  $T(i,j,n+1)$ . Then the ratio

$$\frac{T(i,j,n+1)}{T(i,j,n)} = \frac{C(i,j,n)}{C(i,j,n+1)}$$

where  $C(i,j,n)$  is the coefficient of  $T(i,j,n)$ , is easily found. The three types of behavior of the solution for different values of the ratio  $T(i,j,n+1)/T(i,j,n)$  are (7:282):

The IM and CN methods, for the problems used in this study, result in A being a real, symmetric, positive definite matrix. The most efficient method for solving the equation Ab=c for this case is the direct Cholesky square root method (15:105). This method requires on the order of  $N^3/3$  operations, although it is faster than this sounds since the matrix A has only 5 non-zero diagonals (15:99-100). Should a problem result in a non-symmetric matrix, a less efficient method, such as the Gauss-Seidel, would be needed. For this reason, a problem with irregular geometry which does not result in a symmetric, positive definite matrix will take more work to solve than the problems used in this study.

The ADI method results in a tridiagonal matrix A. This is a great advantage, as the equation Ab=c can be solved rapidly using the Thomas method. Since this method only uses on the order of  $8N$  operations, it is very fast (5:111). Note that the larger the number of mesh points  $N$ , the faster the ADI will be relative to the IM and CN due to the order of operations being  $8N$  vs  $N^3/3$ . Additionally, a tridiagonal matrix in band storage mode requires much less storage, which is a significant factor for a system with a large number of mesh points.

$$\begin{aligned}
 (1+2r) T(i,j,n+1) - r[T(i+1,j,n+1) + T(i-1,j,n+1)] \\
 = (1-2r) T(i,j,n) + r[T(i,j+1,n) + T(i,j-1,n)]
 \end{aligned}
 \tag{5a}$$

to advance from time step  $n$  to  $n+1$ , followed by

$$\begin{aligned}
 (1+2r) T(i,j,n+2) - r[T(i,j+1,n+2) + T(i,j-1,n+2)] \\
 = (1-2r) T(i,j,n+1) + r[T(i+1,j,n+1) + T(i-1,j,n+1)]
 \end{aligned}
 \tag{5b}$$

to advance from time step  $n+1$  to  $n+2$ . Note that  $\Delta t$  must remain constant, and that the solution is valid only after both steps are taken (6:53;13:42).

### Systems of Equations

The EX method results in one equation per mesh point to solve for the temperature at  $t + \Delta t$  directly. The other methods, however, result in systems of equations which must be solved simultaneously. For  $N$  interior mesh points, this is represented in matrix form as

$$\underline{A}\underline{b}=\underline{c}$$

where  $\underline{A}$  is a  $N \times N$  matrix,  $\underline{b}$  is a vector composed of the new temperature at  $t + \Delta t$ , and  $\underline{c}$  is a vector composed from the old temperatures and boundary conditions. This equation is then solved for  $\underline{b}$ .

### Fully Implicit (IM) Formulation

The fully implicit method computes the temperature at the new time step based on temperatures at neighboring nodal points which are also at the new time. A simple extension of the one dimensional case (8:58) results in a series of equations of the form

$$(1+4r) T(i,j,n+1) - r[T(i+1,j,n+1) + T(i-1,j,n+1) + T(i,j+1,n+1) + T(i,j-1,n+1)] = T(i,j,n) \quad (3)$$

which must be solved simultaneously.

### Crank-Nicolson (CN) Implicit Formulation

The Crank-Nicolson method weighs the fully explicit and fully implicit equally and combines the two methods. The result is a series of equations which again must be solved simultaneously. The equations are of the form (13:42)

$$(2+4r) T(i,j,n+1) - r[T(i+1,j,n+1) + T(i-1,j,n+1) + T(i,j+1,n+1) + T(i,j-1,n+1)] \\ = (2-4r) T(i,j,n) + r[T(i+1,j,n) + T(i-1,j,n) + T(i,j+1,n) + T(i,j-1,n)] \quad (4)$$

### Peaceman-Rachford (ADI) Formulation

The ADI method alternates solving one space direction explicitly and the other implicitly. The method results in a series of simultaneous equations to solve of the form (5:110;10:33)

Standard textbooks in this field cover all the variations from which finite differences may be formulated (5:59;7:234;8:25-28). The result of using finite differences is that a partial differential equation may be replaced by a series of finite difference equations. The solution of the finite difference equations on a computer then gives the answer at each nodal point.

### Heat Diffusion Equation In Finite Difference Form

The four primary methods of solving the heat diffusion equation with finite differences are the fully explicit, fully implicit, Crank-Nicolson implicit, and Peaceman-Rachford alternating direction implicit methods. They are found in numerous texts and journals in the field of heat conduction. As a reminder, for this study,  $h=\Delta x=\Delta y, \alpha=1$ , and  $r=\alpha\Delta t/h^2=\Delta t/h^2$ .

#### Fully Explicit (EX) Formulation

The explicit name implies the form of this solution. It computes temperature at each nodal point in terms of the old temperatures of the previous time step. The formula is (13:41),

$$\begin{aligned} T(i,j,n+1) = & r[T(i+1,j,n) + T(i-1,j,n) + T(i,j+1,n) \\ & + T(i,j-1,n)] + (1-4r)T(i,j,n) \end{aligned} \quad (2)$$

This method is the most straight forward of the four methods as it only requires the solution of an independent algebraic equation for each point for every new time step.

## II. Finite Difference Methods

### Finite Difference Equations

To formulate two dimensional finite difference equations, time and space are divided into discrete intervals  $\Delta t$ ,  $\Delta x$ , and  $\Delta y$ , forming a mesh or grid of nodal points. Instead of continuous values, there are only discrete values of variables and functions, so that  $x = i\Delta x$ ,  $y = j\Delta y$ , and  $t = n\Delta t$  where  $i, j$ , and  $n$  are integers. Then a function such as temperature,  $T(x, y, t)$ , is replaced with a function with values only at mesh points,  $T(x, y, t) = T(i\Delta x, j\Delta y, n\Delta t)$ , which notationally is represented as  $T(i, j, n)$ .

Once the grid has been established, the partial differentials in an equation are replaced with finite differences. These are built from Taylor series expansions of the function evaluated at a point, for example, adding the Taylor series expansions

$$T(x + \Delta x) = T(x) + \Delta x T'(x) + \frac{\Delta x^2}{2} T''(x) + O(\Delta x^3) + \dots$$

and

$$T(x - \Delta x) = T(x) - \Delta x T'(x) + \frac{\Delta x^2}{2} T''(x) - O(\Delta x^3) + \dots$$

yields the central difference to a second derivative,

$$T''(x) = \frac{d^2 T(x)}{dx^2} = \frac{T(x + \Delta x) - 2T(x) + T(x - \Delta x)}{\Delta x^2} + O(\Delta x^2)$$

### Computer

The computer used was a VAX 11/780, which is a 32 bit machine. Double precision was used to minimize round off error. Graphs were drawn with a CDC CYBER computer using DISSPLA. All programs were written in FORTRAN 77.

## IV. Results

This chapter presents the results of numerous computer runs to compare the behavior and characteristics of the different finite difference methods. First the two problems and their analytical solutions are presented. Then the results for accuracy, oscillations, and time are presented. Finally, a brief summation of errors in Chiver's thesis is given.

### Problem Description

To compare the four finite difference methods, two problems with known analytical solutions were solved. After getting results for the first problem, it became apparent that the problem was inadequate for evaluating the usefulness of the methods for a practical engineering problem. This was because the solution rapidly tends toward zero, and the errors and oscillations were so small that their interpretation was difficult. A second problem which more closely resembles a practical engineering problem was then selected and solved.

### Problem #1

The first problem is

$$\frac{\partial T(x,y,t)}{\partial t} = \frac{\partial^2 T(x,y,t)}{\partial x^2} + \frac{\partial^2 T(x,y,t)}{\partial y^2}$$

in the region  $0 < x < 1$ ,  $0 < y < 1$ , and  $0 < t$ , with the initial condition

$$T(x,y,0) = \sin(\pi x) \sin(\pi y)$$

and boundary conditions

$$T(0,y,t) = T(1,y,t) = T(x,0,t) = T(x,1,t) = 0$$

The analytical solution is

$$T(x,y,t) = \exp(-2\pi^2 t) \sin(\pi x) \sin(\pi y)$$

which is easily found using separation of variables and verified by substitution. The solution found by Chivers (3:5,55) is erroneous in that the initial condition was not properly applied. The problem is similar to one in Mitchell (6:66) except for the boundary conditions, and the solution is the same. For purposes of comparison, the solution was computed for a time of 1.0 seconds.

#### Problem #2

The second problem is

$$\frac{\partial T(x,y,t)}{\partial t} = \frac{\partial^2 T(x,y,t)}{\partial x^2} + \frac{\partial^2 T(x,y,t)}{\partial y^2}$$

in the region  $0 < x < 1$ ,  $0 < y < 1$ , and  $0 < t$ , with the initial condition

$$T(x,y,0) = 0$$

and boundary conditions

$$T(0,y,t) = T(1,y,t) = T(x,0,t) = T(x,1,t) = 400.0$$

This problem and its analytical solution is virtually identical to the one presented by Shih and Skladany (12:410) except that here it is not normalized. The analytical solution is

$$T(x,y,t) = 400(1-f(x,y,t))$$

where

$$f(x,y,t) = g(x,t)h(y,t)$$

with

$$g(x,t) = \sum_{n=1}^{\infty} \frac{4}{n\pi} \exp(-n^2\pi^2 t) \sin(n\pi x)$$

and

$$h(y,t) = \sum_{n=1}^{\infty} \frac{4}{n\pi} \exp(-n^2\pi^2 t) \sin(n\pi y)$$

where

$$n = 1,3,5,\dots$$

The solution is found by first normalizing, then using separation of variables (2:173;12:410), and can be verified by substitution. For accuracy comparisons, the solution was computed at times of 0.1 and 0.4 seconds.

## Results of Accuracy Comparisons

### Figures

Figures 2 and 3 present the accuracy results for problem #1, and Figures 4-7 give the results for problem #2. Each figure has two graphs, one plotting the RMS error and one plotting the maximum error for different  $\Delta t$ . In Figures 2, 4, and 6, the mesh spacing is  $h = 0.1$ , and in Figures 3, 5, and 7, the mesh spacing is  $h = 0.05$ , so that the effect of halving the mesh size can be seen.

### Results

The results of all the cases in Figures 2-7 show that for small time steps the ADI and CN methods are more accurate than the IM method. This is expected since they have less truncation error (see Chapter 2). At large time steps the IM becomes more accurate, due to oscillatory solutions for the CN and ADI methods at large time steps. The oscillations are discussed in more detail in the next section. Notice that the CN and ADI solutions are very close in accuracy.

Based on truncation error, the EX method is expected to be about as accurate as the IM method. As Figures 2, 6, and 7 show, however, there are regions where it is the most accurate. This occurs with small  $\Delta t$ , which require many time steps to reach a solution at the desired time. The CN, ADI, and IM methods, requiring solutions of simultaneous equations for each iteration, accumulate more round off error, giving the EX method an overall accuracy advantage in these cases. Note that the EX method gives unbounded error when  $r > 1/4$ .

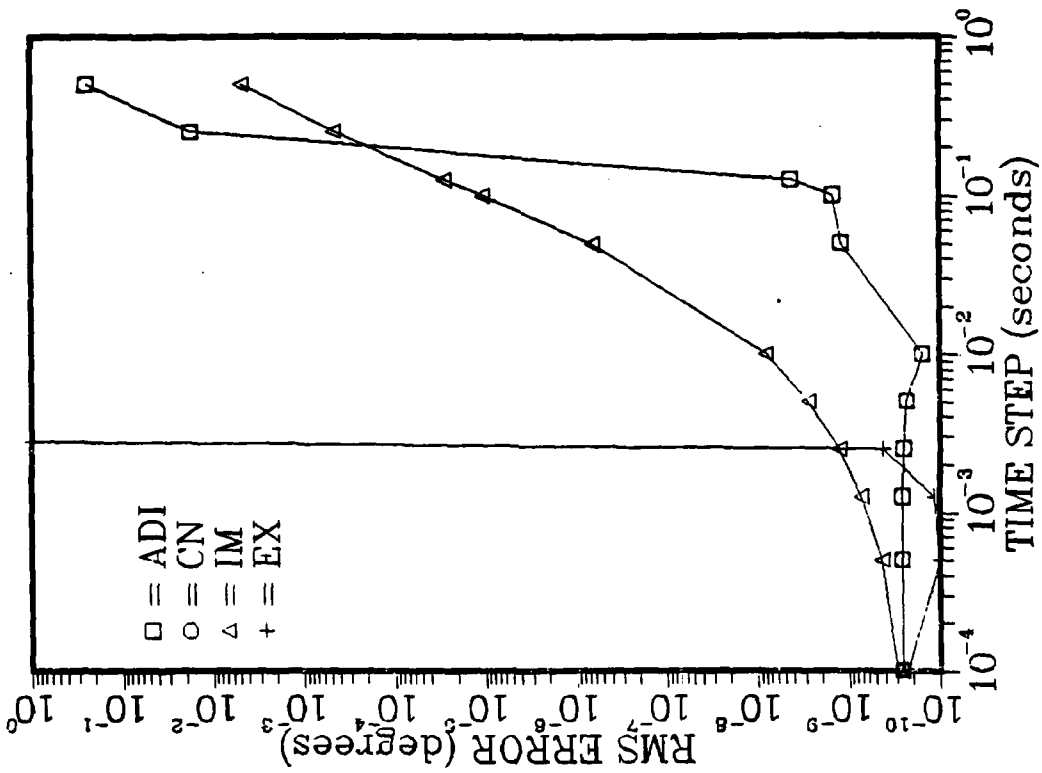
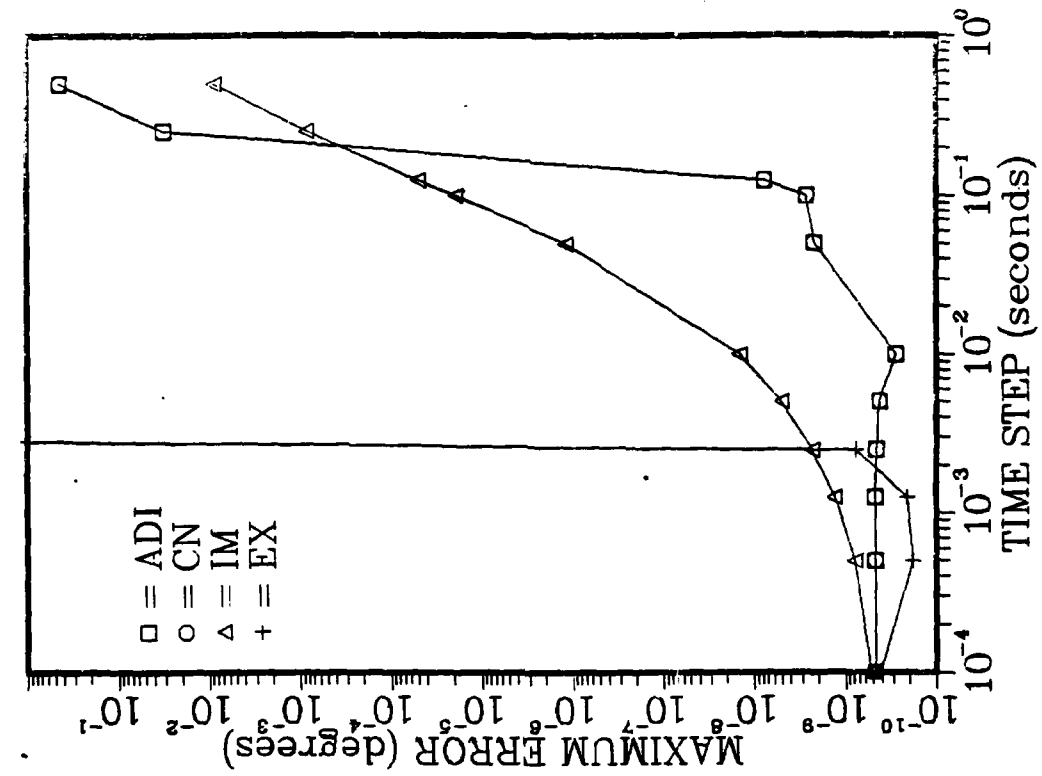


Figure 2. Error vs Time Step Problem #1  
 Time=1.0  $\Delta x = \Delta y = h = 0.1$

