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A PRIORI TIME STEP ESTIMATE FOR
SPHERICAL AND RADIAL FIELD PROBLEMS

presented by

Munawar Hussain Chaudry

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**A PRIORI TIME STEP ESTIMATE FOR SPHERICAL AND RADIAL FIELD
PROBLEMS**

By

Munawar Hussain Chaudry

A THESIS

**Submitted to
Michigan State University
In partial fulfillment of the requirements
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ABSTRACT

A PRIORI TIME STEP ESTIMATE FOR SPHERICAL AND RADIAL FIELD PROBLEMS

By

Munawar Hussain Chaudry

The objective of this study was to develop an a priori time step estimate for three single step methods used to solve the system of ordinary differential equations associated with radial and spherical field problems.

The hypothesis was that the a priori time step estimate has the general form $(\Delta t)\lambda_1 = C$ for the unconditionally stable methods and $(\Delta t)\lambda_{\max} = C$ for conditionally stable methods, where C is a constant to be determined by numerical experimentation, and λ_1 and $\lambda_{\max}$ are the lowest and highest eigenvalues in the system of ordinary differential equations.

Numerical solutions of step change problems were used to determine the coefficient C for each solution procedure in time and each type of physical problem. The final a priori time step equations developed in this study were

Central Difference Method: $(\Delta t)\lambda_1 = 0.050$ for $N \geq 11$

Backward Difference Method: $(\Delta t)\lambda_1 = 0.025$ for $N \geq 11$

Forward Difference Method: $(\Delta t)\lambda_{\max} = 1$ for $N \geq 11$

where N is number of nodes in space. Each equation can be used for both the spherical and the radial problem.

The time step equations were validated by using different problems involving a different set of material properties and boundary conditions.

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CHAPTER ONE

INTRODUCTION

No other field of mathematics has shown a recent increase in importance to the engineers comparable to that of numerical methods, nor has any other field developed as rapidly. The main reason for this evolution is the developments in digital computers. Indeed, each new generation of computers invites new tasks in numerical analysis; in this connection even a small improvement in the algorithm may have great impact on time, storage demand, accuracy and stability. This opens up a wide area of research with a view toward improving accuracy of the software/techniques used for numerical solutions.

Mathematical modeling of physical problems is an important tool in engineering analysis because it provides the opportunity to study a problem and obtain an approximate solution without going into expensive and/or time consuming physical and manufacturing processes. Most of the time-dependent problems in engineering and other branches of science are modeled in the form of *Partial Differential Equations (PDEs)*. One group of these equations is referred to as *Parabolic* or *Diffusion Equations*, which have the general form

$$c \frac{\partial U}{\partial t} = k \nabla \cdot (\nabla U) \quad (1.1)$$

where c is the capacitance coefficient, k is the conductivity/stiffness coefficient and U is the unknown variable, that is, temperature, moisture contents, pressure head, and so on.

Equation (1.1) applies to transient heat conduction in solids, gas diffusion/drying of granular materials, flow of fluids, and transport of solutes in a porous media. Many engineering and mathematics books deal with the derivation of PDEs and their solution

of the above problems. Powers (1987), Ozisik (1980), Patankar (1980), and Churchill (1987) are a few examples.

The analytical solution of a partial differential equation is very difficult to obtain for complicated field problems. Partial differential equations are often converted into a system of ODEs by applying numerical procedures like the finite element method (FEM) or the finite difference method (FDM). This conversion of time and space-dependent partial differential equations (PDEs) into a time-dependent system of ordinary differential equations (ODEs) has been discussed in many books dealing with numerical solution of PDEs; some of them are Segerlind (1984), Smith (1985), and Narasimhan (1978). A system of ODEs has the general form

$$[C] \{ \dot{U} \} + [K] \{ U \} - \{ F \} = \{ 0 \} \quad (1.1)$$

where $[C]$ is the capacitance matrix coming from the transient term in the PDEs, $[K]$ is the stiffness matrix coming from the second partial derivative with respect to space and $\{F\}$ is the forcing function. Since the forcing function, $\{F\}$, in the partial differential equations is often zero, $\{F\}$ is zero until the boundary conditions are incorporated.

Finite element or finite difference methods are used to solve (1.2) in the time domain. The FEM shows clear advantages over the FDM in the space domain in solving (1.1). This advantage, however, does not extend to the time domain, Segerlind (1984). There are numerous finite difference schemes available in the literature for solving (1.2) in the time domain. Different schemes require a different criterion to ensure numerical stability and to minimize oscillations. Various authors have discussed the solution procedures in detail but have always based the size of the *time step* on their art and experience. The authors seldom discuss the entity of *time steps* with respect to accuracy.

There is no clearly defined technique, available to select the time step needed to reach an accurate solution, particularly in two and three-dimensional problems.

Mohtar (1994) pioneered the development of empirical equations that can be used to estimate the time step required to solve (1.2) accurately when using one of Euler's forward difference method, the central difference method or the backward difference method. Mohtar developed equations to compute optimal time steps using the lowest eigenvalue of the system of ODEs as the basic parameter. He compared numerical results with analytical solutions to establish the empirical equations. Time step prediction equations were developed for one-dimensional problems and two-dimensional problems where the grid consisted of square elements. Each prediction equation given by Mohtar had the general form $\lambda_1 \Delta t = CN^b$ where λ_1 is the lowest eigenvalue for the system of ODEs, N is number of nodes in the region, C and b are empirically determined coefficients and Δt is the time step.

Tan (1995) extended the work done by Mohtar into radial coordinates, as a first step towards solving axisymmetric problems. Tan also developed empirical time step estimate with a form similar to that of Mohtar (1994). Tan pioneered the technique of using a numerical solution with a highly refined grid in space and very small time steps to generate reference values. Tan used the central difference method to generate reference values because it is second order accurate, Gear (1971). Since most complex field problems either do not have an analytical solution or the analytical solution is also based on a series solution with truncated terms, use of a numerical technique to generate a set of reference values seems appropriate. Tan's approach to generating the reference set simplifies the research procedure.

The general objective of this study is to extend of the work done by Mohtar (1994) to spherical shapes and to re-look at the radial field problems studied by Tan (1995) in the light of recent redefinition of numerical methodology.

The study of transient heat transfer in spherical as well as radial coordinates is applicable to numerous engineering problems including:

1. Development of instant heat and its study in the gun barrels, rocket tubes, and missile launchers, during and after fire. It can also assist us in determining the optimum rate of fire for a weapon.
2. The study of a gun shell, movement of projectile in the air and its terminal ballistics can be facilitated.
3. Heat dissipation study in piston, cylinder, crankshaft and other components of automotive engines exposed to combustion or frictional heat.
4. Cooling or heating of a large number of natural products and the cooling of processed products in food containers.
5. Grain drying is governed by a diffusion equation. Accurate numerical schemes are critical in the optimal design of grain dryers. Parameters such as the time needed to dry the grain and the rate of drying are critical in determining the dryer specification. The same can be said about the drying of other organic products.

The results of this study should make it easier to perform a numerical study of these subject areas.

CHAPTER TWO

REVIEW OF LITRATURE

The solution of the time dependent field problems using the finite element method was discussed only briefly in early finite element books. Heubner (1975) discusses the derivation of the capacitance matrix $[C]$, for transient heat transfer but never discusses the solution of the resulting system of ODEs. Zienkiewicz (1971) and Segerlind (1976) discussed the numerical solution of the system of ODEs but did not discuss any of the problems that can arise during the solution process and they did not compare the different types of elements.

Recent books cover the time dependent problem in more detail but may mislead an inexperienced analyst. Allaire (1985), concentrates most of his discussion on Euler's single step explicit method with one-dimensional problems. This method is known to be unstable and is not the most accurate of the single step methods. Allaire does not discuss any solution in two or three dimensions and makes no comparison between linear and quadratic elements in the one-dimensional case.

Segerlind (1984) discusses some practical aspects of the numerical methods related to oscillations and physical realities. He warns the reader to avoid using the quadratic elements because of physical reality problems but does not describe the exact significance of the errors.

Until recently, most application oriented books in heat transfer and ground water flow focused their discussion on numerical solutions using finite difference methods and did not go into detail on the finite element method. Jaluria and Torrence (1986) discuss

the three node triangular element for solving heat transfer problems but do not make any comparisons with a two-dimensional finite difference solution. These authors do not discuss any of the other types of two-dimensional elements. Their discussion could lead one into thinking that the *three node triangular element* is the most appropriate for a numerical scheme. Segerlind (1984) indicated that the four node quadrilateral element is superior to the three-node triangle. The presentation in Jaluria and Torrence (1986) can be contrasted with Patankar (1980) who limits the discussion of the finite element method to two pages and does not give any equations for the method. Patankar recommends the use of the backward difference scheme in time due to its "friendliness" for all values of time and grid size and advocates a control volume approach for the space dimensions. Patankar (1991) presented a heat transfer "computer program" called CONDUCT. This program uses the backward difference scheme to solve a heat transfer problem in time, but Patankar never discusses selecting a time step when solving transient problem.

Shih (1984) has a chapter on accuracy and error bounds. Most of his discussion analyzes the error bounds for different orders of the finite element method. Shih does not discuss any estimate for Δt when solving time dependent problems. He does, however, have a chapter on the comparison between finite difference and finite element methods. He covers smoothness of the basic function, numerical instabilities, higher order accurate discretization schemes and the incorporation of mixed boundary conditions. Shih does not give any numerical results and concludes with the statement, "*Much work remains in comparing these two powerful methods in a rigorous and conclusive manner*".

Shih (1984), Jaluria and Torrence (1986) and Segerlind (1984) avoid explicit numerical evaluation of the time step. They discuss stability and numerical oscillation

problems but none of the authors gives a procedure for estimating the time step as it relates to the accuracy of the computation. The typical scenario is to present a numerical solution procedure and compare it with an analytical solution of the PDE using one or more time step values. The authors, however, never said how they determined what numerical value of the time step to use. Dhat and Touzot (1984) comment that the time step value that eliminates stability and numerical oscillations may not produce accurate calculations. They also do not give any suggestions on how to select the time step value.

Gear (1971) and Stoer and Bulirsch (1980) discuss the mathematical approaches to determine a time step value. They define an error as being the difference between two solutions with time steps of Δt and $\Delta t/2$ and use this error to determine an appropriate step size. This approach however, does not give much information on how to select a starting value for Δt and requires two or more solutions before a time step is defined.

Myers (1977) discusses the critical time step, applicable to two-dimensional heat conduction transient problems. His discussion, however, centers on estimating the maximum eigenvalue for use in the Euler stability criterion or the Crank-Nickolson oscillation criterion of $\lambda_{\max}(\Delta t) \leq 2$ where $\lambda_{\max}$ is the maximum eigenvalue. Myers does not discuss the determination of Δt as it relates to the accuracy of the integration.

Another approach for selecting Δt is to limit the maximum change in any nodal value to a certain percent of its previous value. This approach is used in some commercial finite element software when solving nonlinear problems. This method suffers from the need to repeat the calculations if the time step is too large and also does not give any information on how to select a starting value for Δt .

Reddy (1984) has a section on time dependent problem, that is consistent with much of the mathematical literature. Reddy describes the stability in terms of the roots of the characteristic equations and the eigenvalues of the global system. Roots of that equation should be bounded by one to avoid numerical oscillations. Reddy gives a time step estimate for structural dynamics problems. He states that $\Delta t = T_{\min}/\pi$, where $T_{\min}$ is the smallest period of natural vibration associated with the approximate problem gives an accurate solution. According to Reddy, another estimate to Δt can be obtained from the condition that the smallest eigenvalue of the characteristic equation be less than one.

Smith (1985) discusses the explicit Euler's method for solving the non-dimensional form of (1.1). Smith rearranged the difference equation and defined a term $r = \delta t / (\delta x)^2$. During the discussion of stability, Smith stated that the explicit method is stable for r with values less than 0.5. The implicit Crank-Nicolson has the advantage of being stable for all values of r . Smith recommends $r = 1$ for an accurate solution for the Crank-Nicolson method. Smith also discussed convergence and stability for some time stepping schemes and gave a time step expression that satisfies both criteria. No criterion for selecting a time step based on accuracy was given. The term r defined by Smith does not include material properties since the thermal diffusivity coefficient, cp/k , was defined as one.

Allaire (1985) called Smith's r term the Courant Number. Allaire's variable included the material properties. In addition to illustrating stable and non-stable schemes, Allaire defined an oscillatory stable scheme as having spatial oscillation that eventually dies out with the solution converging to the correct steady state values. Allaire showed the following criteria to be true for the single step methods:

$0 < r \leq 0.25$ No oscillation

$0.25 < r \leq 0.5$ Oscillatory and stable

$0.5 < r$ Unstable (Euler's method only)

The solutions given by Allaire have no indication of instability for values of $r < 0.5$. Allaire discussed a “weighted explicit-implicit scheme”. His scheme reduces to the explicit method and has stability criterion of $r < 0.5$ when his parameter θ equals zero. Allaire showed that the Crank-Nickolson method and the fully implicit methods are accurate for values of r up to 1.335.

Jaluria and Torrance (1986) defined Allaire's (1985) Courant number as the Froude number, F_o . These authors suggested using values of F_o less than 0.5 for the implicit method although lower values gave better accuracy. They never give any example of what the lower values should be.

Wood and Lewis (1975) studied seven different finite difference time marching schemes. They compared methods based on an accuracy criterion. The authors related accuracy to oscillations and stability. They determined the critical non-oscillatory time step for the Crank-Nickolson (C-N) based on the maximum eigenvalue. They showed numerically that when increasing the time step beyond a critical time step, oscillations occurred. Wood and Lewis observed inaccurate values in backward difference scheme for some time step values. They did not state that accuracy is a separate consideration in the numerical solution of parabolic equations that needed to be addressed and adjusted accordingly.

Wood (1990) gives an extensive list of time stepping schemes. His list included most of the known schemes and some new ones. He studied stability, consistency, and

oscillations where the term "time step" was mentioned at several places. For many of these schemes, numerical results were tabulated using various time steps and the corresponding error was presented. The author showed that these methods were consistent with the analytical solution. Wood also refers to the use of time step adjustment where the size of the time step changes after every set of calculations but never give any formula for determining a time step value.

Ortega (1990) defined and discussed three types of errors that are all associated with the time step. The discretization (global) error, convergence error, and rounding error. He did not indicate how to define the numerical value for the time step that will minimize these errors.

Rushton and Tomlinson (1971) used the alternating direction approach as a numerical scheme. They studied stability and found that for different boundary conditions the Courant number, C , that generates accurate time steps changes. For a sudden change of pressure head on the boundary, C should be less than 1.0. For a draw down at a well, C should be less than 0.05. For a sudden change in discharge at a well, C should be less than 0.5. The authors suggest that a trial and error procedure is still required for selecting the optimal Δt value.

Henrici (1977) had an extensive discussion about the error propagation for the difference methods in solving the PDE. His theoretical treatment did not include discussion of the time step size needed for accurate results.

Williams (1980) and Fried (1979) both studied the numerical solutions of PDE and used the time step criteria that satisfied stability requirements. Williams used a term equivalent to the Courant number and stated that it should be less than 0.5. Fried used the stability criteria ($\Delta t = 2/\lambda_{\max}$).

Haghighi and Segerlind (1988) solved the coupled heat and mass transfer equations using the finite element method. They used Maadooliat's (1983) non-oscillation criteria as well as the physical reality conditions that Segerlind (1984) discussed in his book.

Nripendra and Kunze (1991) presented a finite element solution for temperature distribution in storage bin. They used the Crank-Nicolson scheme for the time domain. They presented comparisons between numerical and exact solutions. There was no mention of time step in their paper.

Irudayaraj (1991) and Irudayaraj et. al. (1990) applied the finite element method to the solution of a coupled heat and mass transfer problem. Both papers used the stability criteria for selecting the time step. There was no check whether this time step ensured accurate results. The author's calculated results did not agree with experimental data in the literature. The same stability criterion was followed by Liu et. al. (1984). These authors used a modified Runge-Kutta method to solve the parabolic system. Their work did not discuss solution accuracy.

Peraire et. al. (1988) studied the finite element solution of fluid flow. They used the Courant stability criteria of ($\Delta t \leq K \cdot h_e / (u + c)$), where c is local speed of sound, h_e is the average element length, u is the velocity, and K is a constant.

Alagusundaram, et al. (1991) applied the finite element method to model the diffusion of carbon dioxide in grain bins. Their calculated results did not compare well with the measured values. They listed several reasons for this discrepancy. They did not mention how they determined the time step. They did not state what time step value they used and did not state whether the size of the time step might be one reason for the inaccuracy of their calculation.

Cleland and Earle (1984) studied the freezing time of food material using six finite difference methods. They ensured accuracy by reducing the time step until the numerical results converged to a consistent value. They encountered a stability problem and a physical reality violation that they called "jumping" and said it was related to the latent heat. Although there is evidence of accuracy in their solutions, there is no evaluation of a time step expression that could be translated to other problems.

Abdalla and Singh (1985) simulated the thawing of food using the finite element method. They presented comparisons between analytical and predicted values but they did not state what time step value they used.

Segerlind and Scott (1988) were among the first to deal with the time step estimates from the accuracy perspective. They presented a time step estimate for one and two-dimensional problems that produced accurate results. They did not give any derivation for their estimate and stated that much of it was based on their experience. They did not show any evidence that their time step estimates really work. However, they have stated an important observation that a time step based on the oscillation criterion is conservative. The time step could exceed this criteria by a factor of two before oscillations were observed.

Ne-Zheng Sun (1989) studied numerical solutions for the coupled ground water flow and advection-dispersion equation. He applied a variation of the linear finite element method and compared his solution with analytical ones. No indication was given as to what time step was used in his analysis.

Scientists reporting new time stepping schemes seem to discuss stability and oscillations only. Yu and Heinrich (1987), Segal and Praagman (1986), Fong and Mulkey (1990), Rigal (1990). Schreyer (1981) used the stability time step requirement ($\Delta t < C h^2/2$), where C is the thermal capacitance when performing a numerical solution for the heat conduction equation. None of these authors discussed the accuracy of the solutions.

Shu-Tung Chu and Hustrulid (1968), and De Baerdemaeker, et al. (1977) did not define a time step estimate when they discussed the numerical solution of the diffusion equation. Scott (1987) uses the following arbitrary accuracy criteria $\Delta t = (\text{time to steady state})/100$. In other words Scott assumes that running the problem for 100 time steps should be sufficient to ensure an accurate solution. Although this estimate might be a good starting point for some problems, no justification for its use was given.

Maadoliat (1983) studied stability and physical reality oscillations of the finite element numerical solution. He concluded with a set of conditions that must be satisfied in order to avoid both numerical problems and recommends a time step estimate accordingly. He did not consider the accuracy criteria.

Mohtar (1994) was among the first researchers to define the time step value based on an experimental accuracy criterion. He investigated the one-dimensional problem and two-dimensional problems consisting of square elements. The general procedure developed by Mohtar was to:

1. Define a measure of the error,
2. Convert the PDE to a system of ODE using the finite element method in space.
3. Solve a problem using several different values of the time step and several subdivisions of the problem in space,
4. Plot the error value against the number of nodes and select the time step value, Δt , that produced a specified error,
5. Empirically fit an equation to the time step data using lowest eigenvalue as the basic parameter, and
6. Checked the equations by solving a different set of problems.

In one-dimensional problems, Mohtar (1994), defined the accuracy ratio as

$$e = \frac{\sum_{j=1}^n \sum_{i=1}^m |NODE_{ij} - APDE_{ij}|}{\sum_{j=1}^n \sum_{i=1}^m |AODE_{ij} - APDE_{ij}|} \quad (2.1)$$

where NODE is the numerical solution for the system of ODEs, APDE is the analytical solution for the PDEs, AODE is the analytical solution for the system of ODEs, and n and m are the number of sampling points in the space and time domain respectively. The dynamic time step equation developed by Mohtar for the three single step methods applied to one-dimensional problems are:

Forward difference in time

$$\Delta t = 0.27 \frac{N^{-1.6}}{\lambda_1} \quad (2.2)$$

Central difference in time

$$\Delta t = 1.13 \frac{N^{-1.18}}{\lambda_1} \quad (2.3)$$

Backward difference in time

$$\Delta t = 30.6 \frac{N^{-3.91}}{\lambda_1} \quad (2.4)$$

In each equation, Δt is the time step value, N is the number of nodes in space and λ_1 is the lowest eigenvalue for the system. The time step estimates were validated using four different problems with analytical solutions: A sine wave variation and a linear variation in the initial conditions with boundary temperatures known and two problems with uniform initial conditions and derivative boundary conditions. The problems were solved using fractions or multiples of the calculated time steps. Time step values of one-half, two and three-times Δt were used along with the error ratio

$$e = \frac{\sum_{i=1}^m NODE_i}{\sum_{i=1}^m APDE_i} \quad (2.5)$$

The accuracy ratio for $\Delta t/2$ and Δt were equivalent. The results for multiples of two and greater were less accurate than the results for Δt .

In two-dimensional problems, Mohtar (1994), defined the accuracy ratio as

$$e = \frac{\sum_{j=1}^n \sum_{i=1}^m \frac{|NODE_{ij} - APDE_{ij}|}{NODE_{ij}}}{mn} \quad (2.6)$$

where $NODE$ is numerical solution for the system of ODEs, $APDE$ is the analytical solution for PDE, m is the number of sampling points in the space domain, and n is the number of sampling points in the time domain. The sampling points in the time domain were at 9.5, 19, 28.6, 38.1, 47.6, 57.1, 66.7, 76.2, 85.7 and 95.2 percent of the time to steady state defined by $t_{ss}=(4/\text{lowest eigenvalue})$.

The accuracy ratio, (2.1), used with one-dimensional problems became too difficult to evaluate for larger two-dimensional problems. Mohtar (1994) restricted the two-dimensional grid to square elements to allow a comparison of the finite element and finite difference formulations in space. Using the error estimate (2.5) and a five-percent error in the calculated values when compared to the analytical solution of the PDE, Mohtar developed the empirical time step estimates for two-dimensional square grid given below. Equation (2.7) through (2.9) are for the finite difference formulation in space while next three are for the finite element formulation in space.

Finite difference method in space

Forward difference in time:

$$\Delta t = 1.19 \frac{N^{-1.01}}{\lambda_1} \quad (2.7)$$

Central difference in time:

$$\Delta t = 1.6 \frac{N^{-0.55}}{\lambda_1} \quad (2.8)$$

Backward difference in time:

$$\Delta t = 0.05 \frac{N^{-0.1}}{\lambda_1} \quad (2.9)$$

Finite element method in space

Forward difference in time:

$$\Delta t = 1.8 \frac{N^{-1.04}}{\lambda_1} \quad (2.10)$$

Central difference in time:

$$\Delta t = 1.6 \frac{N^{-0.55}}{\lambda_1} \quad (2.11)$$

Backward difference in time:

$$\Delta t = 0.05 \frac{N^{-0.1}}{\lambda_1} \quad (2.12)$$

The above equations are valid when the number of nodes used with the finite difference formulation in space is equal to or greater than nine. The equations for the finite element method in space are valid when the number of nodes is equal to or greater than twenty-five.