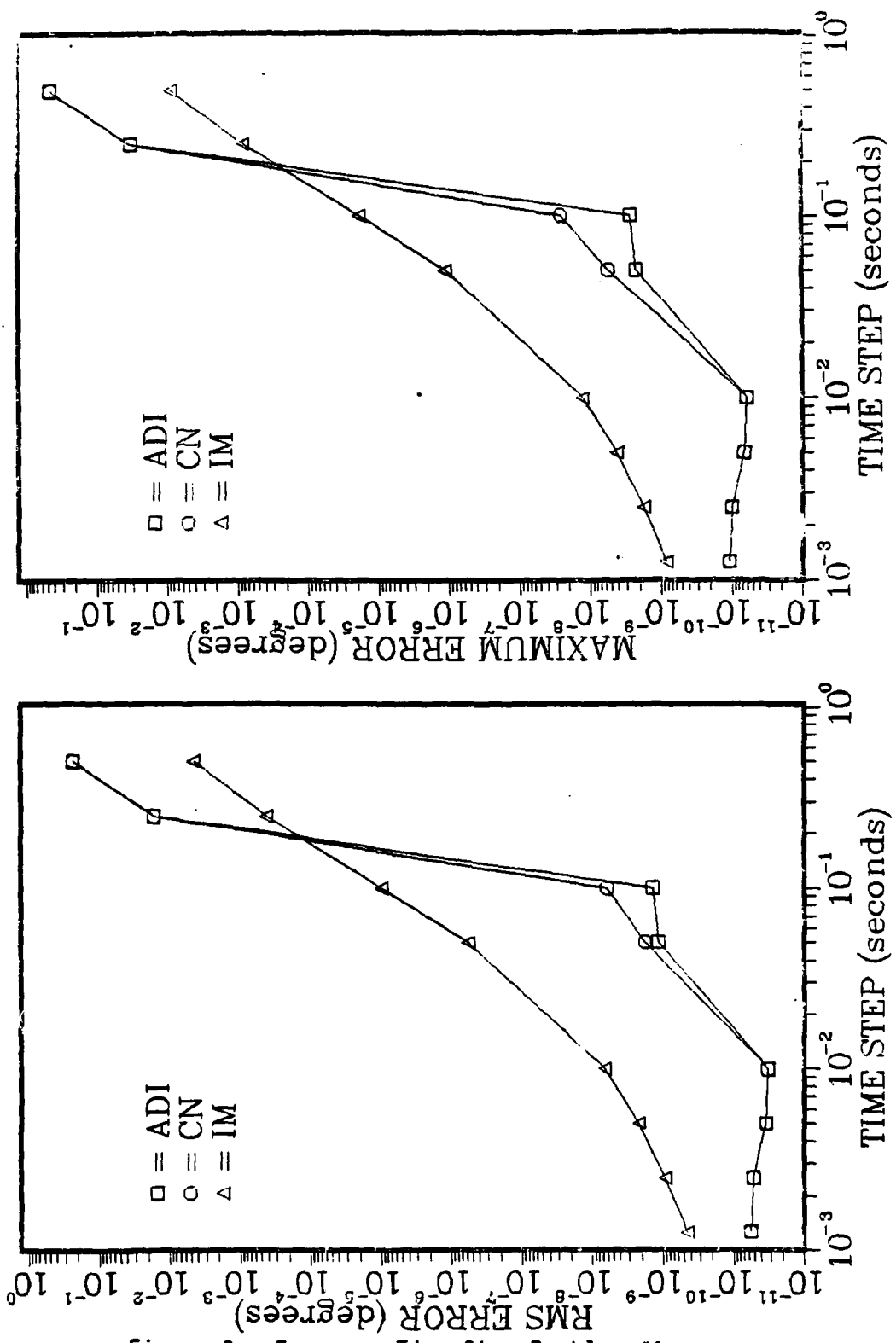


Figure 3. Error vs Time Step Problem #1  
 Time=1.0  $\Delta x=\Delta y=h=0.05$

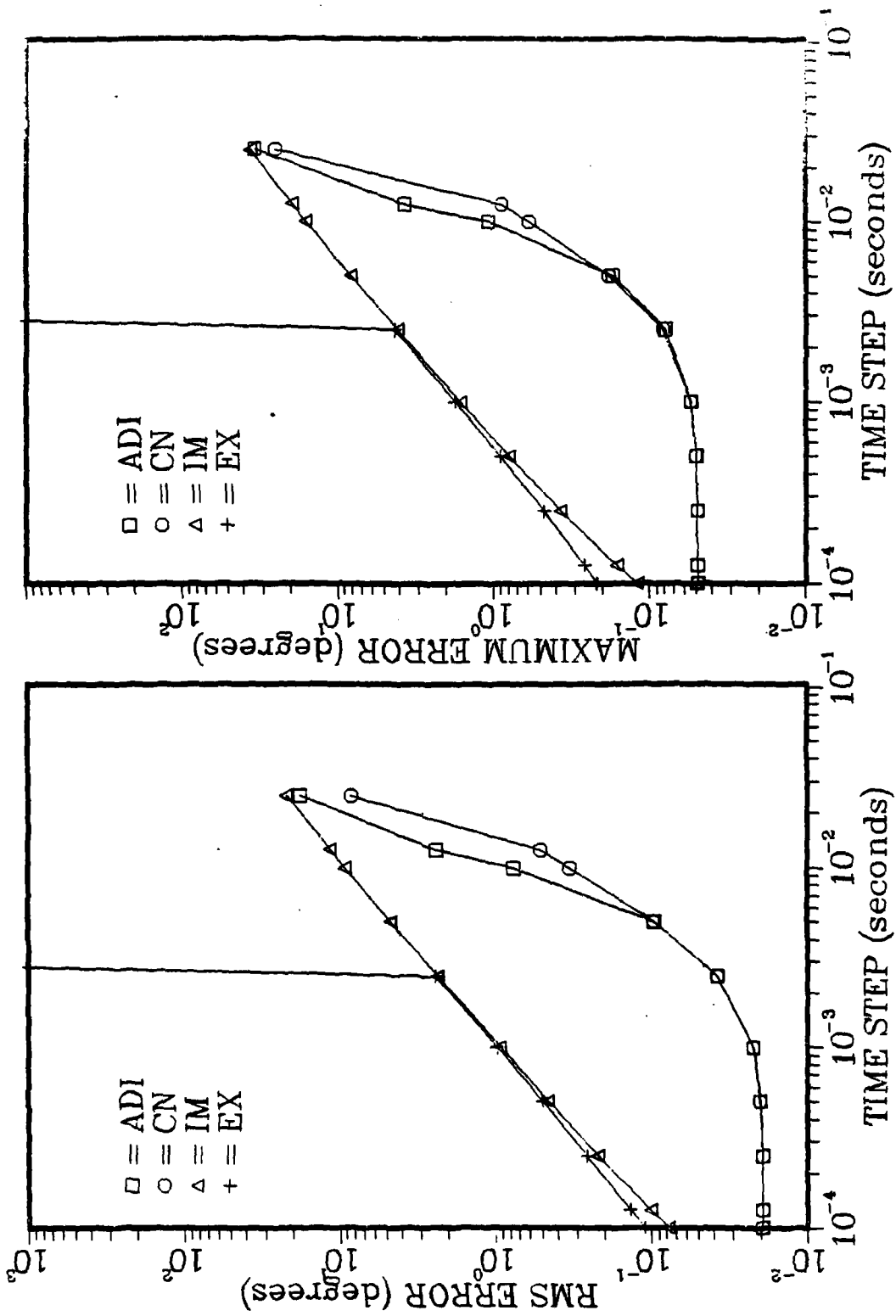


Figure 4. Error vs Time Step Problem #2  
 $1.0 = \Delta t = \Delta x = \Delta y = h$

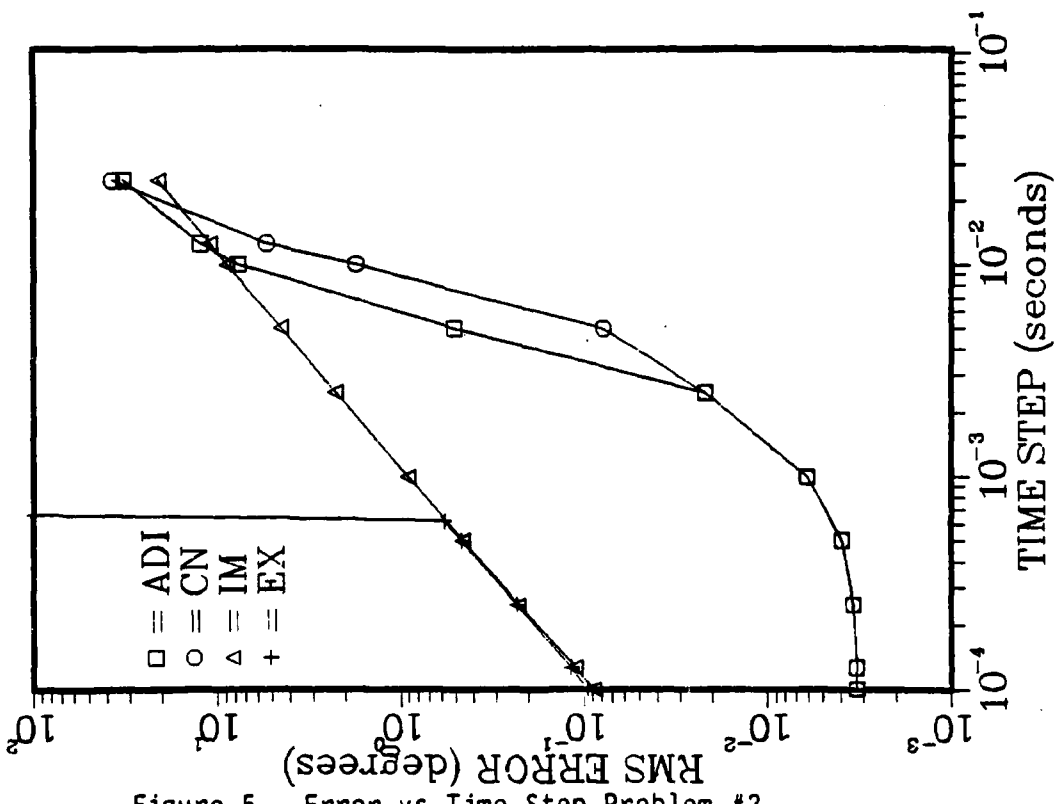
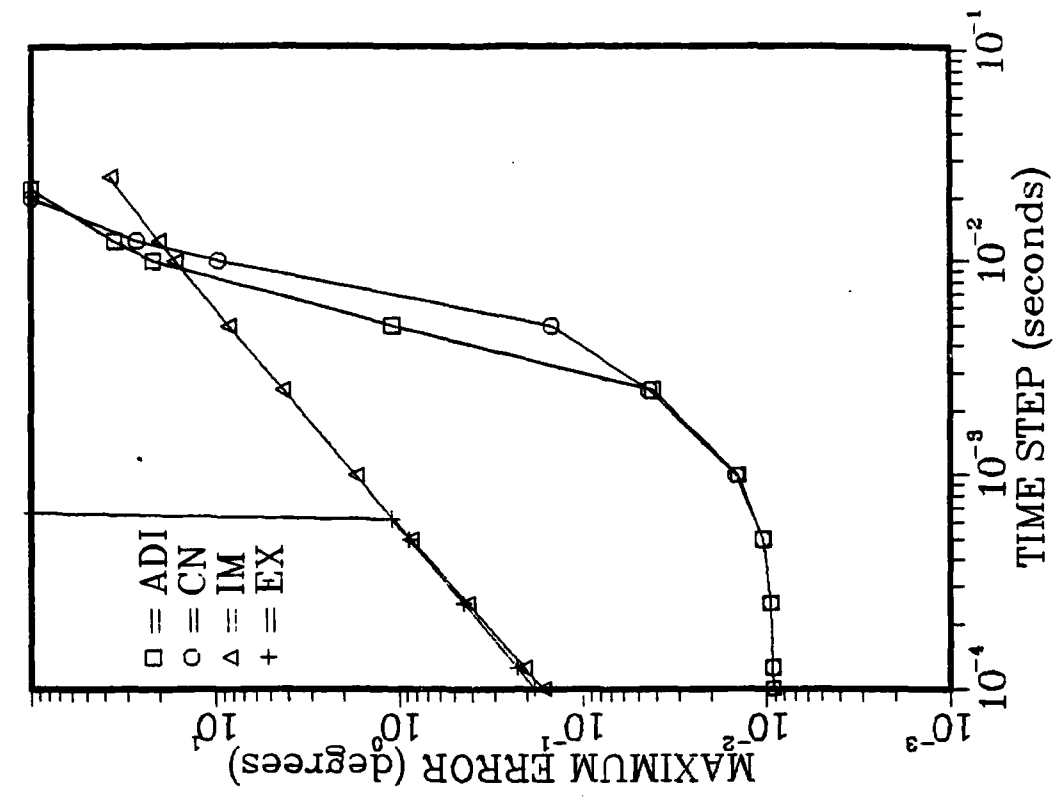


Figure 5. Error vs Time Step Problem #2  
 Time=0.1  $\Delta x = \Delta y = h = 0.05$

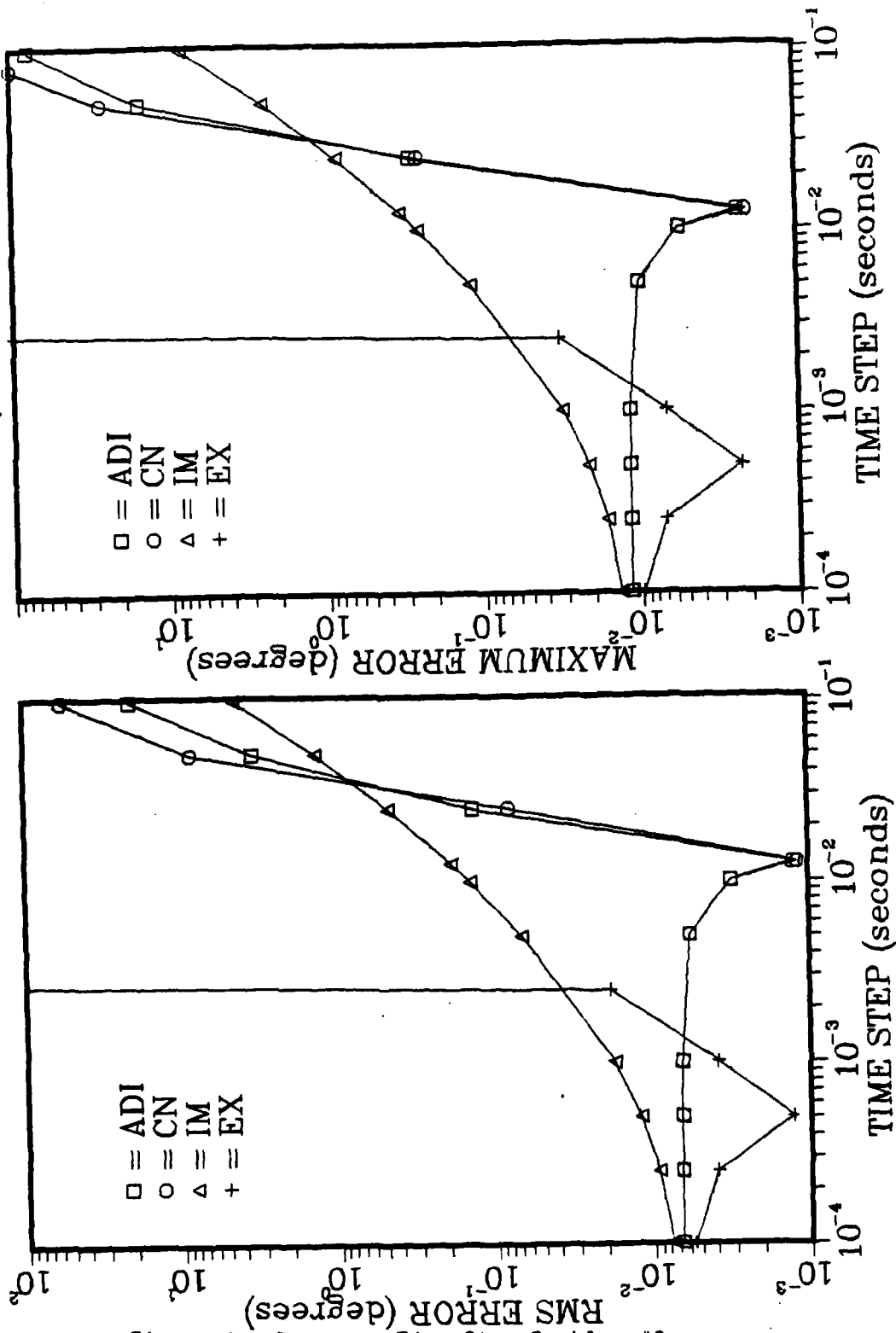


Figure 6. Error vs Time Step Problem #2  
 $1.0=h=\Delta x=\Delta y$   
 $\text{Time}=0.4$