Tan (1995) carried forward the work of Mohtar (1994) and developed empirical equations for calculating the time step required to numerically solve the system of ODEs related to time dependent radial field problem. The specific objectives of his study were to develop an empirical time step estimate for the three single step integration methods that satisfy an accuracy criterion and validate the time step equations by solving different set of problems.

Tan (1995) used the central difference solution scheme with a very small time step size and a highly refined grid in space to generate a set of reference values instead of using an analytical solution. The analytical solution of radial problems involves numerical evaluation of the series that define Bessel functions. Tan thought it was more appropriate to simply use a numerical solution to generate the reference values.

Tan's study used the linear radial element and the three single step integration methods in time. He used FEM in space and the lumped formulation for the capacitance

matrix. The time step equations were presented using the same format as used by Mohtar (1994). The equations are as follows:

Forward difference method in time:

$$\Delta t = 3.91 \frac{N^{-2.13}}{\lambda_1} \quad (2.13)$$

Central difference method in time:

$$\Delta t = .12 \frac{N^{-1.81}}{\lambda_1} \quad (2.14)$$

Backward difference method in time:

$$\Delta t = 5.28 \frac{N^{-1.66}}{\lambda_1} \quad (2.15)$$

CHAPTER THREE

OBJECTIVES

After studying a large amount of literature on the solution of time dependent field problems, the need for a priori time step estimate seems obvious. An a priori time step estimate would eliminate the present trial-and-error procedure. A very good time step estimate would allow the user to generate an accurate solution while satisfying numerical stability and oscillations criteria. The specific objective of this study was to develop an a priori time step estimate for three single-step methods used to solve the system of ordinary differential equations associated with the radial and spherical field problems. This study uses the finite element method in the space domain and lumped formulation in time.

The general hypothesis was that the a priori time step estimate has the general form

$$(\Delta t)\lambda_1 = C$$

for the unconditionally stable methods and

$$(\Delta t)\lambda_{\max} = C$$

for conditionally stable methods. These equations presented are similar to those developed by Mohtar (1994) and Tan (1995). The number of nodes in the space dimension, N , has been deleted as a basic parameter. It is well known that increasing the number of nodes in space increases the solution accuracy. It is also well known but often forgotten that the physical parameters that occur in PDEs are generally accurate to two significant digits and occasionally to three. (c.f. tables in Perry et al. 1984). A large number of nodes in the space dimension significantly increases the solution time and

generates accuracy beyond that justified by the number of significant digits in the basic parameters.

Some of the limits on this study included:

1. Radial and spherical field problems were investigated.
2. Finite element solution was adopted in space domain by using linear one-dimensional elements.
3. In the time domain single-step solution procedure was adopted. The numerical schemes used were: The forward difference, central difference and backward difference methods.
4. The capacitance matrix was formulated by using lumped (diagonal) formulation.

CHAPTER FOUR

THEORETICAL CONSIDERATIONS

Galerkin's finite element formulation was used to obtain the element matrices for both the space and time domains. The finite element technique is preferred over the finite difference method because both of the resulting matrices, $[C]$ and $[K]$, are positive definite, symmetric, and their eigenvalues are real and positive. The stiffness matrix $[K]$ is singular before boundary conditions are imposed. The finite difference method in space produces an unsymmetrical stiffness matrix. The global matrices, $[C]$ and $[K]$, are built from element contributions using the direct stiffness method, Segerlind (1984). The coefficients in the element matrices depend on the type of interpolation function used to solve the problem. There are two types of formulation for the capacitance matrix $[C]$: consistent and lumped. There are some disadvantages associated with the consistent formulation (Visser, 1965, Wilson and Nickell, 1966, Brocci, 1969, Zienkiewicz, 1977 and Segerlind, 1984, therefore, a lumped formulation was used for the capacitance matrix. The primary objective in this chapter is to briefly discuss the derivation of element matrices for spherical and radial field problems.

4.1 The Spherical Field Problems

Misra and Young (1978) have derived the element matrices for transient heat transfer in a sphere and have presented adequate details. To maintain continuity for the reader, especially for the reader who does not have direct access to the reference, a summary of the derivation is given here.

4.1.1 Governing equation

The differential equation for heat conduction in spherical coordinates, with heat generation within the solid, is given by Carslaw and Jaeger (1959) as

$$D_r \frac{\partial^2 U}{\partial r^2} + \frac{2D_r}{r} \frac{\partial U}{\partial r} + \frac{D_\phi}{r^2 \sin \phi} \frac{\partial}{\partial \phi} \left(\sin \phi \frac{\partial U}{\partial \phi} \right) + \frac{D_\theta}{r^2 \sin^2 \phi} \frac{\partial^2 U}{\partial \phi^2} + Q = D_t \frac{\partial U}{\partial t} \quad (4.1)$$

where D_r , D_ϕ , D_θ , and D_t are the physical parameters and $Q = Q(r,t)$ is the rate of heat generation. The initial and surface conditions and physical properties of a sphere are such that the isothermal surfaces are concentric spheres, therefore, the temperature is only a function of the radius, r , and time, t . The problem can now be studied by rotating a one-dimensional pin in three dimensions and can be integrated over the entire volume. The radial distance can be divided into a finite number of elements. The three dimensional equation, (4.1), reduces to

$$D_r \frac{\partial^2 U}{\partial r^2} + \frac{2D_r}{r} \frac{\partial U}{\partial r} = D_t \frac{\partial U}{\partial t} \quad \text{for } 0 \leq r \leq R \text{ and } t > 0 \quad (4.2)$$

where D_r is the radial thermal conductivity, U is the temperature and D_t is the thermal capacitance term which is the product of the density and the specific heat. The variables r and t are the space and time variables respectively. According to Carslaw and Jaeger (1959) the boundary conditions for (4.2) could be

$$U = U(r) \text{ at } r = R; t > 0$$

or a prescribed convection term at the surface

$$\pm D_r \frac{\partial U}{\partial r} + h(U - U_\infty) = 0 \text{ at } r = R, t > 0$$

where h is the surface heat coefficient and U_∞ is the temperature of the surrounding fluid.

The initial condition given by Carslaw and Jaeger is $U = U(r)$ in $0 \leq r \leq R; t = 0$

4.1.2 Variational statement

The finite elements technique requires developing the element equations from governing differential equations either by obtaining the variational or functional statement of the physical problem or by directly transforming the governing equation using Galerkin's method when the functional statement is not readily available. Misra and Young (1978) derived the element contributions by minimizing the functional statement of a physical problem.

The method for obtaining a variational statement from the governing equation is to rewrite the governing equation in the form of Euler-Lagrange equation, which for several independent variables has been given by Schecter (1967). The equation Schecter gives for spherical coordinates is

$$\frac{\partial F}{\partial U} - \frac{\partial}{\partial r} \left(\frac{\partial U}{\partial r} \right)^2 + \frac{D}{r^2 \sin^2 \varphi} \left(\frac{\partial F}{\partial \varphi} \right)^2 + 2D_t U \frac{\partial U}{\partial t} - 2QU \quad (4.4)$$

where F is the function to be determined. In a transient heat transfer problem, the function F can be split into

$$F = F_I + F_B \quad (4.5)$$

where F_I is the function for internal heat conduction and F_B is the function for boundary conditions.

The function F_I in spherical coordinates is,

$$F_I = \frac{1}{2} \left[D_r \left(\frac{\partial U}{\partial r} \right)^2 \frac{D_\varphi}{r^2} \left(\frac{\partial U}{\partial \varphi} \right)^2 + \frac{D_\varphi}{r^2 \sin^2 \varphi} \left(\frac{\partial U}{\partial \phi} \right)^2 + 2D_t U \frac{\partial U}{\partial t} - 2QU \right] \quad (4.6)$$

which reduces to

$$F_I = \frac{1}{2} \left[D_r \left(\dot{U} \right)^2 + 2\rho c U \frac{\partial U}{\partial t} \right] \quad (4.7)$$

when $U \neq f(\phi, \varphi)$. The variable $\dot{U}$ is $\frac{\partial U}{\partial r}$ in (4.7).

The function F_B is found from

$$\frac{\partial F}{\partial \dot{U}} = 0$$

For the boundary conditions given by (4.3), F_B is

$$F_B = \frac{1}{2} h (U - U_\infty)^2$$

Misra and Young (1978), define the element stiffness matrix $[k^{(e)}]$ as

$$[k^{(e)}] = \int_V \left(D_r \frac{\partial [N]^T}{\partial r} \frac{\partial [N]}{\partial r} \right) dV \quad (4.8)$$

The element capacitance matrix $[c^{(e)}]$, is defined the same for all field problems and is given in Segerlind (1984) as

$$[c^{(e)}] = \int_V D_r [N]^T [N] dV \quad (4.9)$$

The incremental volume dV in (4.8) and (4.9) is $dV = 4\pi r dr$.

4.1.3 Element matrices

Figure (4.1) illustrates the node locations and elements for the axisymmetric heat transfer problems in a sphere. The interval between adjacent nodes is called an element and a typical element 'e' is the interval between nodal points i and j. The temperature within an element is assumed to vary linearly and is given by (Myers, 1971)

$$U^{(e)} = c_1^{(e)} + c_2^{(e)} r = \left(\frac{R_j - r}{L} \right) U_i^{(e)} + \left(\frac{r - R_i}{L} \right) U_j^{(e)} \quad (4.10)$$

The constants c_1 and c_2 have a superscript 'e' because these are different for each element and the superscript 'e' with $U^{(e)}$ indicates the nodal value in an element. After the necessary integration, the element stiffness matrix is given by

$$[K^{(e)}] = \frac{4D_r^{(e)}(R_j^3 - R_i^3)}{3(R_j - R_i)^2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad (4.11)$$

where R_i is the radial distance to node i and R_j the radial distance to node j.

Using the shape function matrix

$$[N] = \begin{bmatrix} \frac{R_j - r}{L} & \frac{r - R_i}{L} \end{bmatrix}$$

in (4.9) and performing the matrix integration, the element capacitance matrix is given by

$$[C^{(e)}] = \frac{4\pi\rho^e c^{(e)}}{60(R_j - R_i)} \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix} \quad (4.12)$$

where

$$c_{11} = 2R_j^5 - 20R_j^2R_i^3 + 30R_jR_i^4 - 12R_i^5$$

$$c_{12} = 3R_j^5 - 5R_j^4R_i + 5R_jR_i^4 - 3R_i^5$$

$$c_{21} = c_{12}$$

$$c_{22} = 12R_j^5 - 30R_j^4R_i + 20R_j^3R_i^2 - 2R_i^5$$

This capacitance matrix is for the consistent formulation. The lumped formulation is obtained from the consistent formulation by placing the sum of each row on the diagonal and placing zeros in the off diagonal positions. The lumped capacitance matrix is

$$[C^{(e)}] = \frac{4\pi\rho^e c^{(e)}}{60(R_j - R_i)} \begin{bmatrix} d_{11} & 0 \\ 0 & d_{22} \end{bmatrix} \quad (4.13)$$

where $d_{11} = c_{11} + c_{12}$ and $d_{22} = c_{12} + c_{22}$. The final equations for d_{11} and d_{22} are

$$d_{11} = 5R_j^5 - 5R_j^4 R_i + 20R_j^2 R_i^3 + 35R_j R_i^4 - 15R_i^5$$

$$d_{22} = 15R_j^5 - 35R_j^4 R_i + 20R_j^3 R_i^2 + 5R_j R_i^4 - 5R_i^5$$

The above mentioned element stiffness matrix, (4.11) and capacitance matrix, (4.13) are used to build the global matrices [C] and [K] using the direct stiffness procedure, Segerlind (1984).