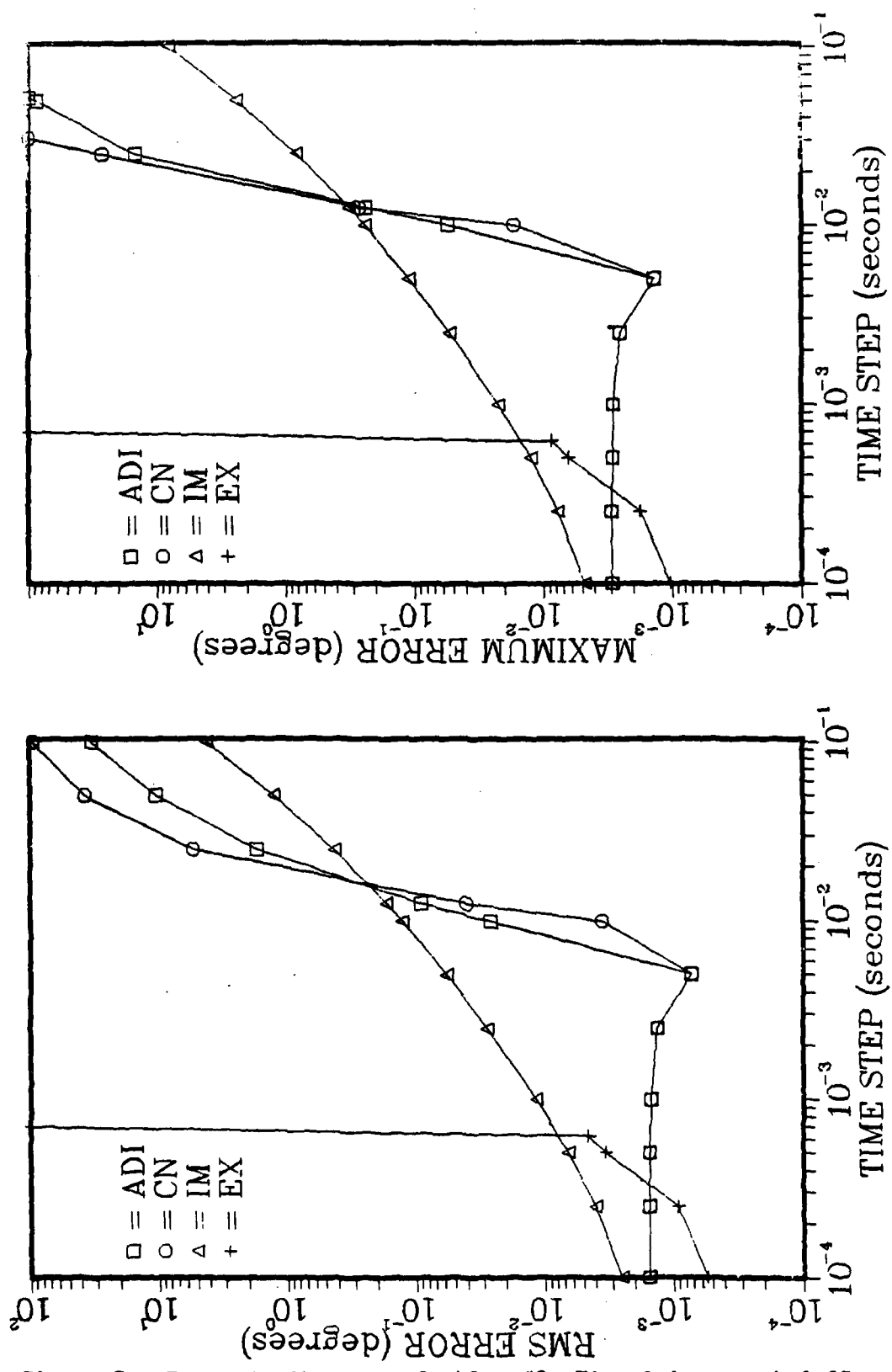


Figure 7. Error Vs Time Step Problem #2 Time=0.4  $\Delta x=\Delta y=h=0.05$

For small time steps ( $10^{-4}$  to  $10^{-3}$ ), the accuracy of the ADI and CN methods remain about the same, while the IM and EX methods have increased error with increasing time step. This is because the truncation error for the ADI and CN methods is of order  $\Delta t^2 + h^2$ , and the  $\Delta t^2$  contribution is negligible for small time steps. The IM and EX methods, however, get contribution to the truncation error from  $\Delta t$ , not  $\Delta t^2$ , so it is not negligible. As a result, at small time steps the IM and EX error increases as time step increases. As the time step increases further, the  $\Delta t^2$  component of truncation error becomes significant, causing increasing error for the ADI and CN solutions as can be seen in Figures 2-7.

A finer mesh is expected to yield a more accurate solution since it reduces the truncation error. For example, for the first problem with a time step of  $\Delta t = 0.01$  and a mesh spacing of  $h = 0.1$ , the order of the truncation error of the ADI method is  $h^2 + \Delta t^2 = (0.1)^2 + (0.01)^2 = 0.0101$ . Cutting the mesh size in half gives error on the order of  $(0.05)^2 + (0.01)^2 = 0.0026$ . The expected ratio of error, then, is  $R = 0.0101/0.0026 = 3.9$ . Figures 2 and 3 show the error ratio is actually  $R = 1.55e-10/3.27e-11 = 4.7$ . Thus the actual improvement in error due to halving the mesh size is about what was expected.

### Oscillatory Solutions

In Chapter 3, stability was examined using the coefficient method. A region of stable oscillations was predicted for the ADI and CN methods. As predicted, the calculations resulted in ADI and CN oscillations for certain values of time step. In some cases, the errors resulting from the oscillations were large enough to render the solution useless for most engineering applications.

### Problem #1 Oscillations

The first problem was of limited usefulness, but did reveal stable oscillations for the CN and ADI solutions. A sample of these oscillations is presented in Figure 8, along with the IM and analytical solutions. The decrease of error with time, indicating stability, is documented in Figure 9. At this value of time step and  $r$ , the EX method was unstable. Also, these oscillations are not symmetric at all four corners. All observed oscillations for this problem began with completely symmetric oscillations, but as time progressed, the nature of the problem (with the solution going to zero) caused the unsymmetric behavior. In all cases, the IM method was stable and did not oscillate.

### Problem #2 ADI Oscillations

The second problem more closely resembles an engineering problem and is much more useful for examining errors caused by oscillations. Figure 10 shows the ADI and analytical solutions for two different times, with a large value of  $r$  for which stable oscillations are predicted. It is clear that the oscillations decreased as time progressed.

Figure 11 confirms that the errors decrease with time, so the solution is shown to be oscillatory but stable. Figure 11 also shows the oscillations induced errors on the order of  $10^0 - 100^0$ , too great an error for most engineering applications.

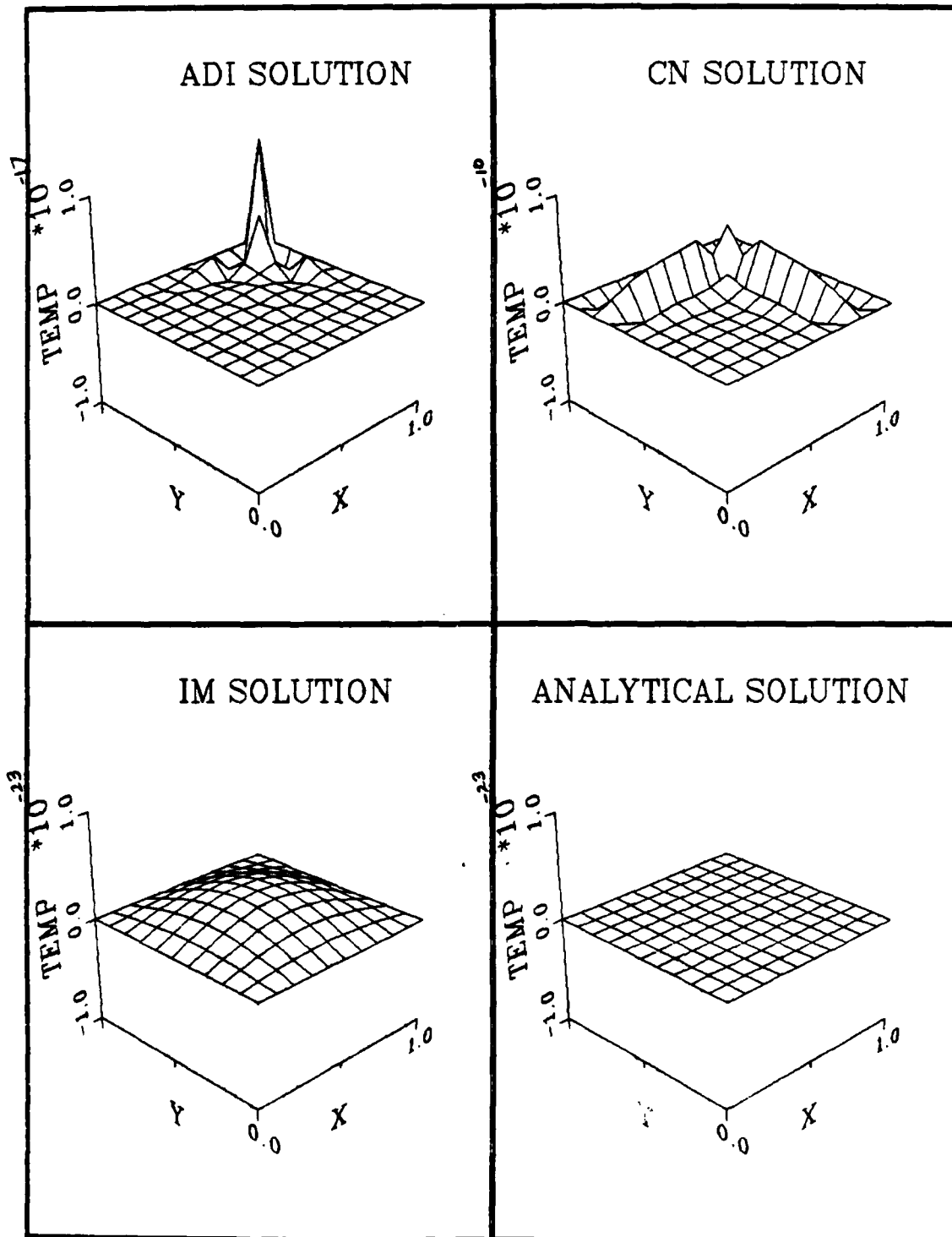


Figure 8. Numerical Solutions Problem #1  
 Time=5.0  $\Delta t=0.1$   $h=0.1$   $r=\Delta t/h^2=10.0$

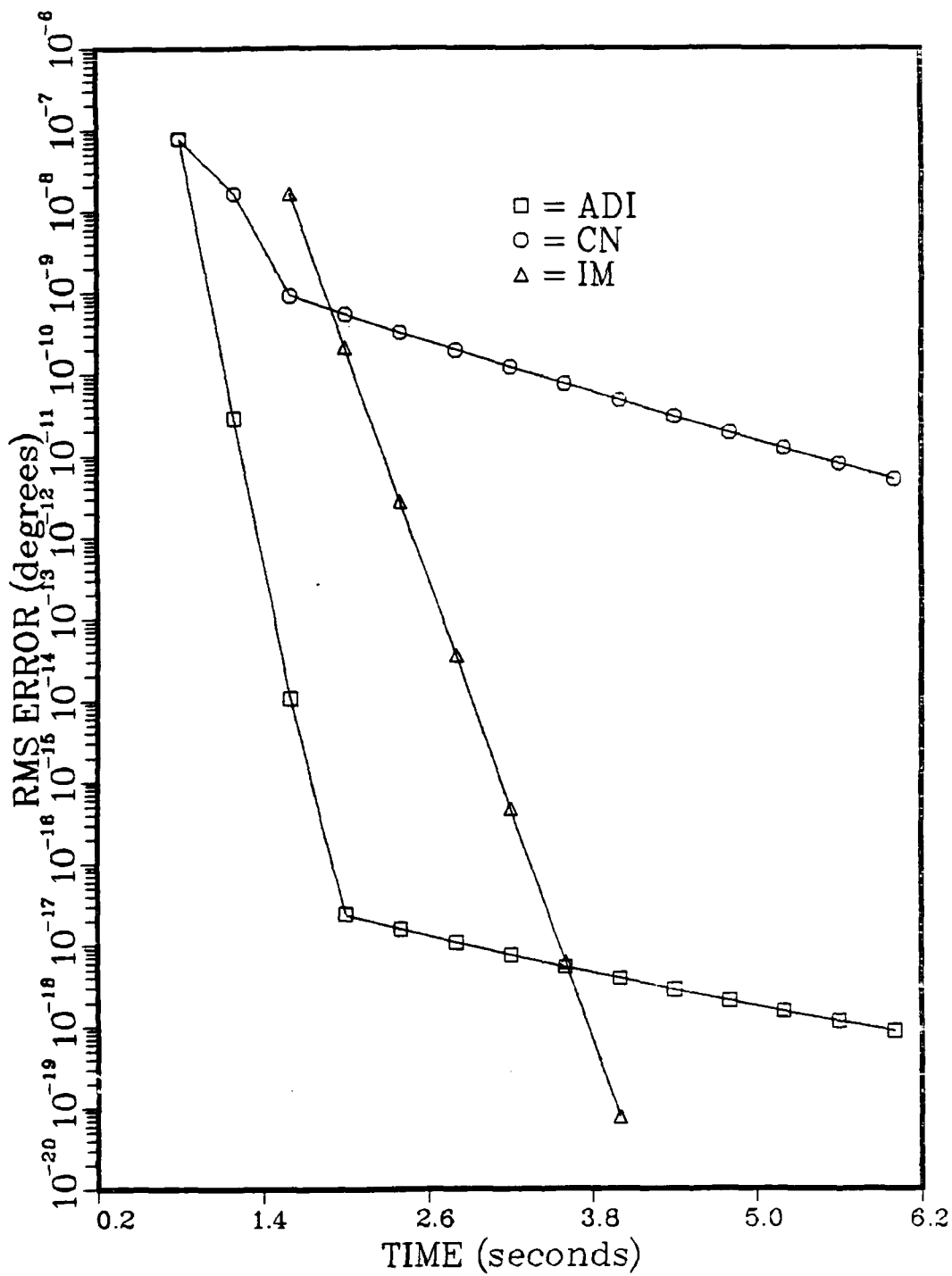


Figure 9. Error Progression With Time Problem #1  
 $\Delta t=0.1$   $h=0.1$   $r=\Delta t/h^2=10.0$

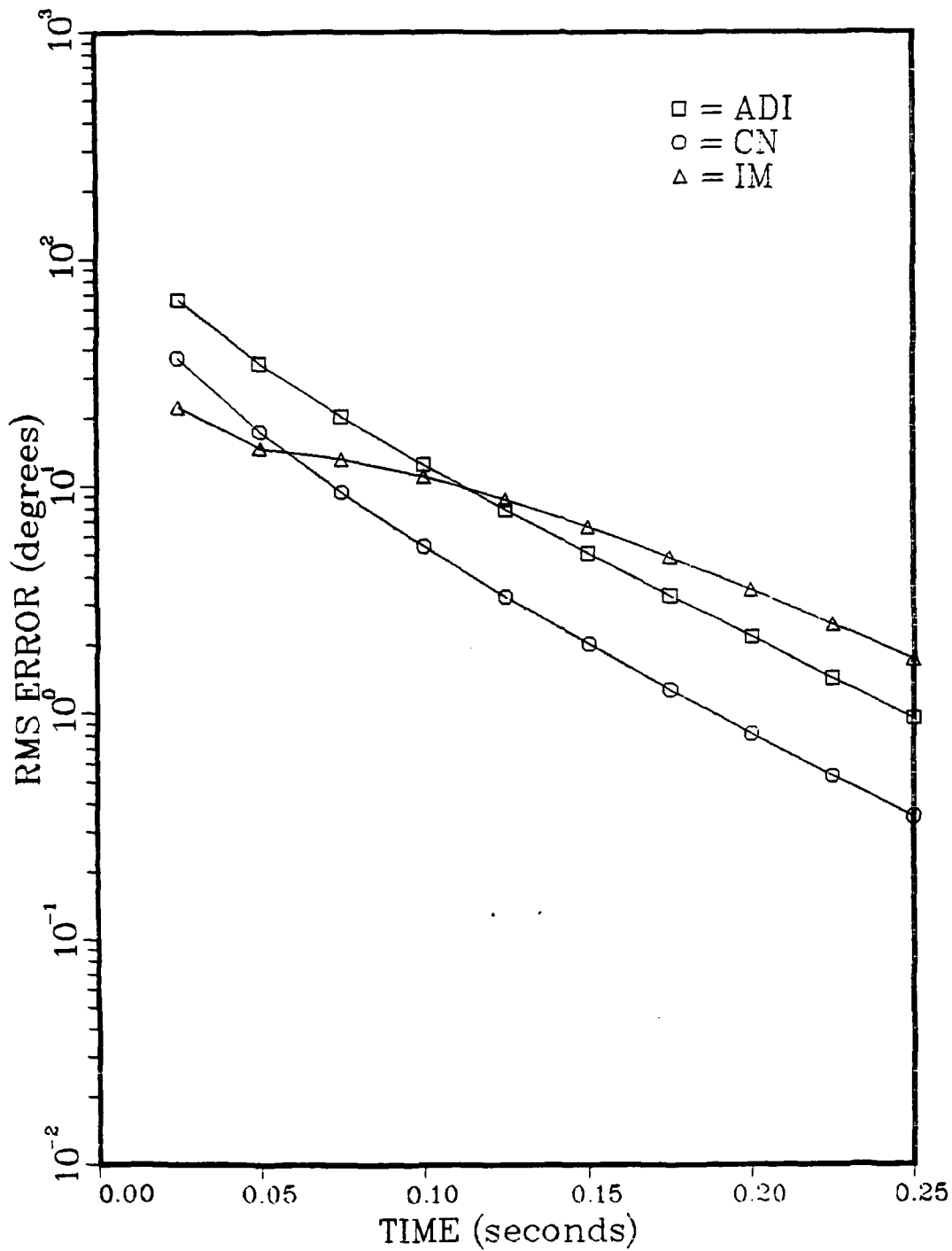


Figure 21. Error Progression with Time Problem #2  
 $\Delta t=0.0125$   $h=0.05$   $r=\Delta t/h^2=5.0$

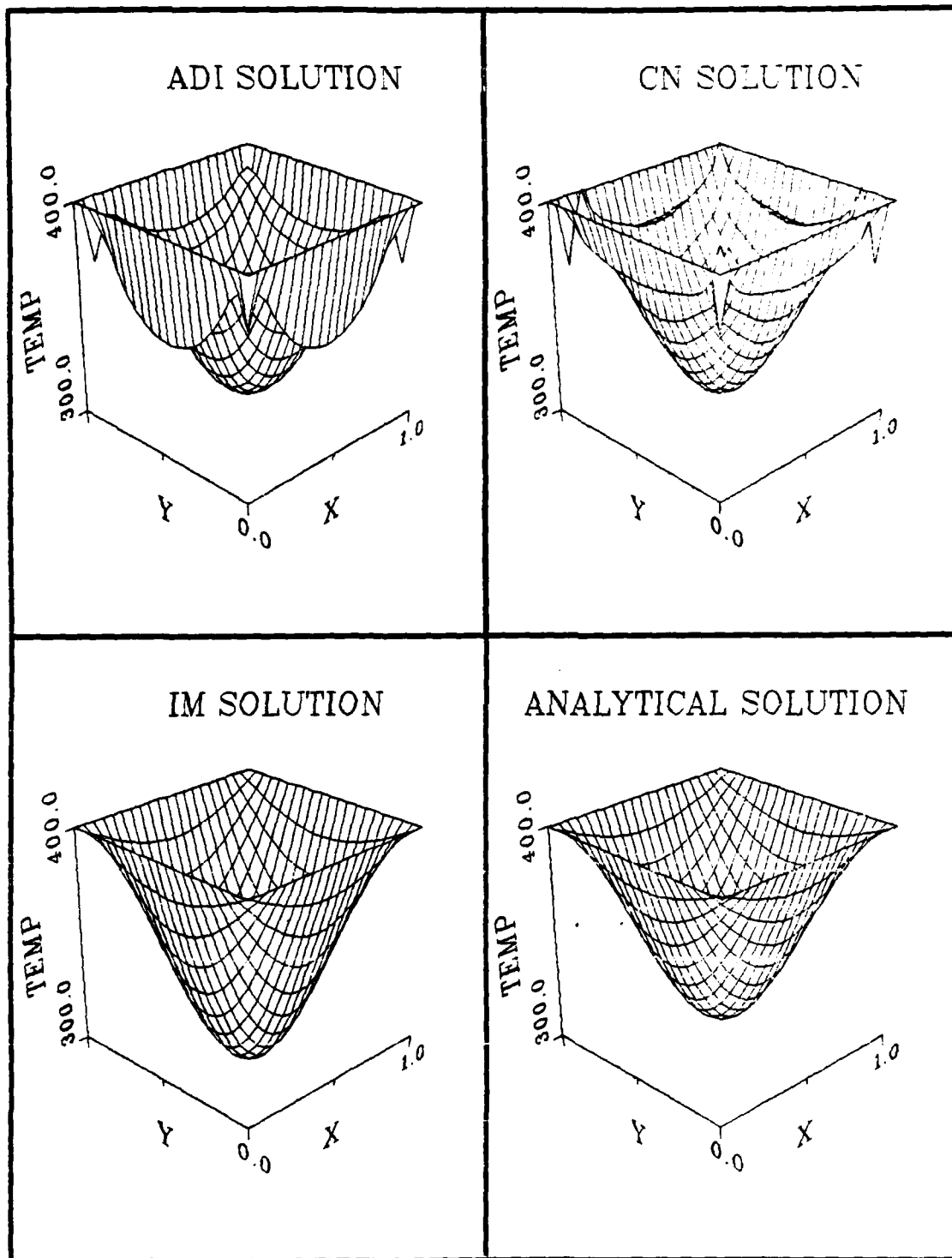


Figure 20. Numerical Solutions Problem #2  
 Time=0.1  $\Delta t=0.0125$   $h=0.05$   $r=\Delta t/h^2=5.0$

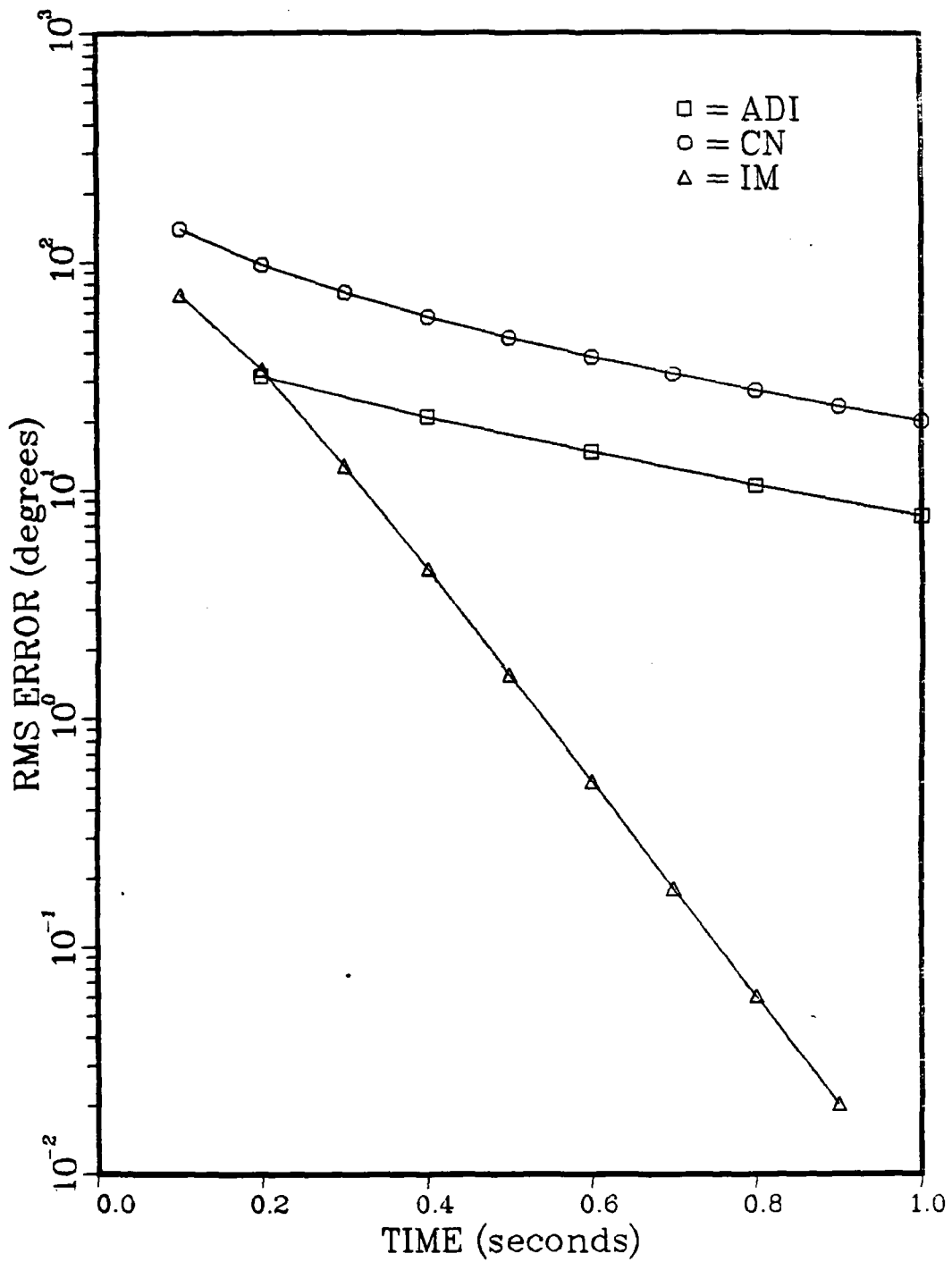


Figure 19. Error Progression With Time Problem #2  
 $\Delta t=0.1$   $h=0.1$   $r=\Delta t/h^2=10.0$

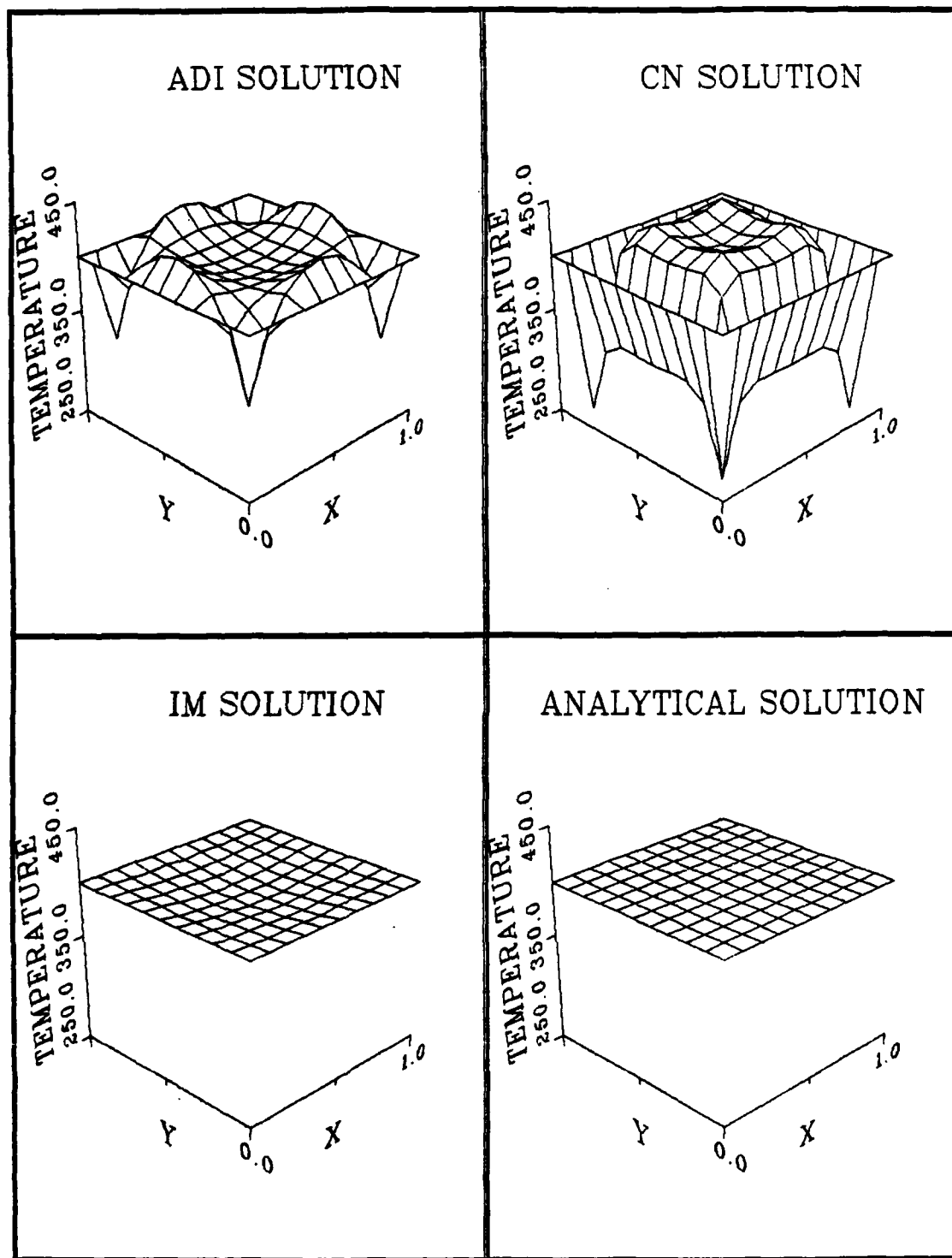


Figure 18. Numerical Solutions Problem #2  
 Time=0.4  $\Delta t=0.1$   $h=0.1$   $r=\Delta t/h^2=10.0$

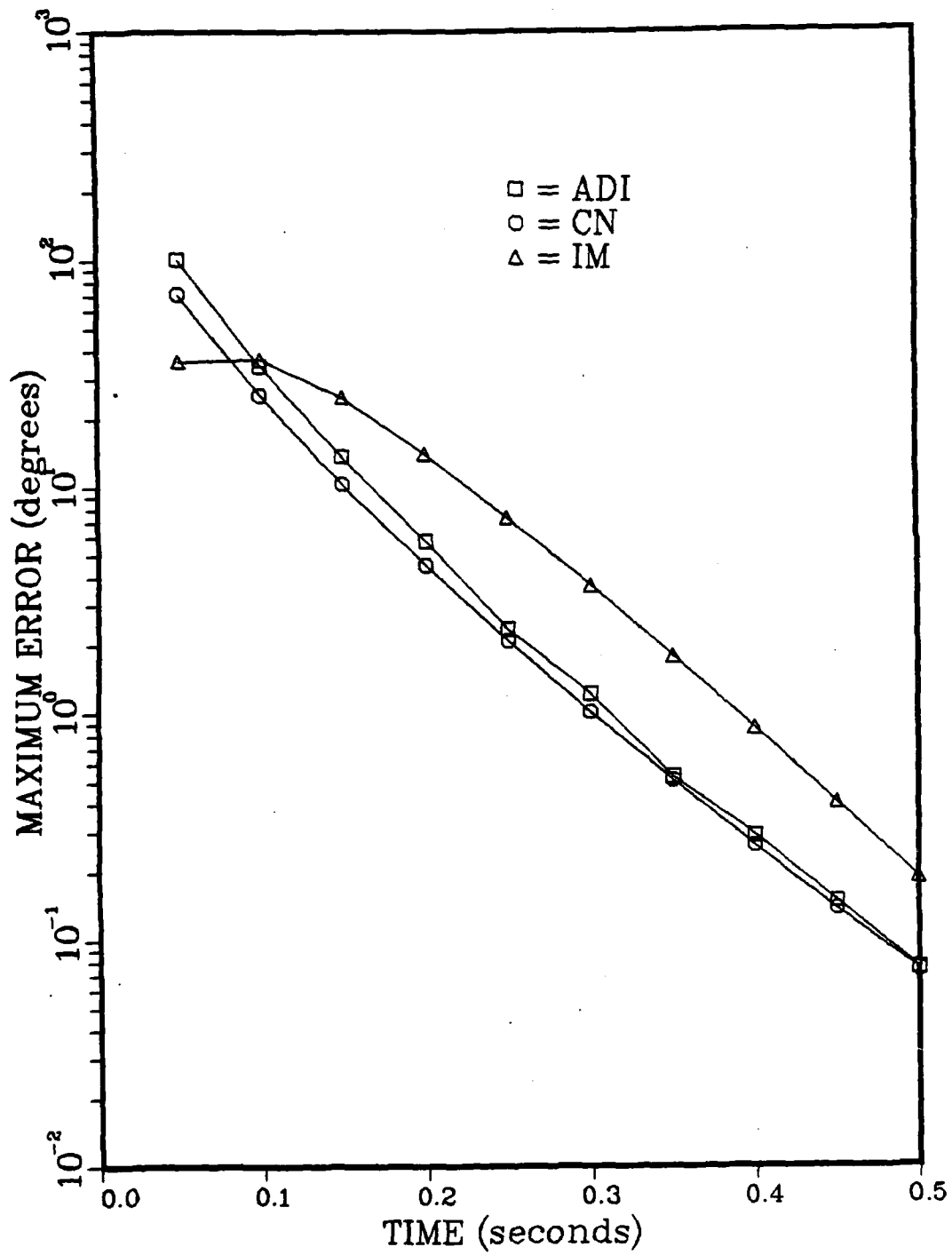


Figure 17. Error Progression With Time Problem #2  
 $\Delta t=0.025$   $h=0.1$   $r=\Delta t/h^2=2.5$