4.2 Radial problem

The field equation in cylindrical coordinates (r, θ , z) is

$$D_r \frac{\partial^2 U}{\partial r^2} + \frac{D_r}{r} \frac{\partial U}{\partial r} + \frac{D_\theta}{r^2} \frac{\partial^2 U}{\partial \theta^2} + D_z \frac{\partial^2 U}{\partial z^2} + Q = D_t \frac{\partial U}{\partial t} \quad (4.14)$$

where D_r , D_θ , D_z and D_t are physical parameters, Q is the source term and U is the unknown. If U is independent of θ then (4.14) reduces to

$$D_r \frac{\partial^2 U}{\partial r^2} + \frac{D_r}{r} \frac{\partial U}{\partial r} + D_z \frac{\partial^2 U}{\partial z^2} + Q = D_t \frac{\partial U}{\partial t} \quad (4.15)$$

If the body is long in z-direction as compared to radius, the end effects are negligible, and (4.15) reduces to

$$D_r \frac{\partial^2 U}{\partial r^2} + \frac{D_r}{r} \frac{\partial U}{\partial r} + Q = D_t \frac{\partial U}{\partial t} \quad (4.16)$$

This equation governs radial heat flow. Assuming that D_r is constant, (4.16) can be written in the compact form

$$\frac{1}{r} \left[D_r \frac{\partial}{\partial r} \left(r \frac{\partial U}{\partial r} \right) \right] + Q = D_t \frac{\partial U}{\partial t} \quad (4.17)$$

The boundary conditions associated with (4.17) are either U is constant or the convection boundary condition

$$D_r \frac{\partial U}{\partial r} = -MU_b + S \quad (4.18)$$

4.2.1 Galerkin's Finite Element Formulation

The weighted residual integral for left side of (4.17) is the volume integral given by Segerlind (1984)

$$\{R^{(e)}\} = - \int_V [N]^T \left(\frac{D_r}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \phi}{\partial r} \right) + Q \right) dV \quad (4.19)$$

The solution of field problems for cylindrical coordinates is discussed in several books. The integral form of the element matrices for radial field problems can be obtained from the cylindrical formulation by deleting all terms associated with the z coordinate. The weighted residual integral associated with Galerkin's finite element formulation for an axisymmetric element is

$$\begin{aligned} \{R^{(e)}\} = & \left(\int_V \left(D_r \frac{\partial [N]^T}{\partial r} \frac{\partial [N]}{\partial r} + D_z \frac{\partial [N]^T}{\partial z} \frac{\partial [N]}{\partial z} \right) dV \right) \{U^{(e)}\} - \int Q [N]^T dV \\ & - \int_V [N]^T \left(D_r \frac{\partial U}{\partial r} \cos \theta + D_z \frac{\partial U}{\partial z} \sin \theta \right) d\Gamma \end{aligned} \quad (4.20)$$

The above is equation (13.21), Segerlind (1984). Deleting the terms associated with the z coordinate direction and noting that the outside normal is always perpendicular to the boundary, $\cos \theta = 1$, the weighted residual integral for the radial element becomes

$$\{R^{(e)}\} = \left(\int_V \left(D_r \frac{\partial [N]^T}{\partial r} \frac{\partial [N]}{\partial r} \right) dV \right) \{U^{(e)}\} - \int Q [N]^T dV - \int_V [N]^T \left(D_r \frac{\partial U}{\partial r} \right) d\Gamma \quad (4.21)$$

The first integral in (4.21) multiplies the column vector of nodal values and defines the element stiffness matrix $[k^{(e)}]$. The integral containing Q becomes $\{f^{(e)}\}$, while the surface

integral is the inter-element requirement for interior element boundaries and the derivative conditions for the element with a node on an internal or external boundary.

4.2.2 Element Stiffness Matrix

The element stiffness and capacitance matrices for the radial field problems are not readily available in the literature. Most authors have chosen to write about the axisymmetric problem, which is solved using two-dimensional elements. The one-dimensional radial element has the equation as the spherical element

$$U^{(e)} = C_1^{(e)} + C_2^{(e)} r = \left(\frac{R_j - r}{L} \right) U_i^{(e)} + \left(\frac{r - R_i}{L} \right) U_j^{(e)} \quad (4.22)$$

where R_i is the radial distance to node i, R_j the radial distance to node j and L is the element length. The row vector $[N]$ is

$$[N] = \left[\frac{R_j - r}{L} \quad \frac{r - R_i}{L} \right] \quad (4.23)$$

and

$$\frac{\partial [N]}{\partial r} = \left[\frac{-1}{L} \quad \frac{1}{L} \right] \quad (4.24)$$

while

$$\frac{\partial [N]^T}{\partial r} = \left[\begin{array}{c} -\frac{1}{L} \\ \frac{1}{L} \end{array} \right] \quad (4.25)$$

The element stiffness matrix $[k^{(e)}]$ is defined by

$$[k^{(e)}] = \int_V \left(D_r \frac{\partial [N]^T}{\partial r} \frac{\partial [N]}{\partial r} \right) dV \quad (4.26)$$

Substitution of (4.24) and (4.25), using $dV=2\pi r dr$ and integrating from R_i to R_j produces

$$[k^{(e)}] = \frac{2\pi \bar{r} D_r}{L} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad (4.27)$$

after using the relationships

$$L = R_j - R_i \quad \text{and} \quad \bar{r} = \frac{R_j + R_i}{2}$$

and noting that

$$\frac{R_j^2 - R_i^2}{2} = L \bar{r}$$

4.2.3 Element Capacitance Matrix

The element capacitance matrix $[c^{(e)}]$, is defined the same for all field problems

$$[c^{(e)}] = \int_V D_r [N]^T [N] dV \quad (4.28)$$

The matrix of shape functions, $[N]$, for the radial problems is defined by (4.14).

Substitution of (4.28), using $dV=2\pi r dr$ and again integrating from R_i to R_j produces the consistent capacitance matrix. Add all of the coefficients in a single row and placing the value on the main diagonal gives the lumped version of capacitance matrix which is

$$[c^{(e)}] = \frac{2\pi D_r L}{6} \begin{bmatrix} R_i + 2\bar{r} & 0 \\ 0 & R_j + 2\bar{r} \end{bmatrix} \quad (4.29)$$

4.3 Closure

The element stiffness and element capacitance for the spherical and radial field problems were developed in this chapter. There are several other details related to the computer implementation that have not been discussed/included. The direct stiffness

procedure for constructing the global matrices and the incorporation of known and/or derivative boundary conditions. These items are in most finite element books and duplicating the information seemed unnecessary.

CHAPTER FIVE

METHODOLOGY

The research in this study is directed at developing an a priori time step estimate that meets a required accuracy criteria. Stability and oscillations were given secondary consideration. It is worthwhile to mention that no numerical algorithm can produce valuable results unless it is stable and free of oscillations. This chapter discusses with the methodology adopted to develop an a priori time step estimate.

5.1 Methodology

The methodology in this study is a refinement of the techniques used by Mohtar (1994), Tan (1995) and Kwon (1998). The basic steps in this procedure are:

1. Define the Physical Problem

This study was limited to the radial and spherical parabolic diffusion equations. Each problem was converted to a system of ordinary differential equations by using the finite element method in space and lumped formulation in time. The investigation was limited to a cooling problem, which goes to equilibrium.

2. Define an Error Norm

An average error norm, L_1 was defined

$$e = \sum \sum \frac{|U_{cal_{ij}} - U_{ref_{ij}}|}{N(U_{max} - U_{min})} \quad (5.1)$$

and used in this study. The numerator is the difference between a set of calculated values in space and time and a set of reference values for the same set of points in space and time. The denominator contains the total number of sampling points, N , and the largest difference between the initial condition and a final value. The

reference values were calculated using a 21-node grid in space and a time step smaller than the time step values used to investigate other solutions.

The maximum error in each solution was also determined and retained as useful data in developing the time step estimate. Mohtar (1994) investigated the use of other error norms including L_2 and L_∞ norms. These norms provided less accurate estimation of the desired time step.

3. Select a Defining Problem

The time step estimate is established using a physical problem that is considered very difficult to solve numerically; a body with a constant temperature (or some other variable) and the boundary temperature is changed instantaneously to another value. This problem was selected because the analytical solution of this problem has all of the frequency components and it has shortest time to steady state. The initial and boundary conditions for both the radial and spherical problems were

$$U(r,0) = 1, 0 \leq r \leq 1 \quad (5.2)$$

with the boundary condition

$$U(1,t) = 0, t > 0 \quad (5.3)$$

Both problems were solved using a radius of one and the physical parameters D_r and D_l were also assigned a value of one.

4. Define the Sampling Points in Space

The sampling points in space have to be defined such that the grid being studied has nodes at the same location as the reference grid. The sequence that satisfies these requirements consists of 6, 11 or 21 nodes. The reference grid also has 21 nodes but smaller time steps. This set of grids is illustrated in Figure 5.1. The calculated value at each internal node in the 6, 11 and 21 node grids was used in the calculation of the error norm.

5. Define the Sampling Points in Time

The sampling points in time were defined at or very near 1/14, 2/14, 3/14, 4/14, 5/14, 6/14, 7/14, 8/14, 9/14, 10/14, 12/14 and 14/14 of the 60 percent of the time to steady state, t_{ss} , which was calculated using

$$t_{ss} = \frac{4}{\lambda_1} \quad (5.3)$$

where λ_1 is the lowest eigenvalue of the system of ordinary differential equations associated with the transient solution. The definition of t_{ss} comes from, $e^{-\lambda_1 t}$, the first term in the analytical solution of a parabolic diffusion equation. This particular term lasts the longest. The value of 4 is used in (5.3) because when $\lambda_1 t = 4$, $e^{-4} = 0.018$ and over 98% of the transient has been completed.

6. Select the Solution Procedure in Time

There are several methods available for solving a system of ordinary differential equations in time. Three single step methods were investigated in this study; the forward difference, central difference and backward difference methods.

SAMPLING POINTS IN SPACE

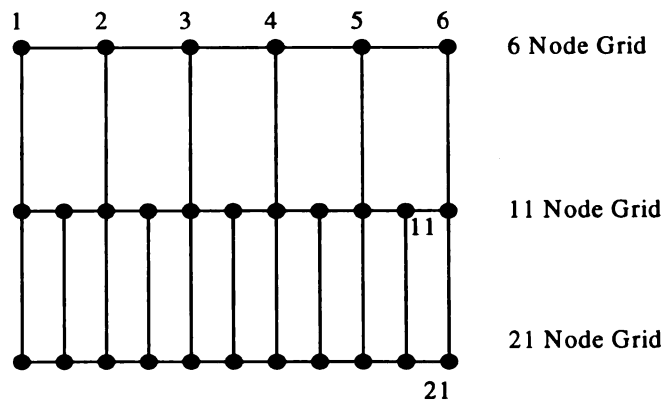


Figure 5.1

7. Define the Accuracy Level

A priori time step estimate must be defined relative to a level of accuracy. The equations in this research were defined for an average error of one-percent and a maximum error of approximately five-percent.