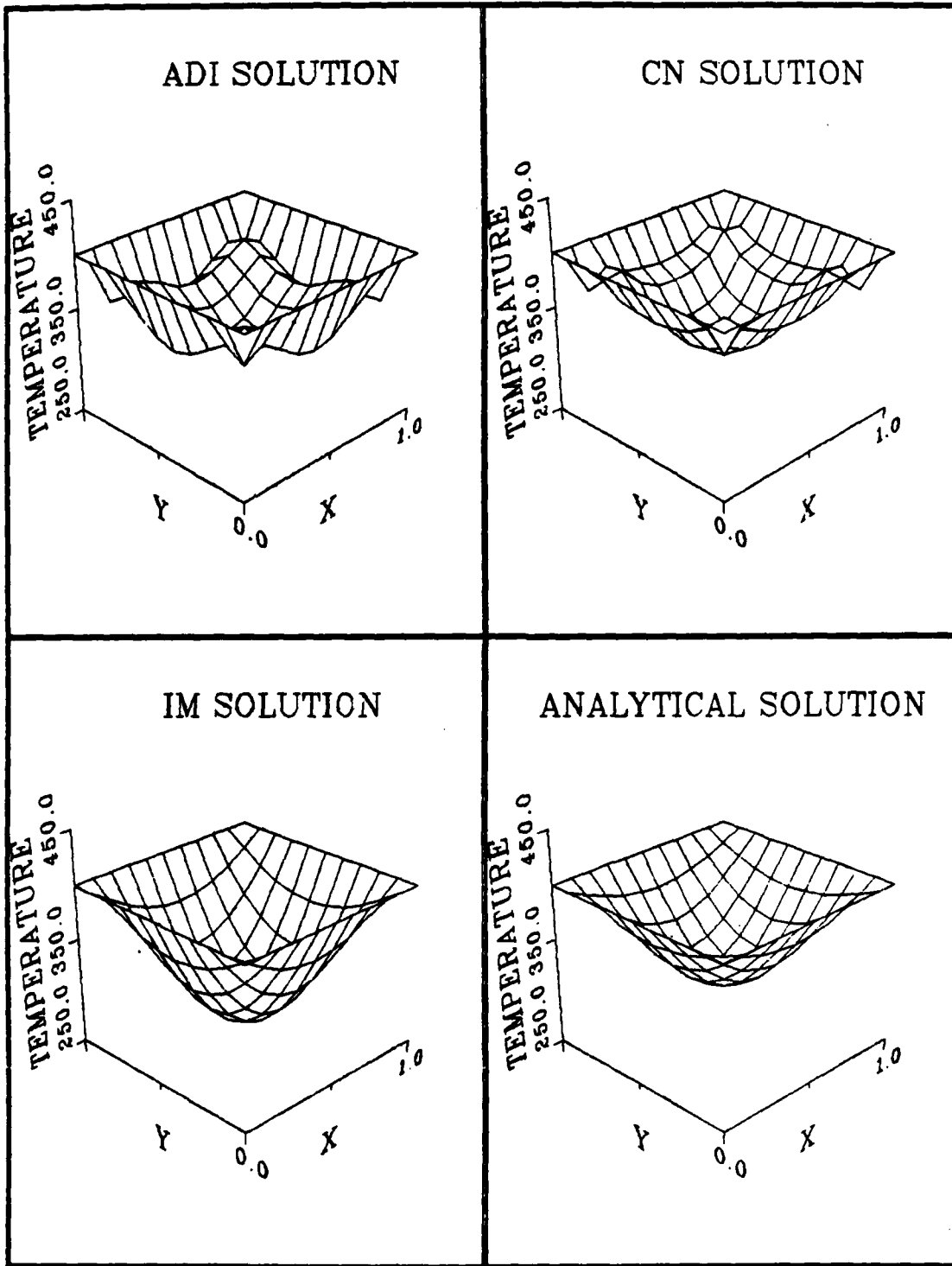


Figure 16. Numerical Solutions Problem #2  
 Time=0.1  $\Delta t=0.025$   $h=0.1$   $r=\Delta t/h^2=2.5$

Figure 16 shows the solutions computed with the ADI, CN, and IM methods for a value of  $r = 2.5$ . Note that this is in the oscillatory region, so the unstable EX method gave no solution. As predicted for this value of  $r$ , the ADI and CN methods resulted in oscillations and the IM method did not. To see if these oscillations are stable, the errors are plotted against time in Figure 17. Clearly the error decreases with time, so all three methods are stable.

Using a larger time step which gives a value of  $r = 10$ , Figure 18 again reveals oscillatory behavior for the ADI and CN methods. Figure 19 shows that the error decreases with time, so the methods are stable. For a finer mesh with  $h = 0.05$ , Figure 20 shows another example of oscillations, this time with a value of  $r = 5.0$ . Figure 21 again demonstrates that the methods are stable, as the error decreases with time.

To examine the effects of the CN oscillations, the maximum error for the CN solutions for different values of  $r$  in the oscillatory region are plotted in Figures 22 and 23. As expected, the larger the time step (and, therefore, the larger  $r$  is), the larger the error. As with the ADI method (Figures 14 and 15), these figures show that in some cases the method can be used despite oscillations. Like the ADI method, if an accuracy criteria of maximum error less than  $1^\circ$  is used, values of  $r$  less than two are usable, values of  $r$  of 4 - 5 marginal, and  $r = 10$  is unusable. Compared to the ADI solutions (Figures 14 and 15), the CN is seen to have about the same amount of oscillations as the ADI methods for small  $r$ , and greater error at large  $r$ .

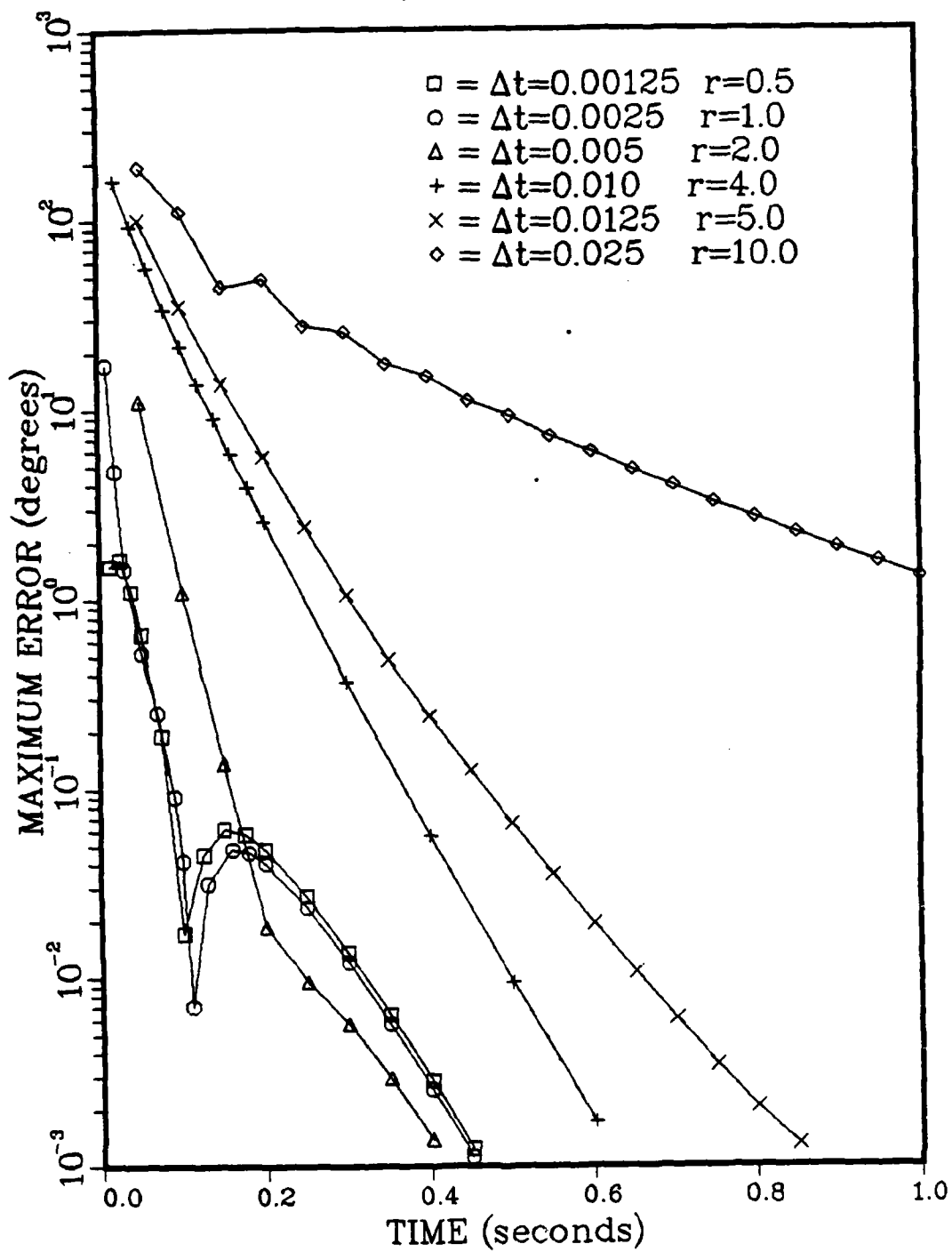


Figure 15. ADI Solutions Problem #2  $h=0.05$   
 Maximum Error vs Time For Various  
 Values Of  $r$  In The Oscillatory Region

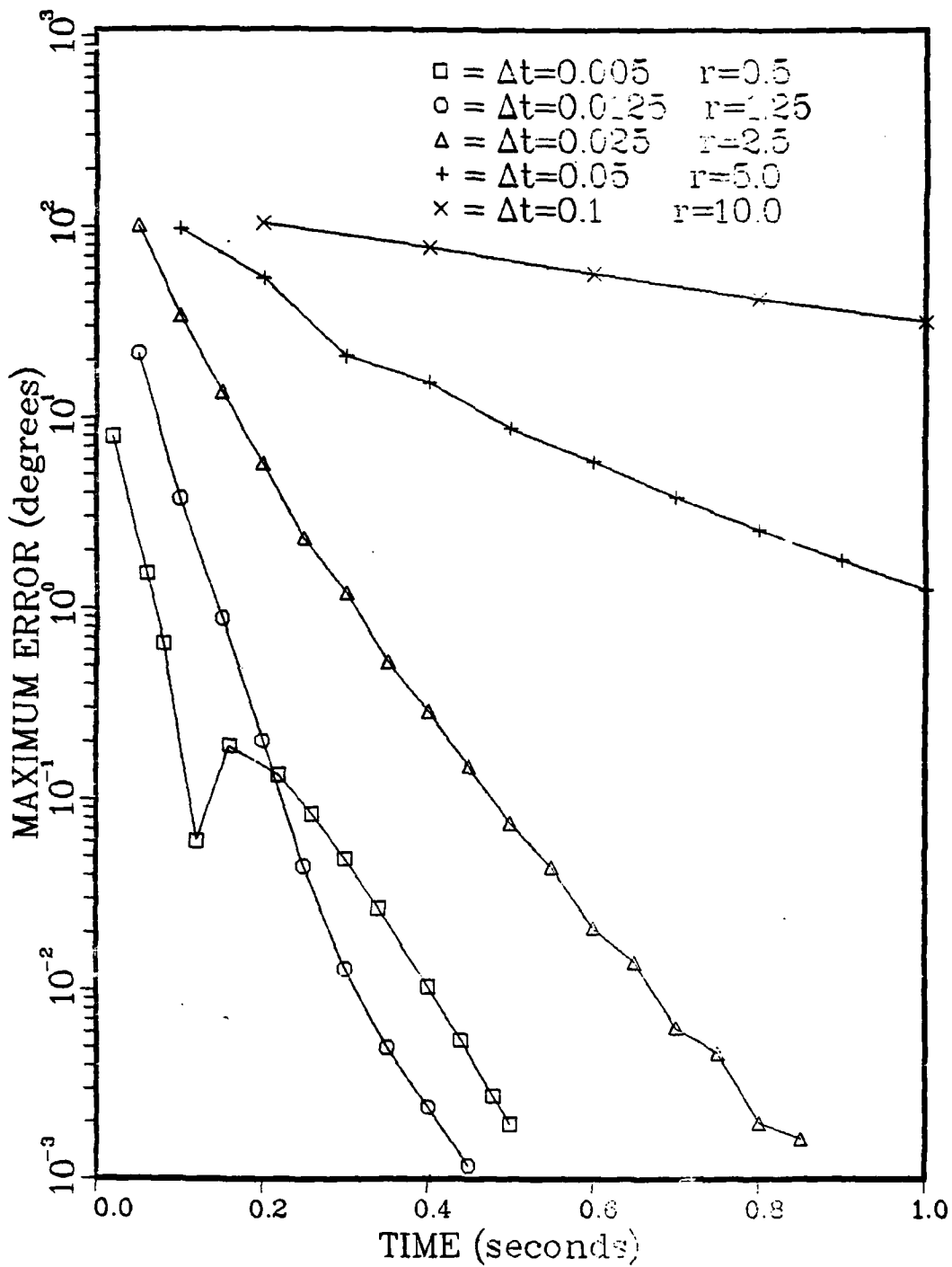


Figure 14. ADI Solutions Problem #2  $h=0.1$   
 Maximum Error vs Time For Various  
 Values Of  $r$  In The Oscillatory Region

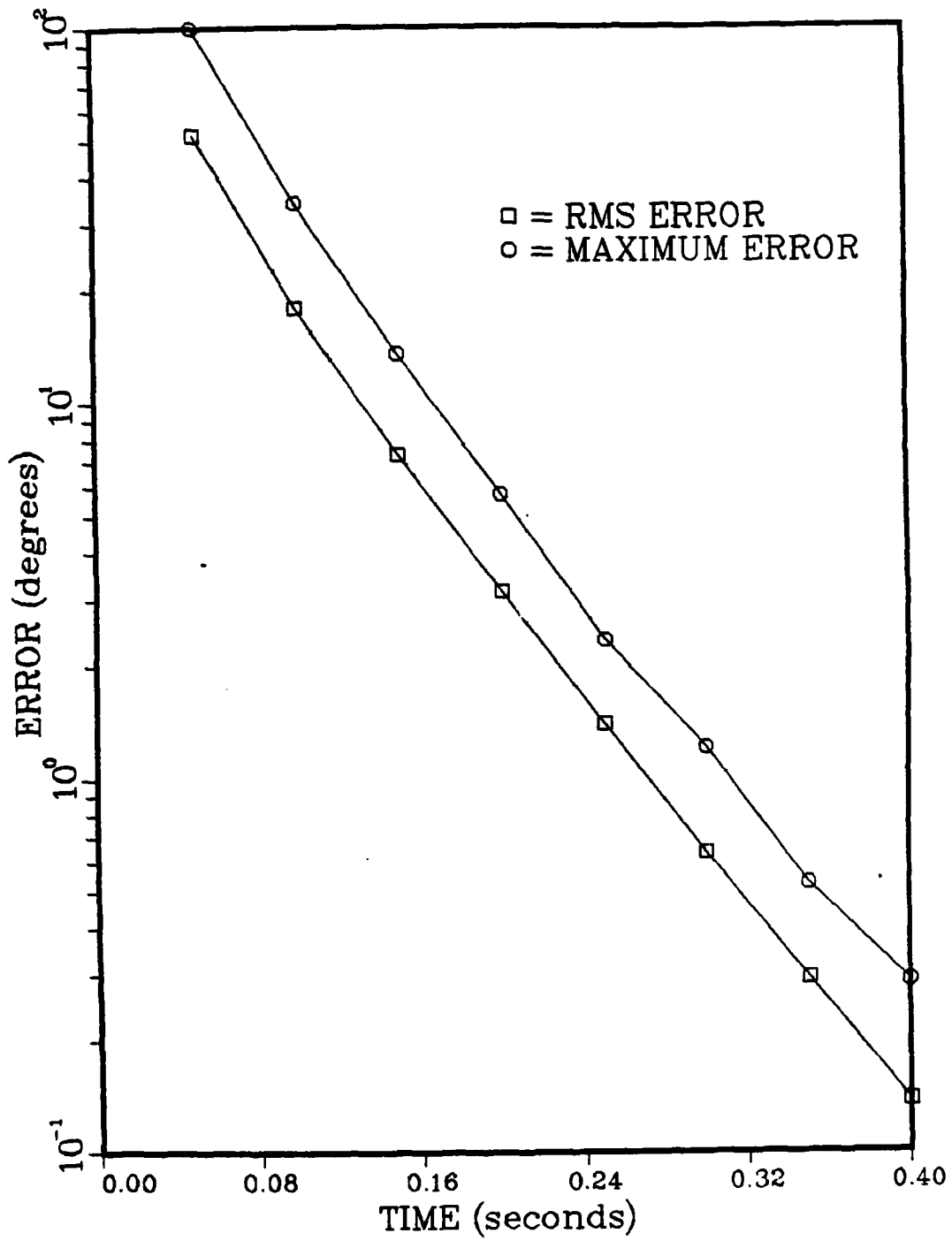


Figure 13. Error Progression With Time ADI Problem #2  
 $\Delta t=0.025$   $h=0.1$   $r=\Delta t/h^2=2.5$