5.2 Computer Software

A finite element program, Segerlind (1987), was modified for use in the numerical experimentation. Some of the results obtained from the Quickbasic®¹ program were also verified using the commercially available mathematical program, MATLAB®². The Quickbasic programs solved the PDEs in space generating the ODEs and then calculated the lowest and highest eigenvalues for the system of equations. The program is capable of evaluating four different capacitance matrices including the lumped and distributed (consistent) matrices. Only the lumped formulation was used during this research. The computer programs were enhanced to minimize the amount of time required for file management and graphing of the calculated values.

¹ Registered Trademark of Microsoft Corporation.

² Registered Trademark of The Math Works, Inc.

CHAPTER SIX

RESULTS: UNIFORM GRID

A large number of experiments was conducted to determine the desired Δt and its relationship with the lowest or largest eigenvalue of the system of ODEs associated with the spherical and radial field problems. Each subdivision of this chapter covers the experiments related to one of the field problems and the solution procedure in time; the central difference, backward difference and forward difference single step numerical schemes. Each time scheme was investigated using grids of 6, 11 and 21 nodes. Sectors 6.4 and 6.5 deal with deriving equations for the a priori time step.

6.1 Reference Values

Reference values were generated by solving a twenty one-node grid using the central difference single-step numerical scheme. The time step (Δt) was kept equal to $0.6t_{ss}/112$ for the unconditionally stable methods and $\Delta t = 0.6t_{ss}/8960$ was used for conditionally stable method. Numerical solutions with 31 and 41 nodes were abandoned because there was minimal improvement in accuracy with a considerable increase in the computational effort.

6.2 Spherical Shapes

For the unconditionally stable schemes, central difference and backward difference, the 6, 11 and 21 node grids were solved in time using a Δt that varied from 0.064 ($0.6t_{ss}/14$) to 0.008 ($0.6t_{ss}/112$). To maintain compatibility of the sampling points in time domain, sampling points for $\Delta t = 0.6t_{ss}/14$ were 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12 and 14;

similarly for $\Delta t = 0.6t_{ss}/56$ the points were 4, 8, 12, 16, 20, 24, 32, 36, 40, 48, 56. The multiples of 14 used in the experiments were 28, 56, 70, 84, 98 and 112.

For the conditionally stable forward difference scheme 6, 11 and 21 node grids were solved in time using a Δt that varied from $(0.6t_{ss}/896)$ to $(0.6t_{ss}/8960)$. All Δt were kept in the multiples of 896 (896 is also a multiple of 14) to maintain compatibility of the sampling points. For example, sampling points with $\Delta t = 0.6t_{ss}/896$ were 64, 128, 192, 256, 320, 384, 448, 512, 576, 640, 766 and 896, and so on. The multiples of 896 used in the experiments were 896, 1792, 3584, 5376, 7168 and 8960. A larger number of time steps was required for the forward difference scheme because of the stability criterion.

Every solution was compared with the reference in space as well as time domain by calculating a L_1 norm, the average error and determining the maximum error. Summary of all the data used in experiments and the values obtained are attached as Appendix A.

The results were plotted for every reading obtained during experiments. The time step was kept on the horizontal axis and the average or maximum error was kept on vertical axis. Details of data including variation of temperature at each sampling point in space and time are lengthy and not attached with this document; however, a summary of results, graphs and analysis for each experiment is presented.

6.2.1 Central Difference Method in Time

6.2.1.1 Six Node Grid

Figure 6.1 graphically represents the average error for a six-node grid. The six-node grid did not produce accurate results. The average error remained above two-percent even for smaller time steps. A more refined grid in space is recommended.

SPHERICAL UNIFORM GRID CENTRAL DIFFERENCE

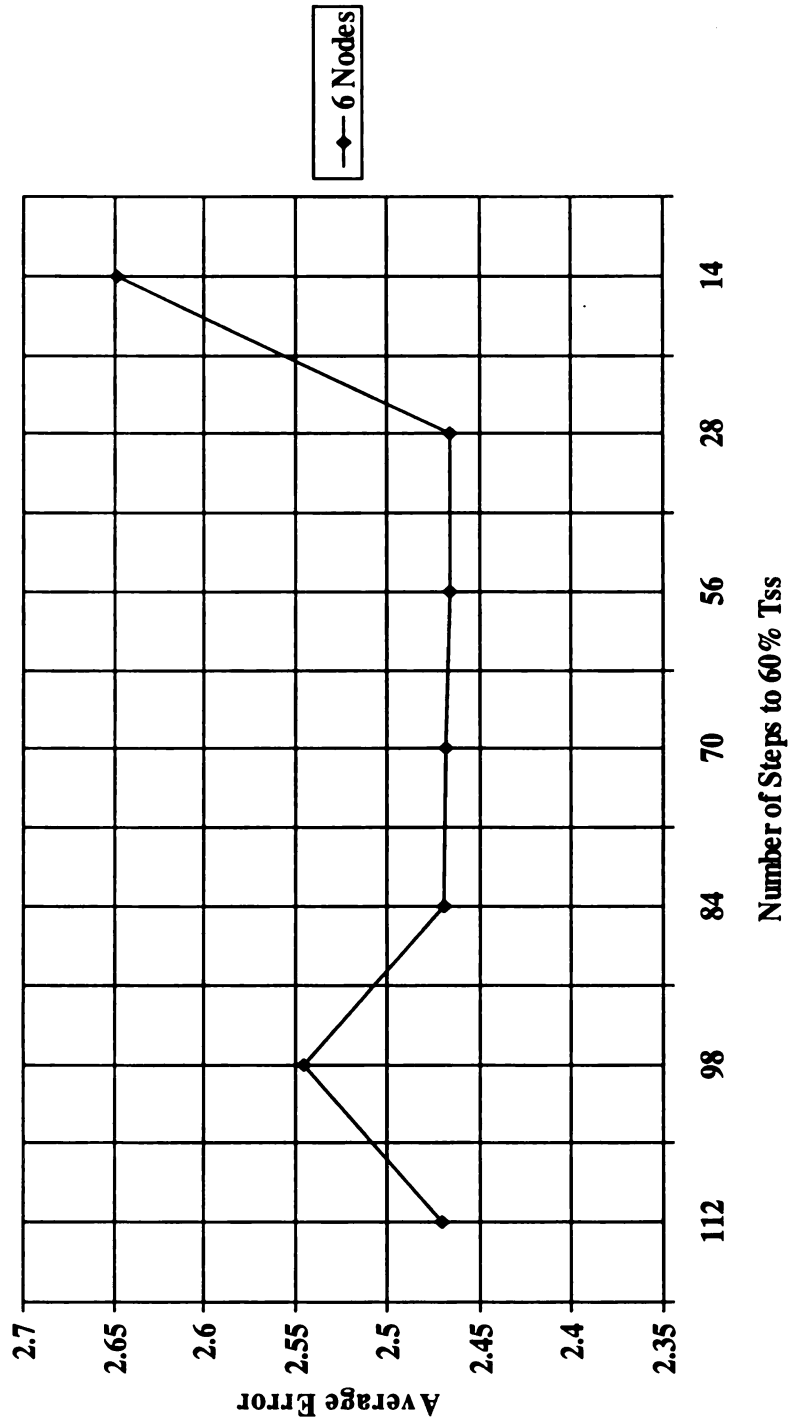


Figure 6.1

6.2.1.1 Eleven Node Grid

The average error for an eleven-node grid is presented in Figure 6.2. The eleven-node grid produced very accurate results with the average error remaining below one percent for all time steps. The error increased sharply for time steps larger than $0.6t_{ss}/28$ or $\Delta t > 0.0032$.

6.2.1.2 Twenty-one Node Grid

Figure 6.3 represents the average error for the twenty-one node grid. The results were very accurate, with the average error remaining below 0.2 percent for several time steps. The error has a sudden increase at time steps larger than $0.6t_{ss}/28$ or $\Delta t > 0.0032$ and exceeds the error in the eleven-node grid.

6.2.1.3 Backward Difference Method in Time

6.2.1.4 Six Node Grid

The average error is presented in Figure 6.4. The six node grid did not produce accurate results. Average error remained above two- percent even for the smallest of time steps.

6.2.1.5 Eleven Node Grid

Figure 6.5 graphically represents the average error. The eleven-node grid produced accurate results below $\Delta t = 0.016$ where the average error remained below 1 percent. The error increased with the time steps larger than $0.6t_{ss}/28$ or $\Delta t > 0.0032$.

6.2.2.3 Twenty-one Node Grid

The average error for the twenty-one node grid is presented in Figure 6.6. The average error was below one percent when more than 56 time steps were used. The error increased for the time steps larger than $0.6t_{ss}/28$ or $\Delta t > 0.0032$.