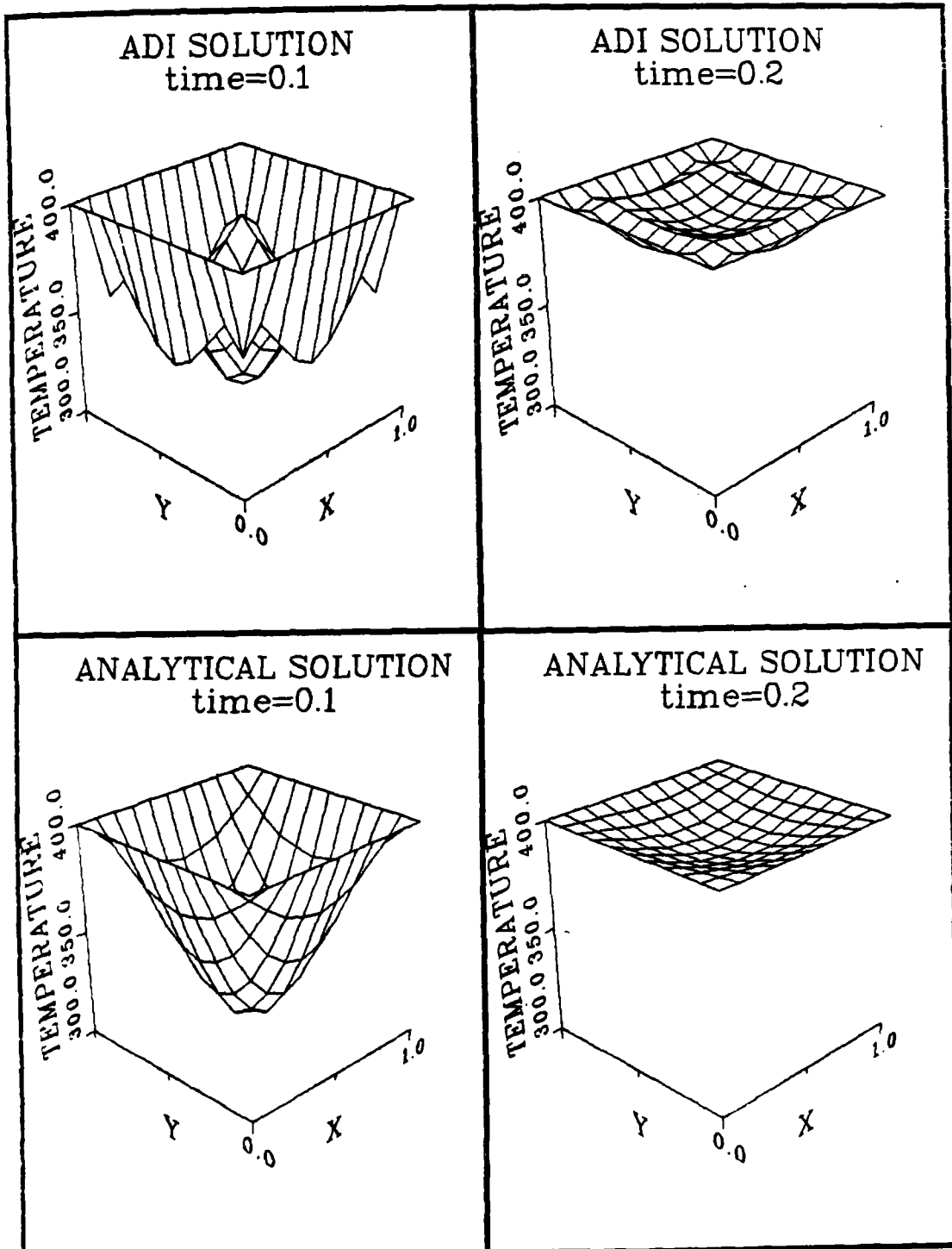


Figure 12. ADI and Analytical Solutions Problem #2  
 $\Delta t=0.025$   $h=0.1$   $r=\Delta t/h^2=2.5$

For a smaller time step and, therefore, a smaller value of  $r$  (still in the oscillatory region), Figure 12 shows the ADI and analytical solutions at two different times. Again, the error decreases with time, as can be seen in Figure 12 and confirmed in Figure 13. In this case, the errors at times greater than about 0.3 seconds are on the order of  $1^\circ$ , and so may be useful for engineering applications.

The ADI method also gives oscillatory solutions for other values of  $r > 1/2$ . The oscillations are sometimes dominated by the other errors and cannot be observed in the solution. Generally, the greater the value of  $r$ , the more severe the oscillations. For all cases of oscillatory solutions, it was found that the error decreased with time, so stability was maintained.

Figures 14 and 15 show the maximum error as time progresses for different values of  $r$  for which oscillations are predicted. Figure 14 is for a mesh spacing of  $h = 0.1$  and Figure 15 is for  $h = 0.05$ . As time increases, the error decreases and the oscillations damp out. It is seen in these figures, however, that at early times the error is large. If the requirement for accuracy in an engineering problem was for the maximum error at any point to be less than  $1^\circ$ , then Figures 14 and 15 show that values of  $r$  of 2 or less may be usable, values of  $r$  of 4 - 5 marginal, and  $r = 10$  unusable. Also, the longer the time of interest, the larger the time step (and thus larger  $r$ ) that can be used since with enough time, all the errors decrease substantially.

#### CN and IM Oscillatory Results

As discussed in Chapter 3, the CN method may have stable oscillations and the IM method is expected to always be stable without oscillations.

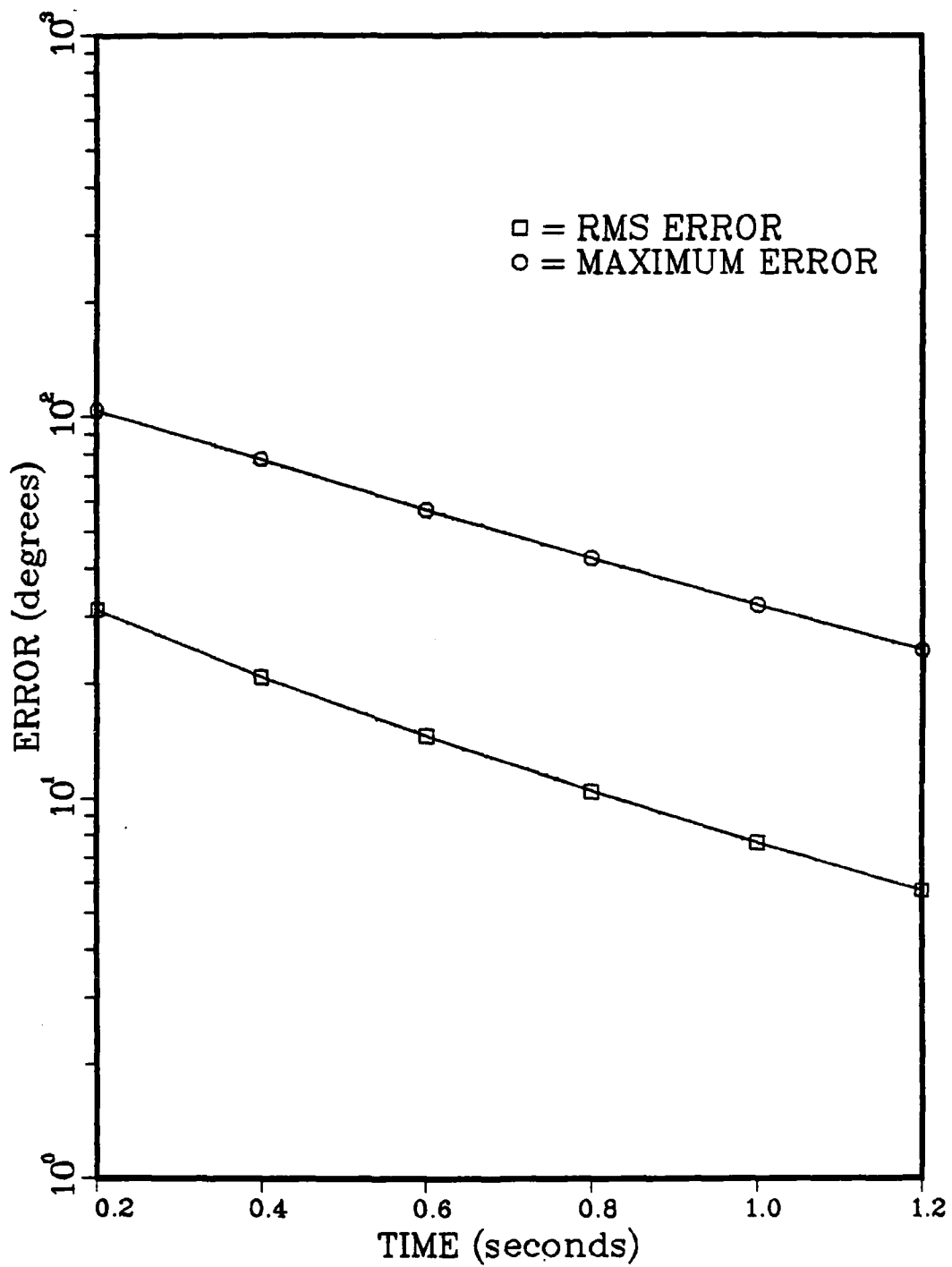


Figure 11. Error Progression With Time ADI Problem #2  
 $\Delta t=0.1$   $h=0.1$   $r=\Delta t/h^2=10.0$

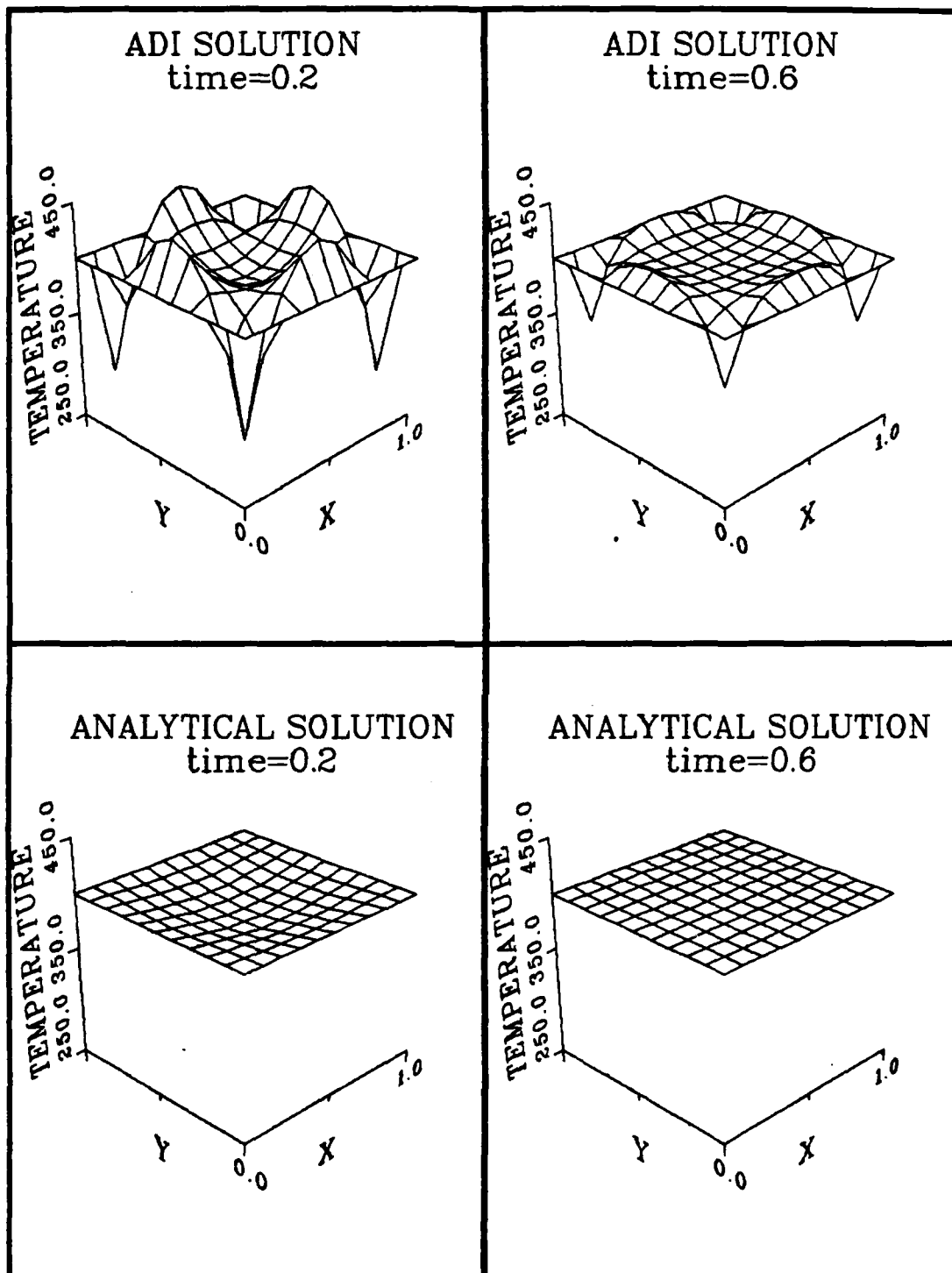


Figure 10. ADI And Analytical Solutions Problem #2  
 $\Delta t=0.1$   $h=0.1$   $r=\Delta t/h^2=10.0$

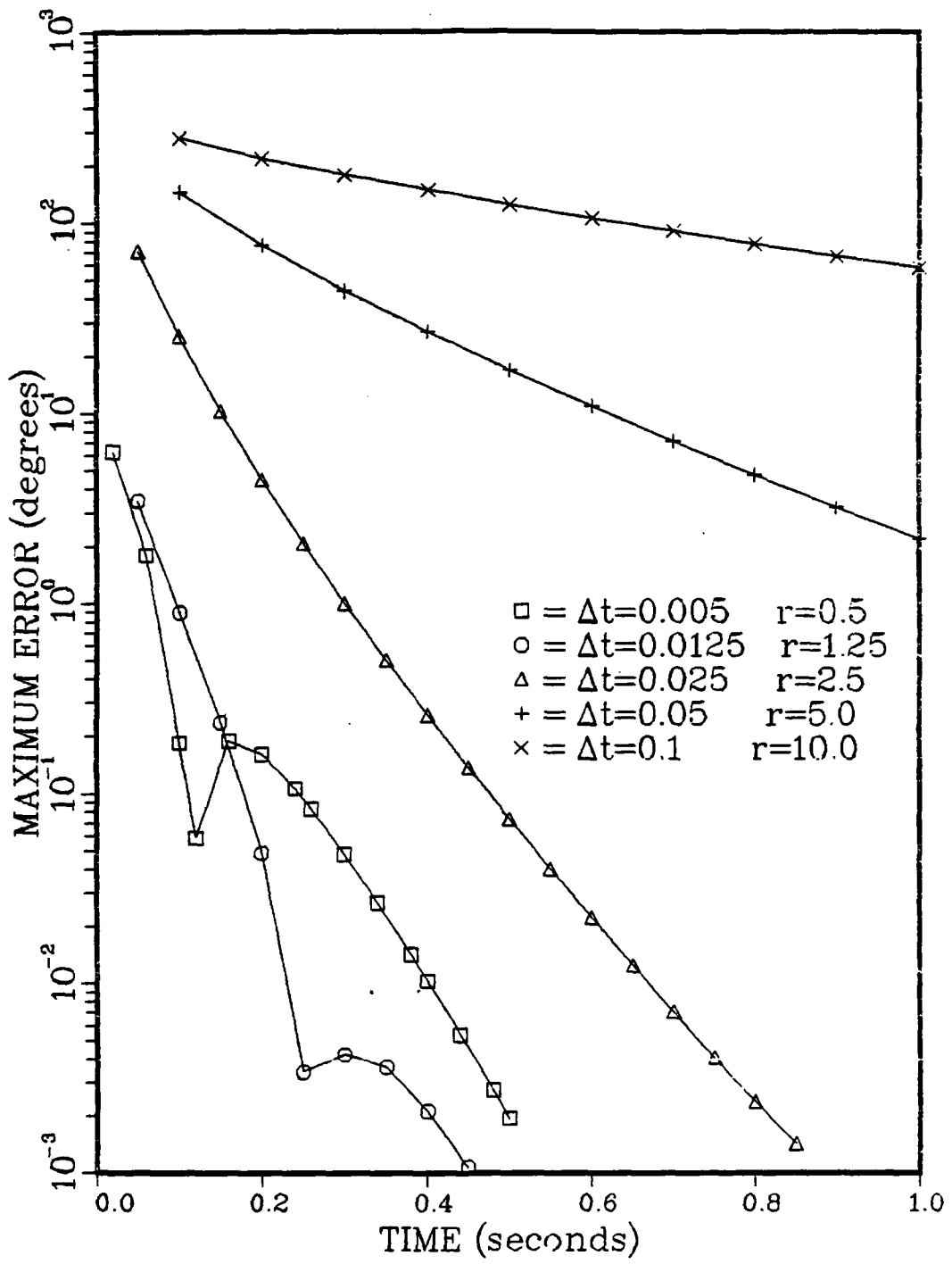


Figure 22. CN Solutions Problem #2  $h=0.1$   
 Maximum Error vs Time For Various  
 Values Of  $r$  In The Oscillatory Region

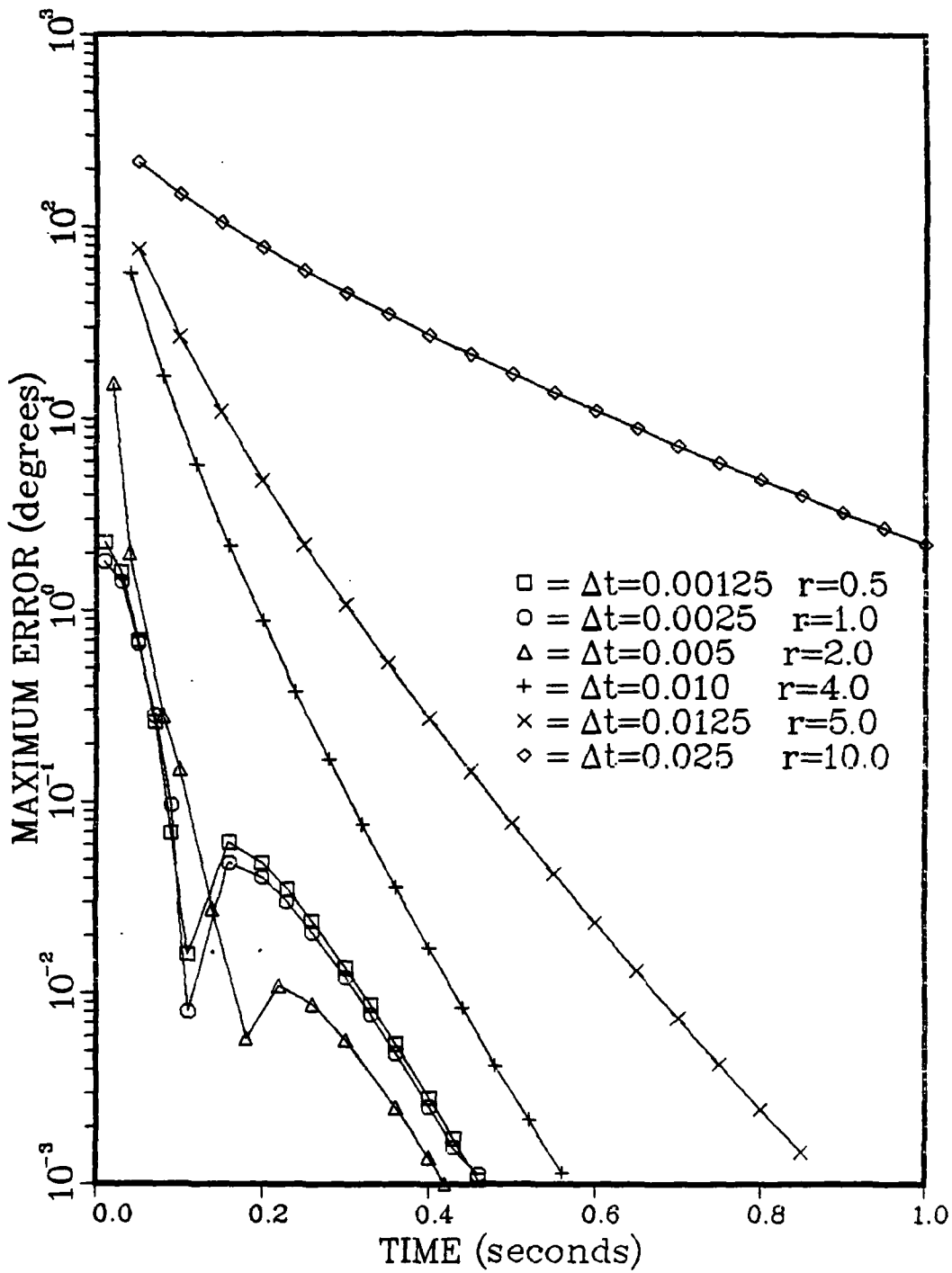


Figure 23. CN Solutions Problem #2  $h=0.05$   
 Maximum Error vs Time For Various  
 Values Of  $r$  In The Oscillatory Region

### Summary of Oscillations

Dozens of cases with different mesh spacing and time steps were run. In all the cases, behavior was as predicted. For values of  $r$  greater than  $1/2$ , both the CN and ADI methods had stable oscillations. Oscillations did not always appear, however; in some cases, the dominant error was truncation error. As  $r$  increased, so did the degree of oscillations. In every case, both oscillatory and non-oscillatory, the CN and ADI solutions were stable.

As predicted, the IM method never oscillated, even for large values of  $r$ . This non-oscillatory behavior did not ensure accuracy, however. Although more accurate than the CN and ADI methods for large time steps, often the IM solution had enough error to be unusable. In every case run, with values of  $r$  up to 200, the IM method was stable. Of course, since  $r = \alpha \Delta t / h^2$ , a different value of  $\alpha$  will affect the choice of time step.

### Computer Time Required

Central processor unit (cpu) time required for calculations was measured. For a set number of iterations, the EX method, which doesn't require solving a system of simultaneous equations, was the fastest. The ADI method, which results in a tridiagonal matrix system, was second fastest. The finer the mesh, the greater the order of the matrix, and so the greater the advantage the ADI method has over the CN and IM methods. This is seen in Figures 24-26, which give the time required to solve representative problems with a coarse mesh spacing of  $h = 0.1$ , a finer mesh of  $h = 0.05$ , and a very fine mesh of  $h = 0.025$ . The relative time advantage of the ADI method increases tremendously as the mesh is refined.

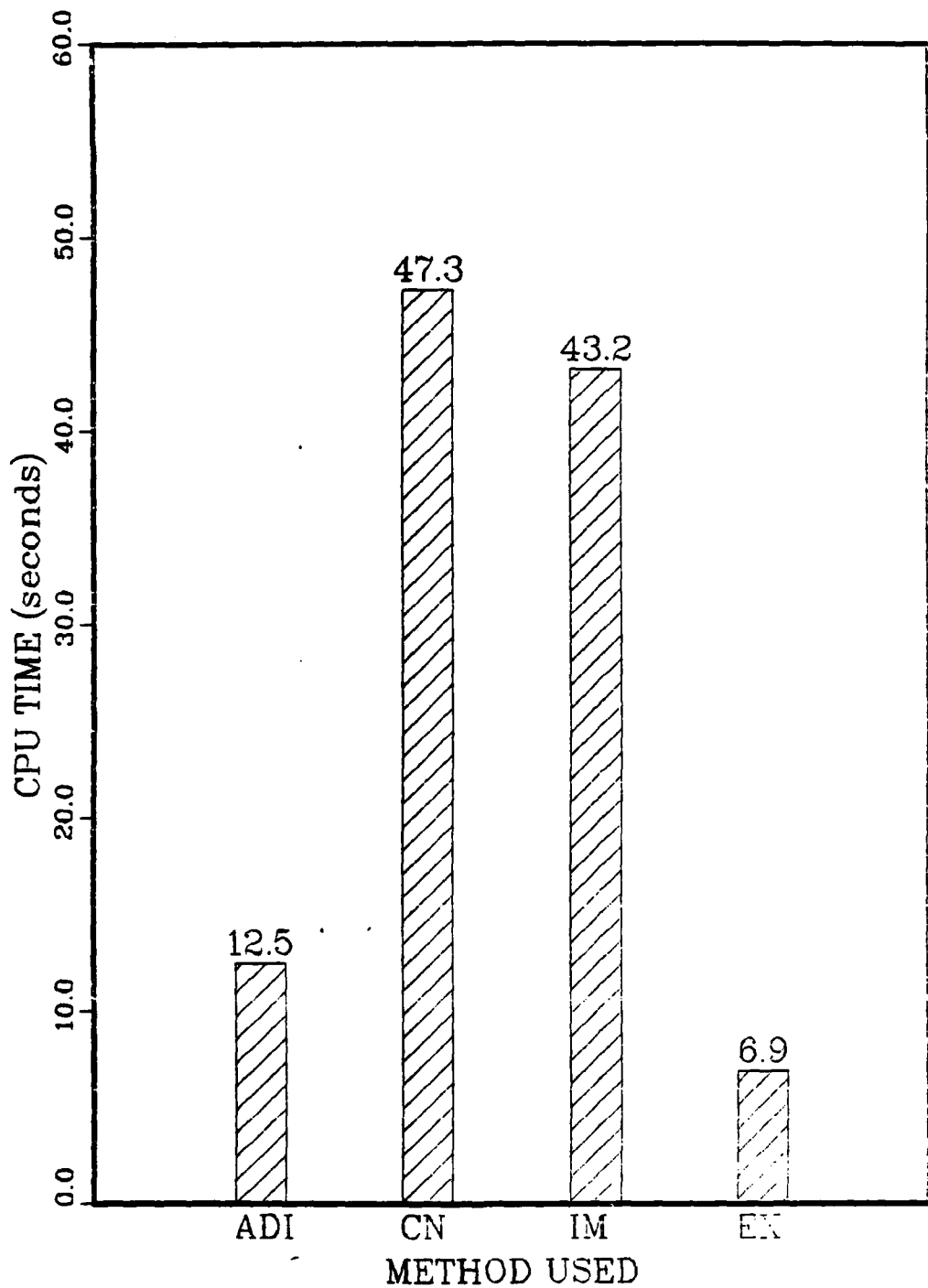


Figure 24. CPU Time Used To Solve Problem #2  
800 Time Steps of  $\Delta t=0.0005$   
Mesh Spacing  $h=0.1$  Time=0.4

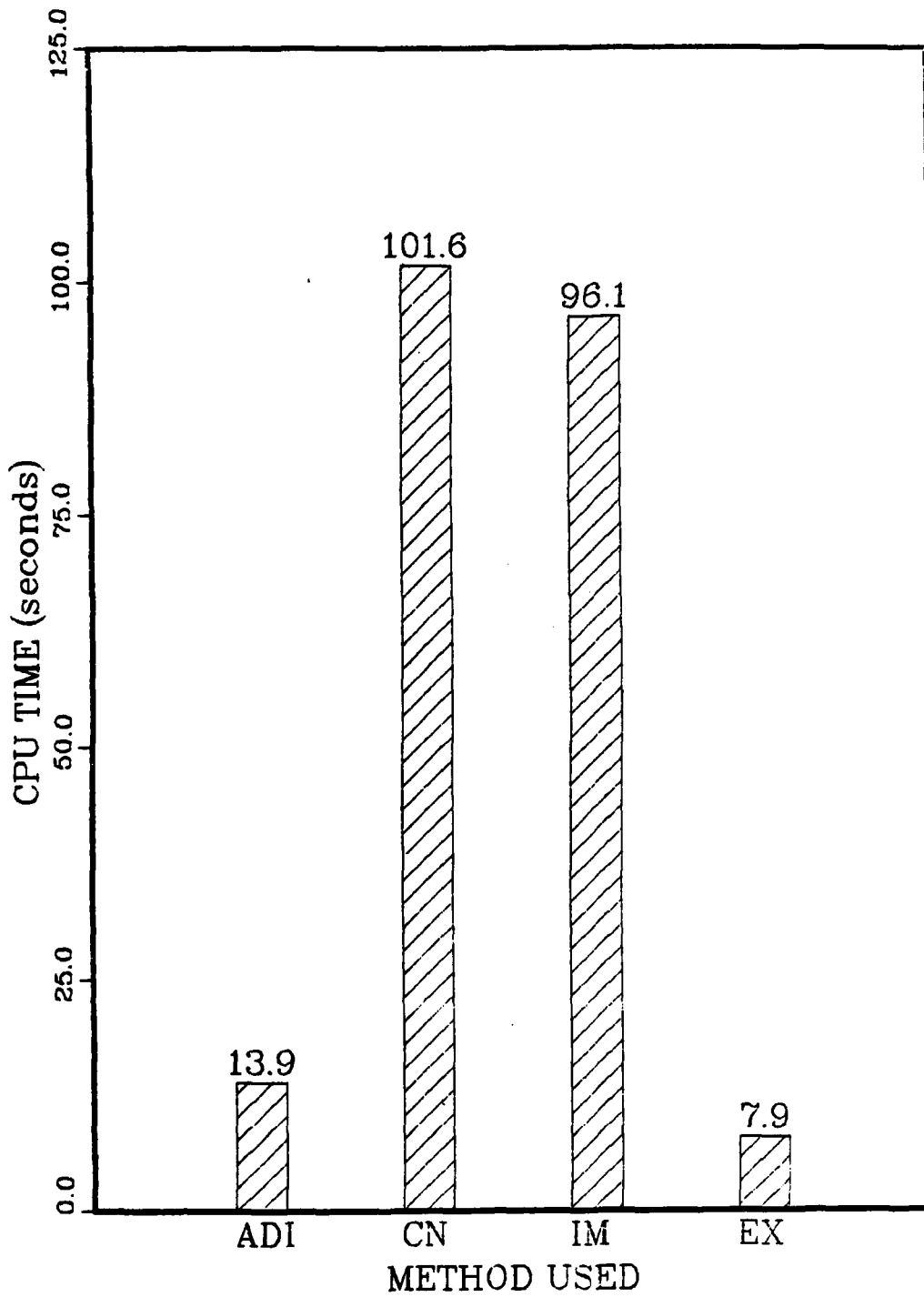


Figure 25. CPU Time Used To Solve Problem #2  
 200 Time Steps of  $\Delta t=0.0005$   
 Mesh Spacing  $h=0.05$  Time=0.1

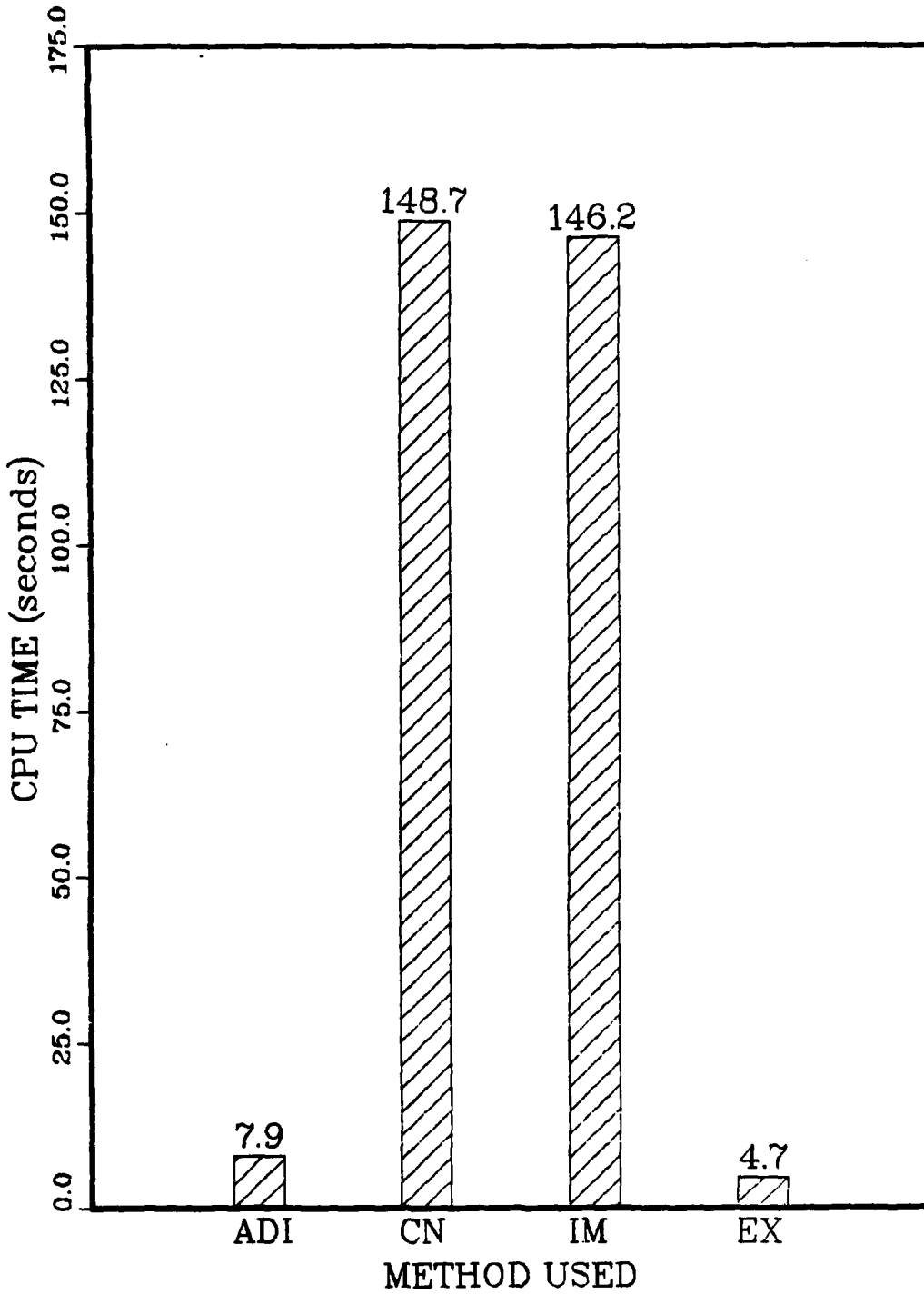


Figure 26. CPU Time Used To Solve Problem #2  
20 Time Steps of  $\Delta t=0.0001$   
Mesh Spacing  $h=0.025$  Time=0.002

The real test of time, of course, is the time required to solve a problem to the desired level of accuracy. To test this, the solution to the second problem was computed at 0.4 seconds using the largest time step for which the maximum error at any grid point was less than  $1^\circ$ . The computations were made for mesh spacings of  $h = 0.1$  and  $h = 0.05$ .