SPHERICAL UNIFORM GRID CENTRAL DIFFERENCE

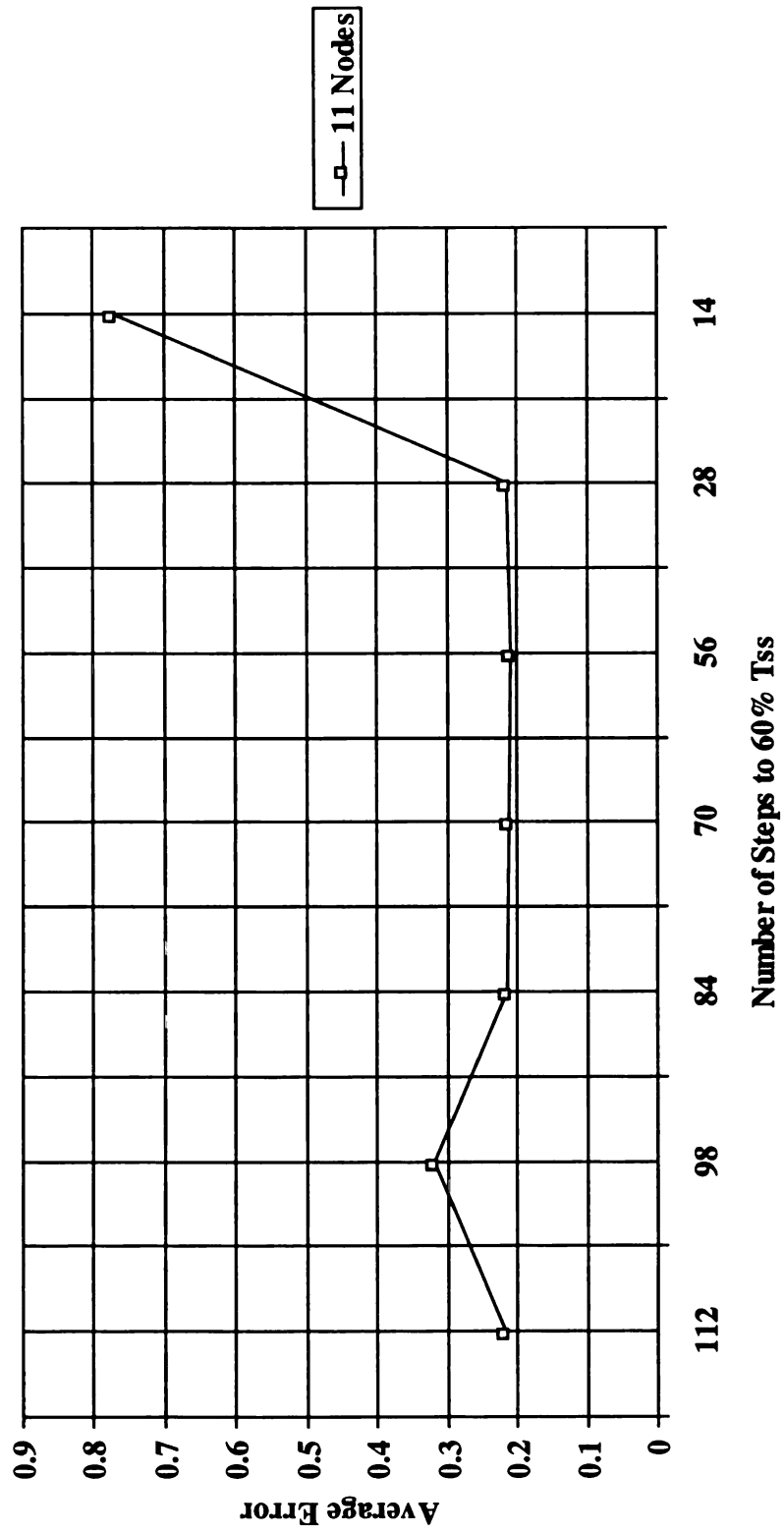


Figure 6.2

SPHERICAL UNIFORM GRID CENTRAL DIFFERENCE

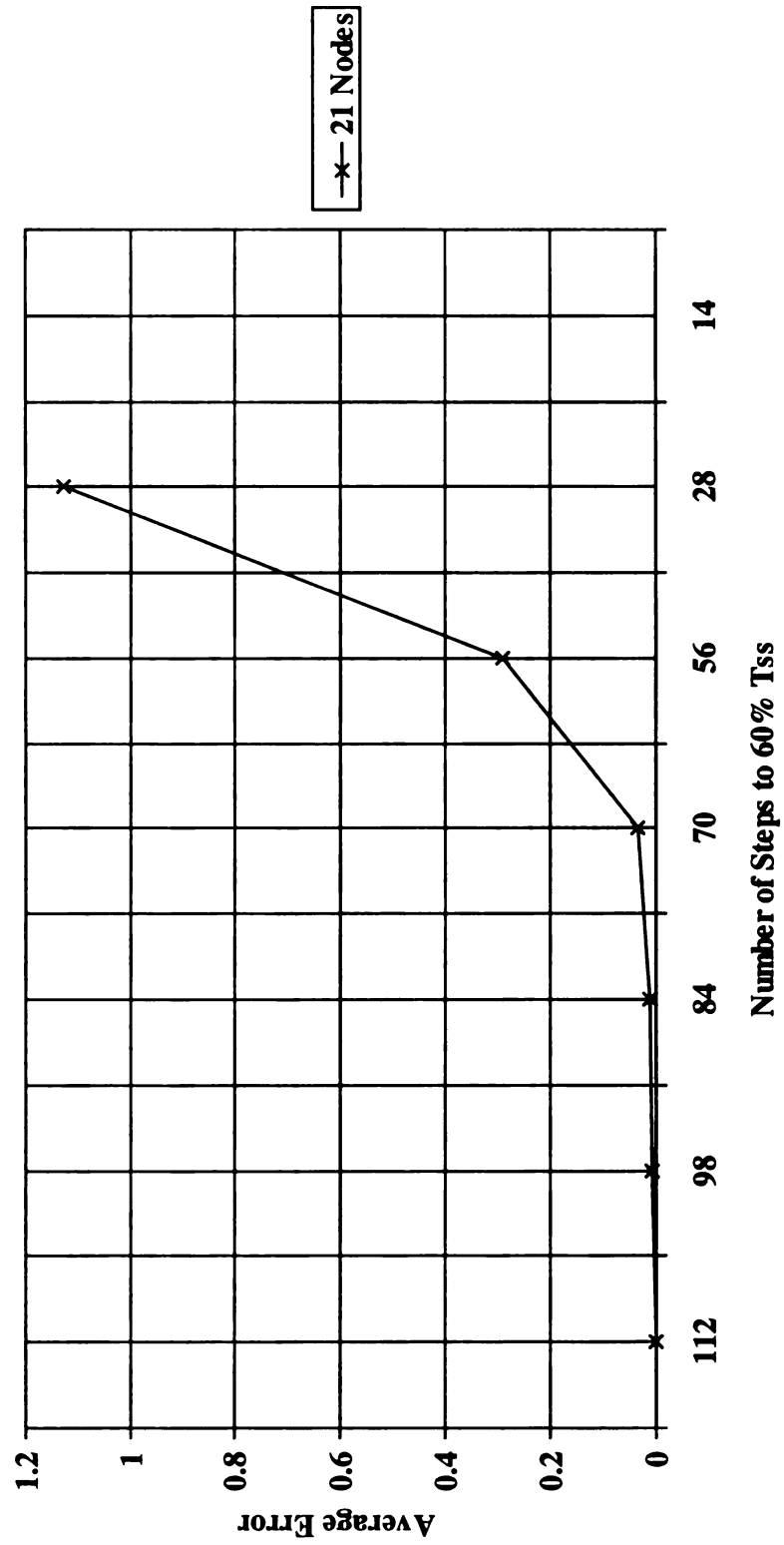


Figure 6.3

SPHERICAL UNIFORM GRID BACKWARD DIFFERENCE

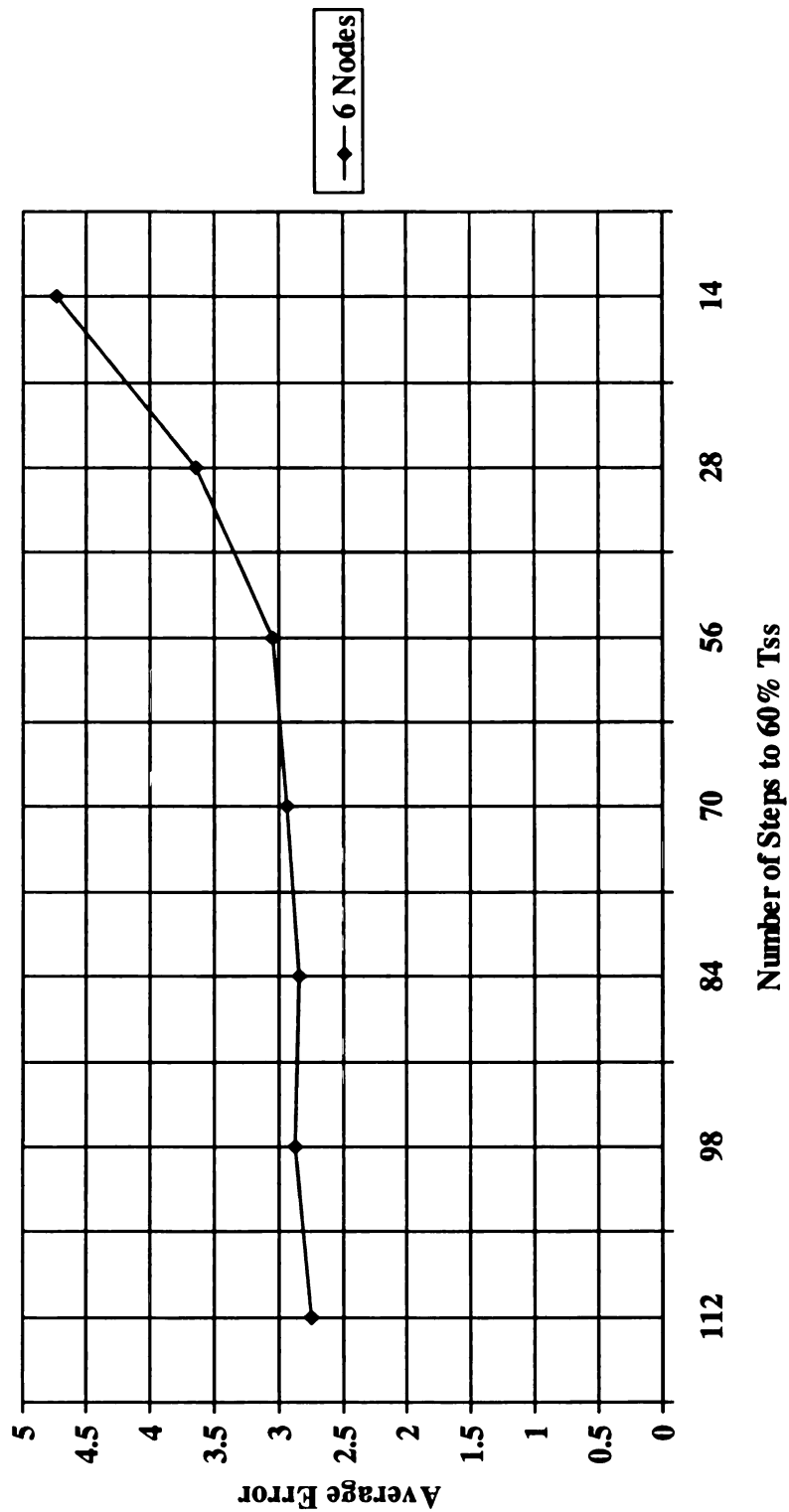


Figure 6.4

SPHERICAL UNIFORM GRID BACKWARD DIFFERENCE

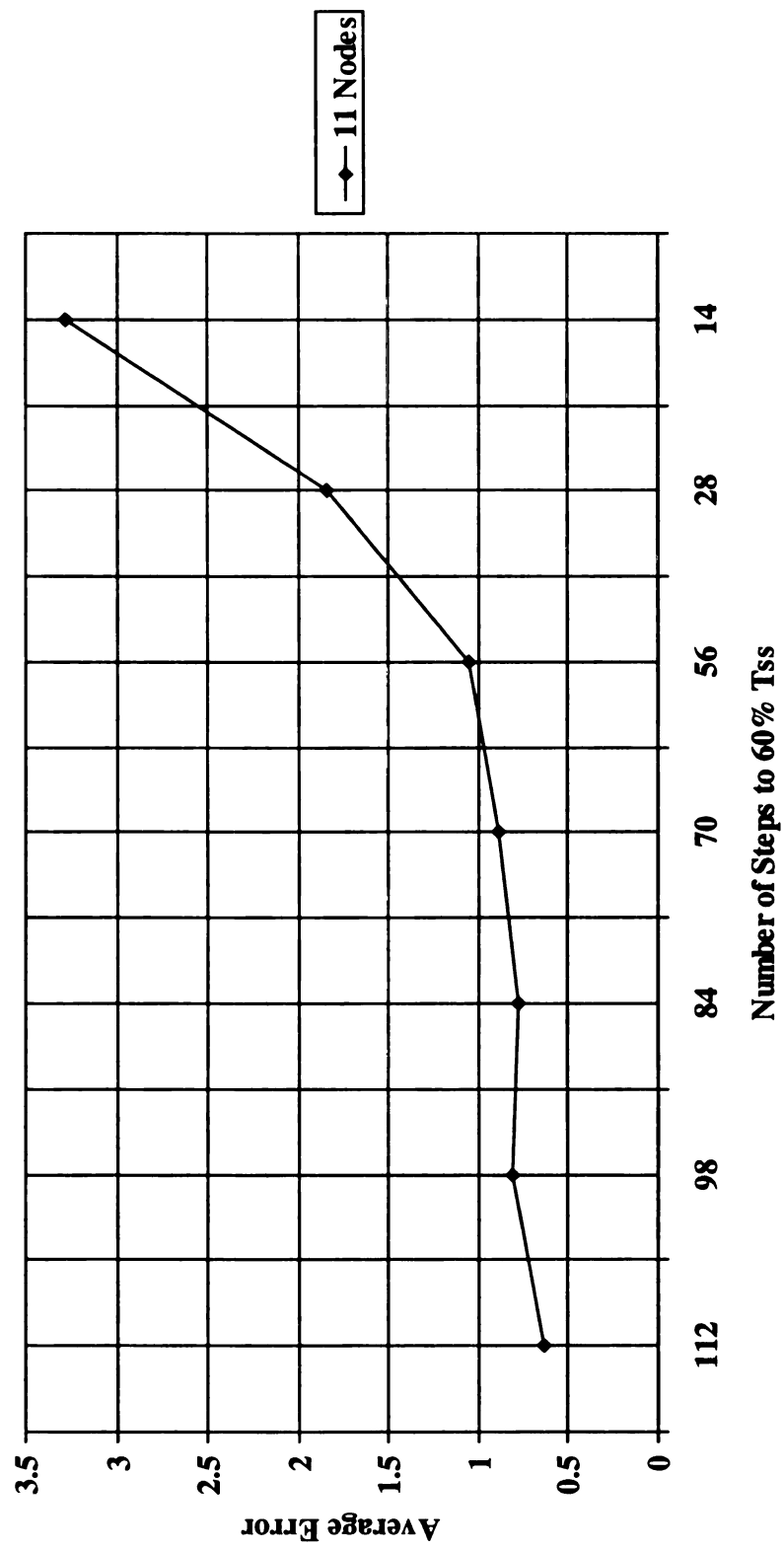


Figure 6.5

SPHERICAL UNIFORM GRID FORWARD DIFFERENCE

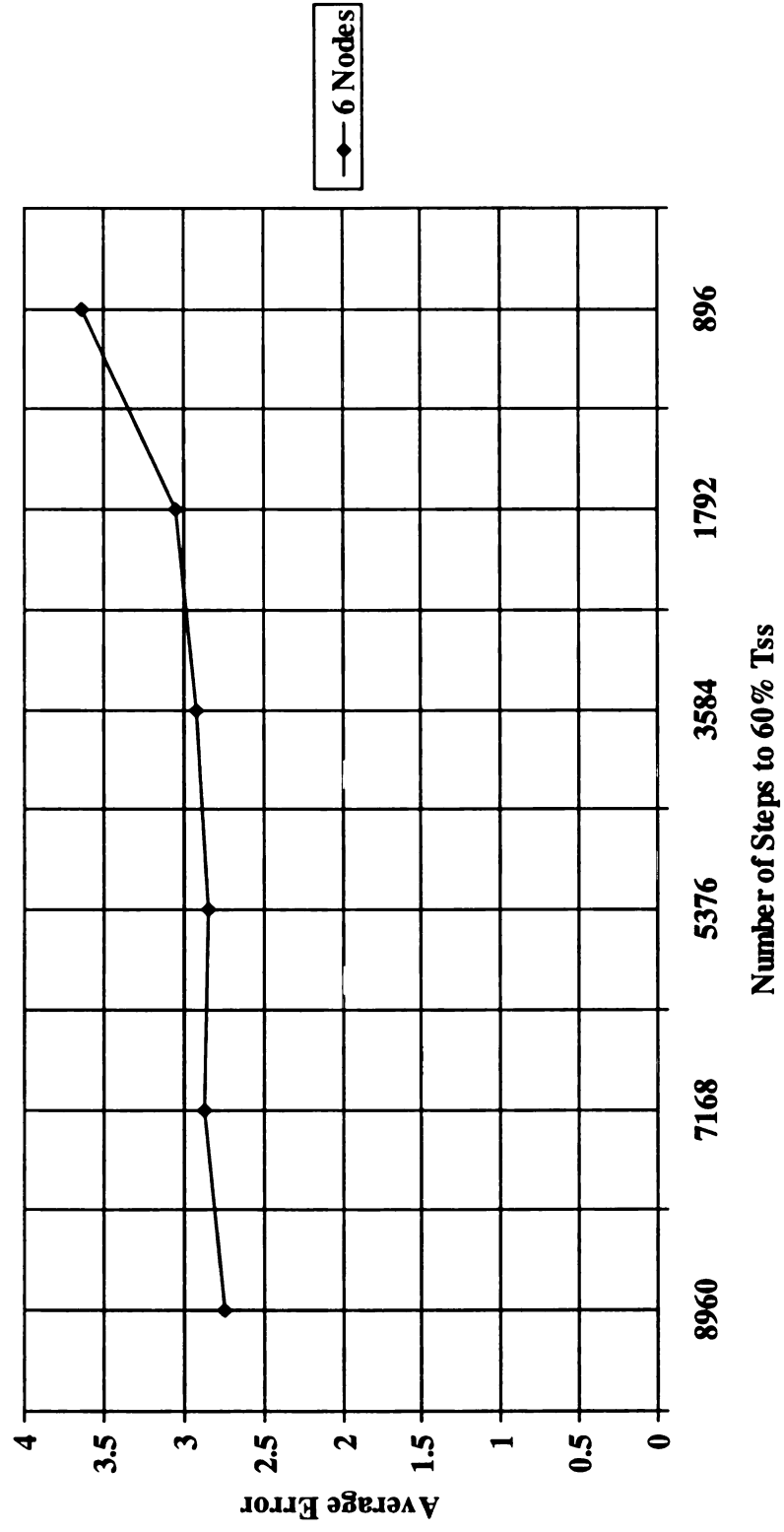


Figure 6.7

6.2.3 Forward Difference Method in Time

The forward difference is a conditionally stable method in which stability and oscillation limits depend upon the maximum eigenvalue, $\lambda_{\max}$, of the system of equations, Segerlind (1984). The reference values were obtained by using a very small time step, $\Delta t = 0.6t_{ss}/8960$.

6.2.3.1 Six Node Grid

Figure 6.7 graphically represents the six node grid. Once again, it did not prove to be accurate and average error remained above one-percent even for small time steps.

6.2.3.2 Eleven Node Grid

The average errors for the eleven node grid are plotted in Figure 6.8. The results were accurate and the average error remained below one percent for smaller time steps but suddenly increased for the time steps larger than $0.6t_{ss}/3584$.

6.2.3.3 Twenty-one Node Grid

The average error for the twenty-one node grid is presented in Figure 6.9. The results were very accurate. Average error remained below 1 percent but suddenly increased for time steps larger than $0.6t_{ss}/3584$.

6.3 Radial Shapes

The procedure and schemes used for radial shapes are similar to those used for the spherical shapes. Results of eleven and twenty-one node grids have reasonable similarity; therefore, they have been combined for the purpose of clarity and brevity.