For the case of  $h = 0.1$ , the stability condition required 160 time steps with  $\Delta t = 0.0025$  for the EX method. The ADI, CN, and IM methods all reached the desired accuracy with 16 time steps of  $\Delta t = 0.025$ . Figure 27 shows that the ADI method is fastest, and the EX the slowest. For such a course grid, the difference is noticeable but relatively small. For a refined mesh spacing of  $h = 0.05$ , the ADI proved far superior. The matrix equation requiring solution has a much larger order than for  $h = 0.1$  (361 compared to 81), and so the advantage of the tridiagonal system is greater. Figure 28 shows the cpu time required for the computations. Oscillatory errors limited the CN and ADI methods to 32 time steps with  $\Delta t = 0.0125$ , and the IM required only 16 time steps with  $\Delta t = 0.025$ . Despite twice as many time steps, the ADI method was nearly four times faster than the IM method. Due to the stability condition, the EX method required 640 time steps with  $\Delta t = 0.000625$ , and was the slowest method.

In summary, the finer the mesh, the more speed advantage the ADI method has. Even with limitations on the time step due to oscillatory behavior, the ADI was the fastest method.

### Chiver's Thesis

The primary error in Chiver's thesis, which was the starting point for this study, was his misinterpretation of the results. He stated

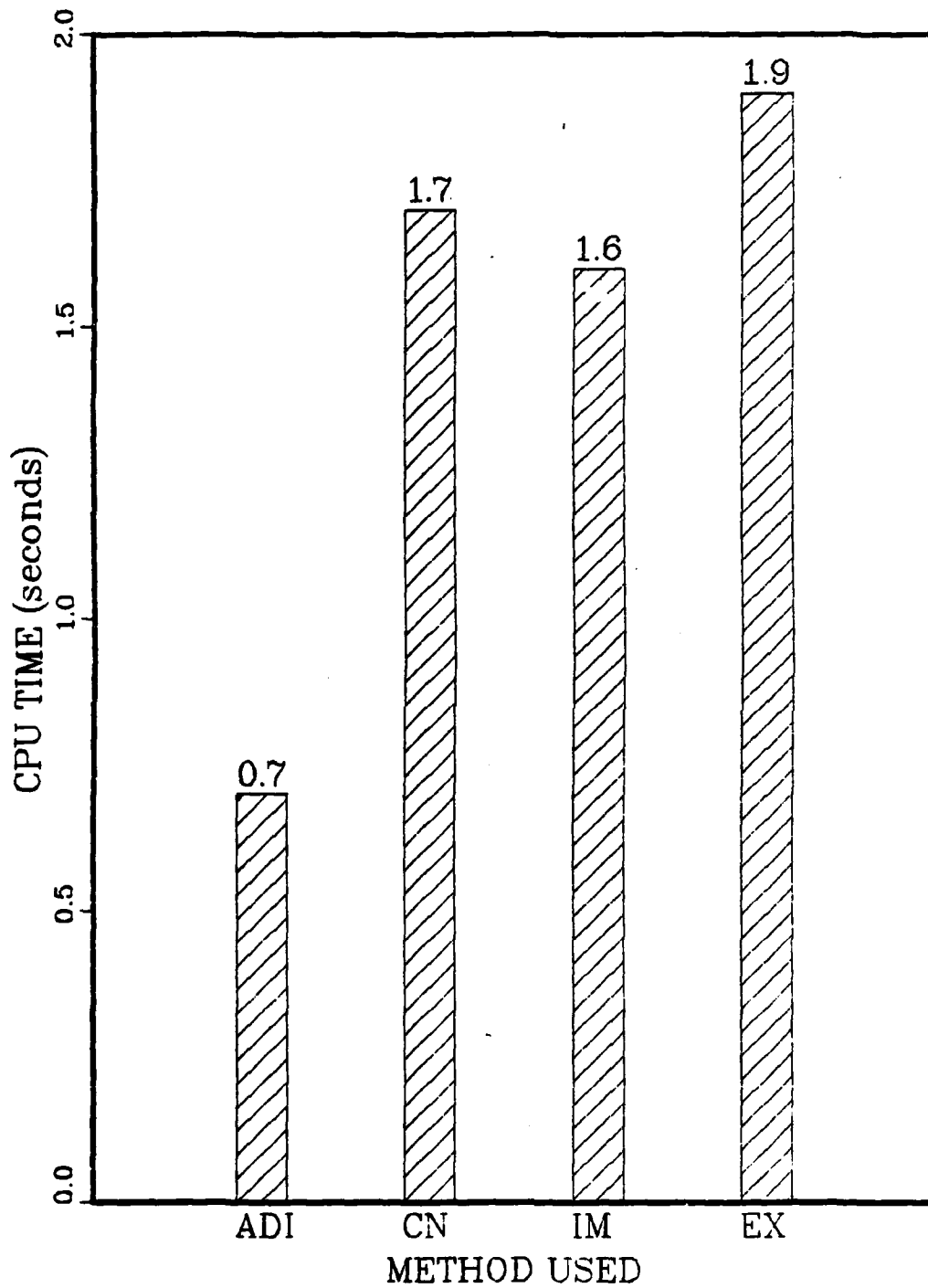


Figure 27. CPU Time Used To Solve Problem #2 To An Accuracy Of Maximum Error Less Than 1.0\*  
Time=0.4 h=0.1

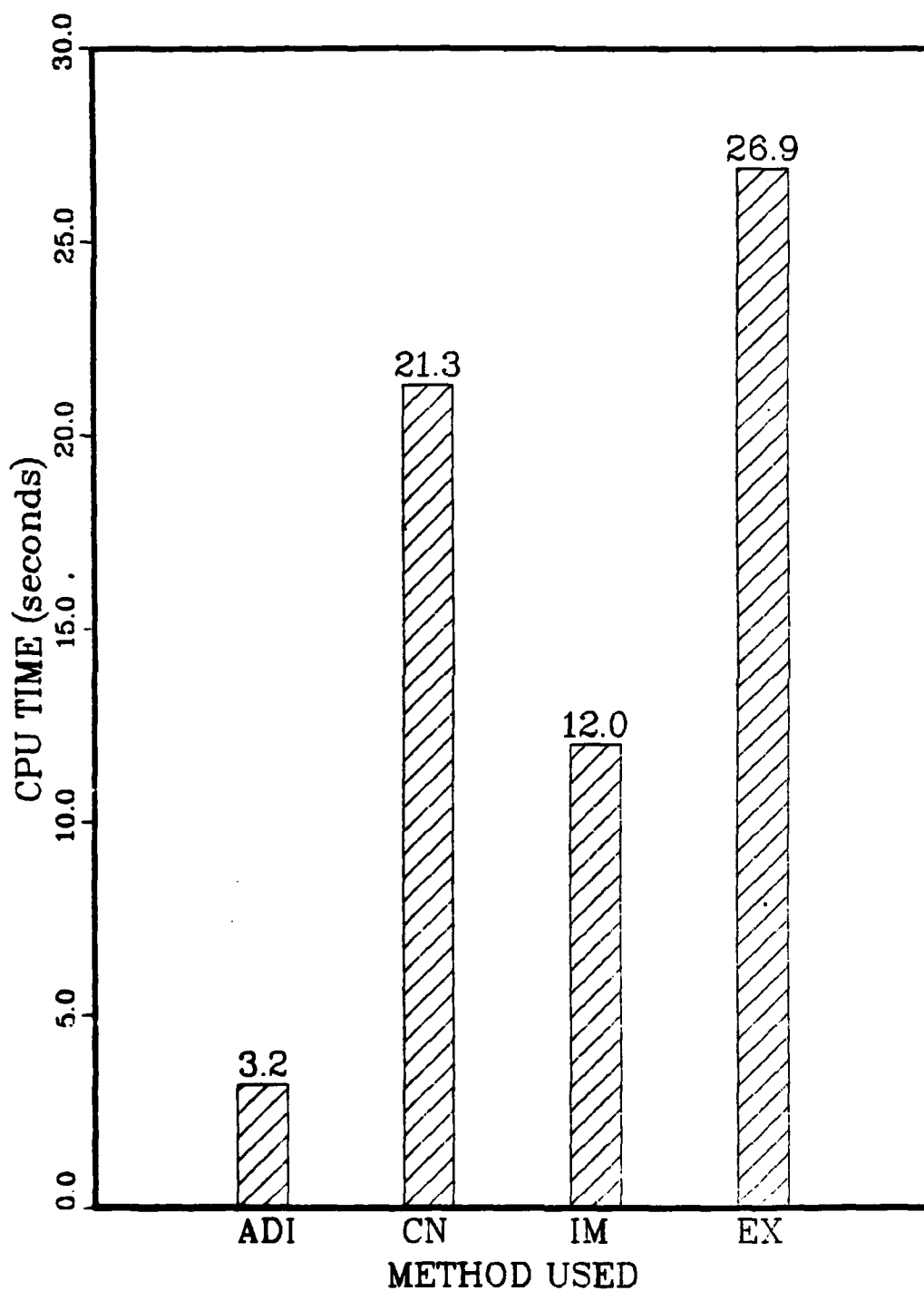


Figure 28. CPU Time Used To Solve Problem #2 To An Accuracy Of Maximum Error Less Than 1.0°  
Time=0.4 h=0.05

that his oscillatory solutions were unstable (3:47), but did not demonstrate that they were, having failed to test for stability by studying error progression with time.

Chiver's results and conclusions on the accuracy of the methods (3:42,47) are not clearly stated and are not documented well enough to support his assertions. He also gives the improper ADI truncation error (3:22) with no reference.

Small errors were the improper application of the initial condition in the derivation of the analytical solution (3:5,55) and a missing factor of two in the Crank-Nicolson formula (3:16). It is likely that these two errors were typographical.

## V. Conclusions and Recommendations

### Conclusions

The comparison of the four finite difference methods did not reveal any unexpected behavior. It was shown that certain stability and oscillatory requirements need to be met, and the results bore this out. Based on the results of this study, the following conclusions can be inferred.

1. The ADI method will yield stable oscillatory solutions with larger time steps. The oscillations may create errors large enough to make the solution unusable. Values of  $r = \alpha \Delta t / \Delta x^2 = \alpha \Delta t / \Delta y^2 = \alpha \Delta t / h^2$  greater than 2 must be used with caution, and values of  $r$  greater than 4 or 5 create oscillatory errors too large to be useful.

2. The oscillations of the CN method are similar to those of the ADI method. Useful values of  $r$  are about the same for the CN method as for the ADI.

3. For small time steps, the CN and ADI are more accurate than the IM method. The time required to run the CN and IM methods are about the same, so a decision between the CN and IM methods should consider the time step required. For large time steps, the IM method was more accurate, but the error can still be too large to be useful.

4. The ADI method, even with restrictions on time step due to oscillations, is faster than the other methods. The finer the mesh size, the greater the speed advantage of the ADI method.

5. As expected, the stability requirement severely limits the EX method to very small time steps.

## Recommendations

Based on experiences studying these methods, the following recommendations for further study are proposed.

1. Irregular geometries will permit the ADI to maintain its tridiagonal form, but the CN and IM will not have symmetric, positive definite matrices. These methods, then, will have to be solved with a slower method than Cholesky (square root) decomposition. A study of irregular geometries may reveal an even more significant speed advantage for the ADI method.

2. Two dimensional problems with Neumann or mixed boundary conditions could investigate complications caused by these boundary conditions.

3. Comparisons of the ADI with Patankar's exponential (power) method (9:32) would be useful for investigating this relatively new method.

4. Comparisons of the methods for spherical and cylindrical geometries may be useful, as these are commonly encountered geometries in engineering.

5. A comparison of the ADI with other methods in three dimensions and a study of oscillatory behavior for three dimensions could give further insight into the ADI method.

6. The stability conditions (analyzed here using the coefficient method) should be extended by using the matrix approach such as Myers (7:284-286) presents for two dimensions.

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## Vita

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SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

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|---|---|---|-----------------------------|
| 1a. REPORT SECURITY CLASSIFICATION<br><b>UNCLASSIFIED</b>   |   | 1b. RESTRICTIVE MARKINGS  |                             |
| 2a. SECURITY CLASSIFICATION AUTHORITY   |   | 3. DISTRIBUTION/AVAILABILITY OF REPORT<br><br>Approved for public release;<br>distribution unlimited. |                             |
| 2b. DECLASSIFICATION/DOWNGRADING SCHEDULE   |   |   |                             |
| 4. PERFORMING ORGANIZATION REPORT NUMBER(S)<br><b>AFIT/GNE/ENP/85M-16 //</b>  |   | 5. MONITORING ORGANIZATION REPORT NUMBER(S)   |                             |
| 6a. NAME OF PERFORMING ORGANIZATION<br><b>School of Engineering</b>   | 6b. OFFICE SYMBOL<br>(If applicable)<br><b>AFIT/EN</b>                | 7a. NAME OF MONITORING ORGANIZATION   |                             |
| 6c. ADDRESS (City, State and ZIP Code)<br><b>Air Force Institute of Technology<br/>Wright-Patterson Air Force Base, OH 45433</b>  |   | 7b. ADDRESS (City, State and ZIP Code)  |                             |
| 8a. NAME OF FUNDING/SPONSORING ORGANIZATION   | 8b. OFFICE SYMBOL<br>(If applicable)                                  | 9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER   |                             |
| 8c. ADDRESS (City, State and ZIP Code)  |   | 10. SOURCE OF FUNDING NOS.  |                             |
|   |   | PROGRAM ELEMENT NO.   | PROJECT NO.                 |
|   |   | TASK NO.  | WORK UNIT NO.               |
| 11. TITLE (Include Security Classification)<br><b>See Box 19</b>  |   |   |                             |
| ● PERSONAL AUTHOR(S)<br><b>Roger F. Kropf, B.A., Capt, USAF</b>   |   |   |                             |
| 13a. TYPE OF REPORT<br><b>MS Thesis</b>   | 13b. TIME COVERED<br>FROM _____ TO _____                              | 14. DATE OF REPORT (Yr., Mo., Day)<br><b>1985 January</b>   | 15. PAGE COUNT<br><b>60</b> |
| 16. SUPPLEMENTARY NOTATION  |   |   |                             |
| 17. COSATI CODES  |   | 18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)                     |                             |
| FIELD   | GROUP   | Numerical Analysis Heat Conduction (Diffusion)  |                             |
| <b>12</b>   | <b>01</b>   | Finite Differences Partial Differential Equations   |                             |
|   |   | Heat Transfer Mathematical Analysis   |                             |
| 19. ABSTRACT (Continue on reverse if necessary and identify by block number)  |   |   |                             |
| Title: <b>OSCILLATORY SOLUTIONS OF THE PEACEMAN-RACHFORD ALTERNATING DIRECTION IMPLICIT METHOD AND A COMPARISON OF METHODS FOR THE SOLUTION OF THE TWO DIMENSIONAL HEAT DIFFUSION EQUATION</b>  |   |   |                             |
| Thesis Chairman: <b>Dr. Bernard Kaplan, Professor of Physics</b>  |   |   |                             |
| <div style="text-align: right;"> <p>Approved for public release: LAW AFB 190-14.<br/> <i>Lynn E. Wolaver</i> 17 April 85<br/> <b>LYNN E. WOLAVER</b><br/>                     Dean for Research and Professional Development<br/>                     Air Force Institute of Technology (AIC)<br/>                     Wright-Patterson AFB OH 45433</p> </div> |   |   |                             |
| 20. DISTRIBUTION/AVAILABILITY OF ABSTRACT<br><b>UNCLASSIFIED/UNLIMITED <input checked="" type="checkbox"/> SAME AS RPT. <input type="checkbox"/> DTIC USERS <input type="checkbox"/></b>  |   | 21. ABSTRACT SECURITY CLASSIFICATION<br><b>UNCLASSIFIED</b>   |                             |
| 22a. NAME OF RESPONSIBLE INDIVIDUAL<br><b>Dr. Bernard Kaplan, Professor of Physics</b>  | 22b. TELEPHONE NUMBER<br>(Include Area Code)<br><b>(513) 255-4498</b> | 22c. OFFICE SYMBOL<br><b>AFIT/ENP</b>   |                             |

19. Abstract

The two dimensional heat diffusion equation with Dirichlet boundary conditions was solved using the fully explicit, fully implicit, Crank-Nicolson implicit, and Peaceman-Rachford alternating direction implicit (ADI) methods. Comparisons of accuracy and time requirements were made.

The possibility that the ADI method has stable oscillatory solutions with large time steps was investigated.

Results of computations revealed that the ADI has stable oscillations for large time steps, in some cases producing large enough errors to render the solution unusable. Time steps greater than twice the square of the mesh spacing divided by the thermal diffusivity must be used with care.

For small time steps, the Crank-Nicolson and ADI methods were the most accurate, and the ADI was the fastest method. The fully implicit method was the most accurate at large time steps, but the ADI, with a smaller time step to reduce the oscillatory error, was still the fastest method to reach a solution with the desired degree of accuracy.

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