SPHERICAL UNIFORM GRID FORWARD DIFFERENCE

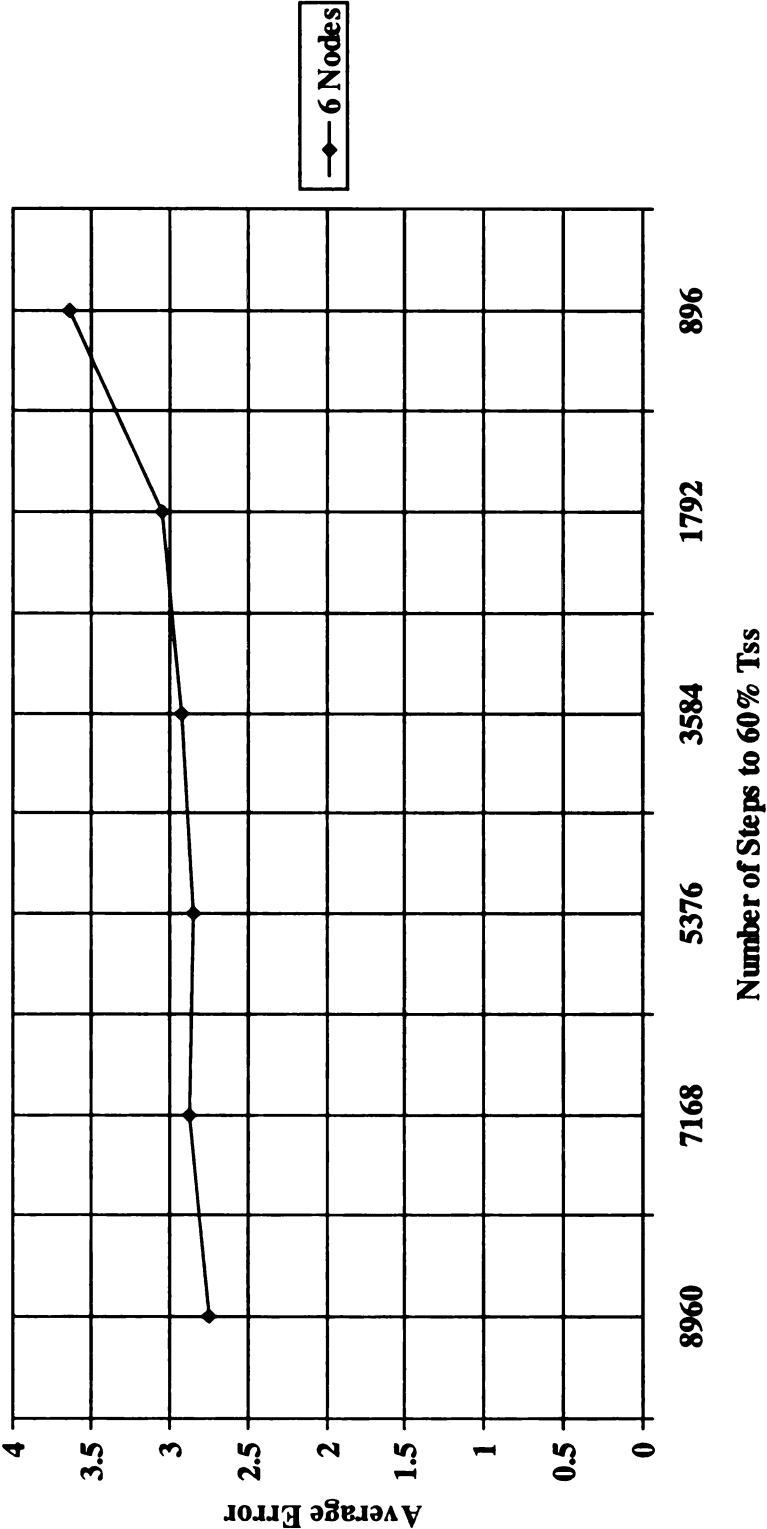


Figure 6.7

SPHERICAL UNIFORM GRID FORWARD DIFFERENCE

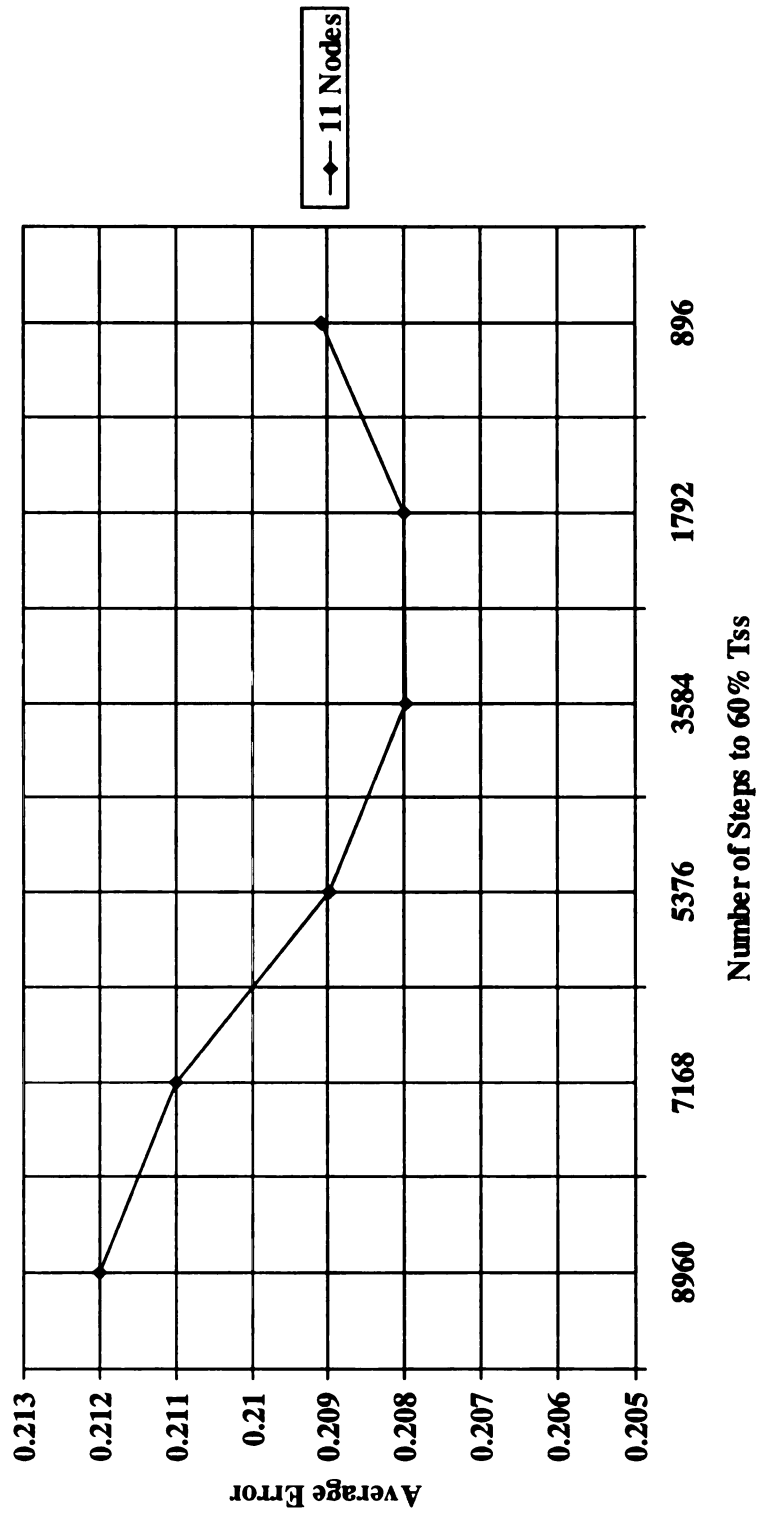


Figure 6.8

SPHERICAL UNIFORM GRID FORWARD DIFFERENCE

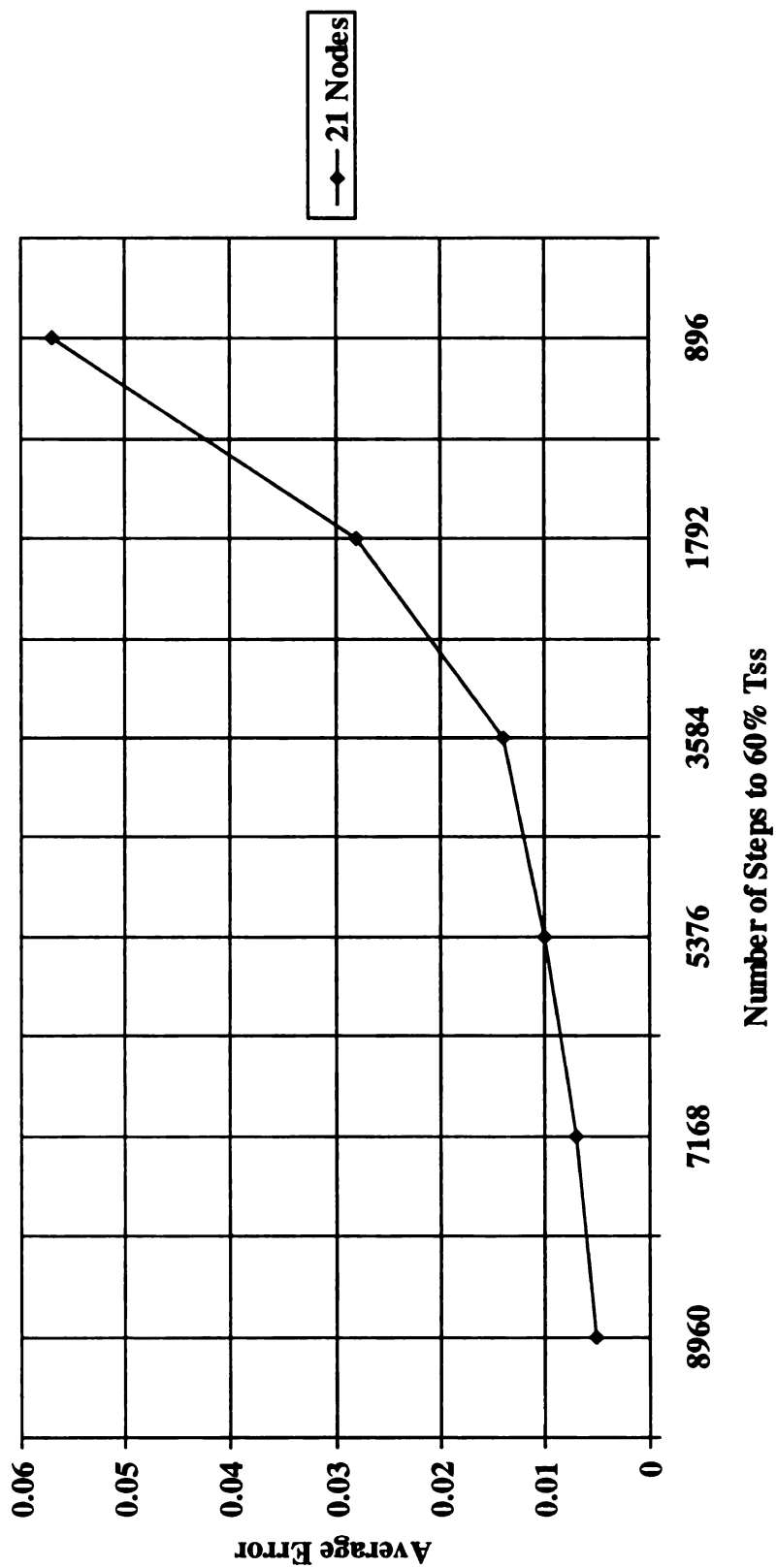


Figure 6.9

6.3.1 Central Difference Method in Time

6.3.1 Six Node Grid

Figure 6.10 exhibits the average error for the six-node grid. The results were inaccurate; average error remained above two-percent.

6.3.1.1 Eleven and Twenty-one Node Grid

Figure 6.11 displays the plot of average error for the eleven and twenty one-node grids. The results for the time steps up to $0.6t_{ss}/56$ are accurate with the average error remaining below 0.5 percent. There is, however, a sharp rise in the error for the time steps larger than $0.6t_{ss}/28$.

6.3.2 Backward Difference Method in Time

6.3.2.1 Six node Grid

Figure 6.12 graphically displays the average error for the six node grid. The results are inaccurate and suggest need for more refined grid in space.

6.3.2.2 Eleven and Twenty-one Node Grid

Figure 6.13 represents the average error for the eleven and twenty-one node grids. The results were accurate with the average error remaining below 0.5 percent for several time steps. The error increases suddenly at time steps larger than $0.6t_{ss}/56$.

6.3.3 Forward Difference Method in Time

6.3.3.1 Six Node Grid

Figure 6.14 displays the average error for the six node grid. The results remain inaccurate and further strengthen the idea of needing a more refined grid in space.

RADIAL UNIFORM GRID CENTRAL DIFFERENCE

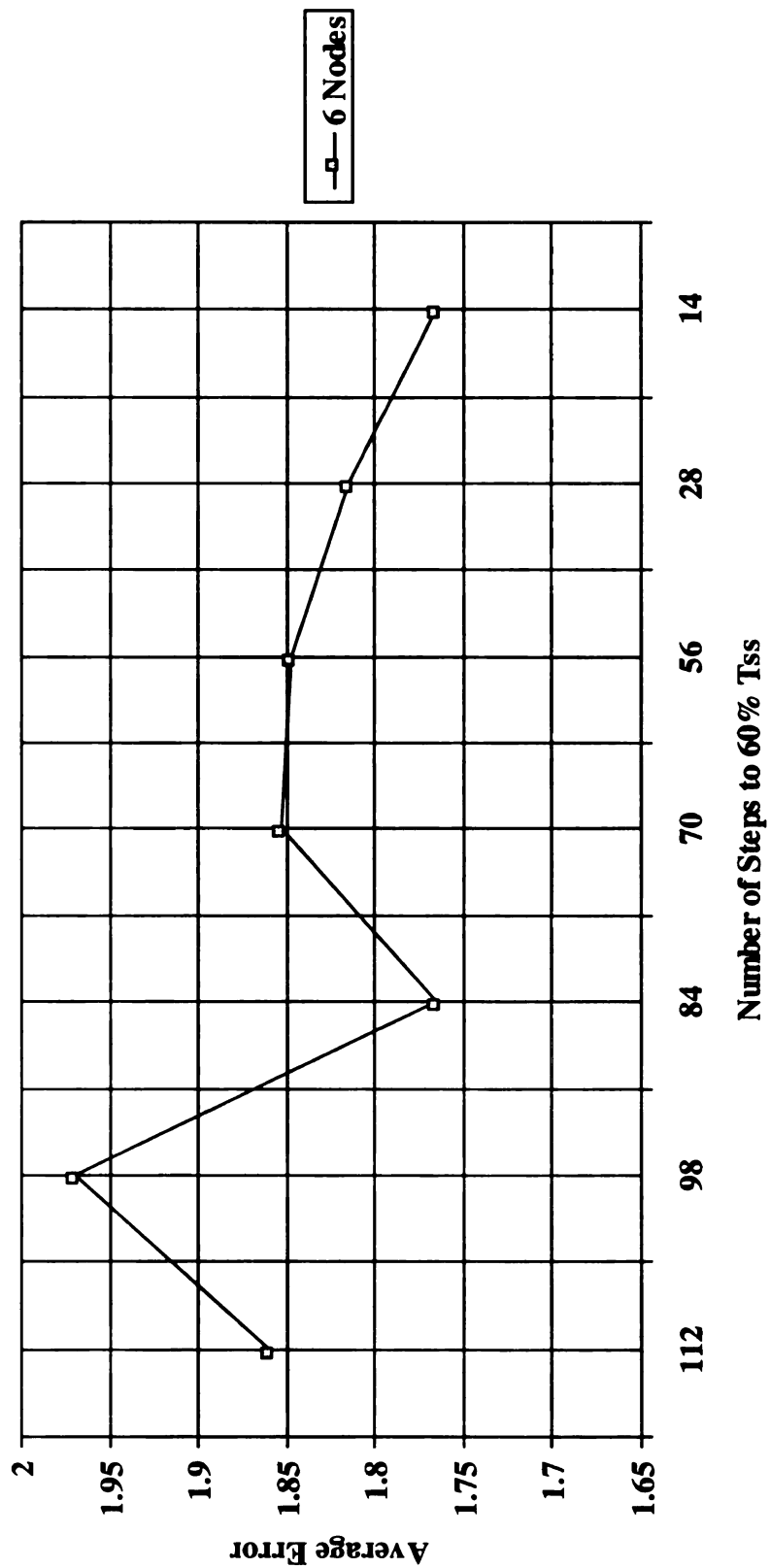


Figure 6.10

RADIAL UNIFORM GRID CENTRAL DIFFERENCE

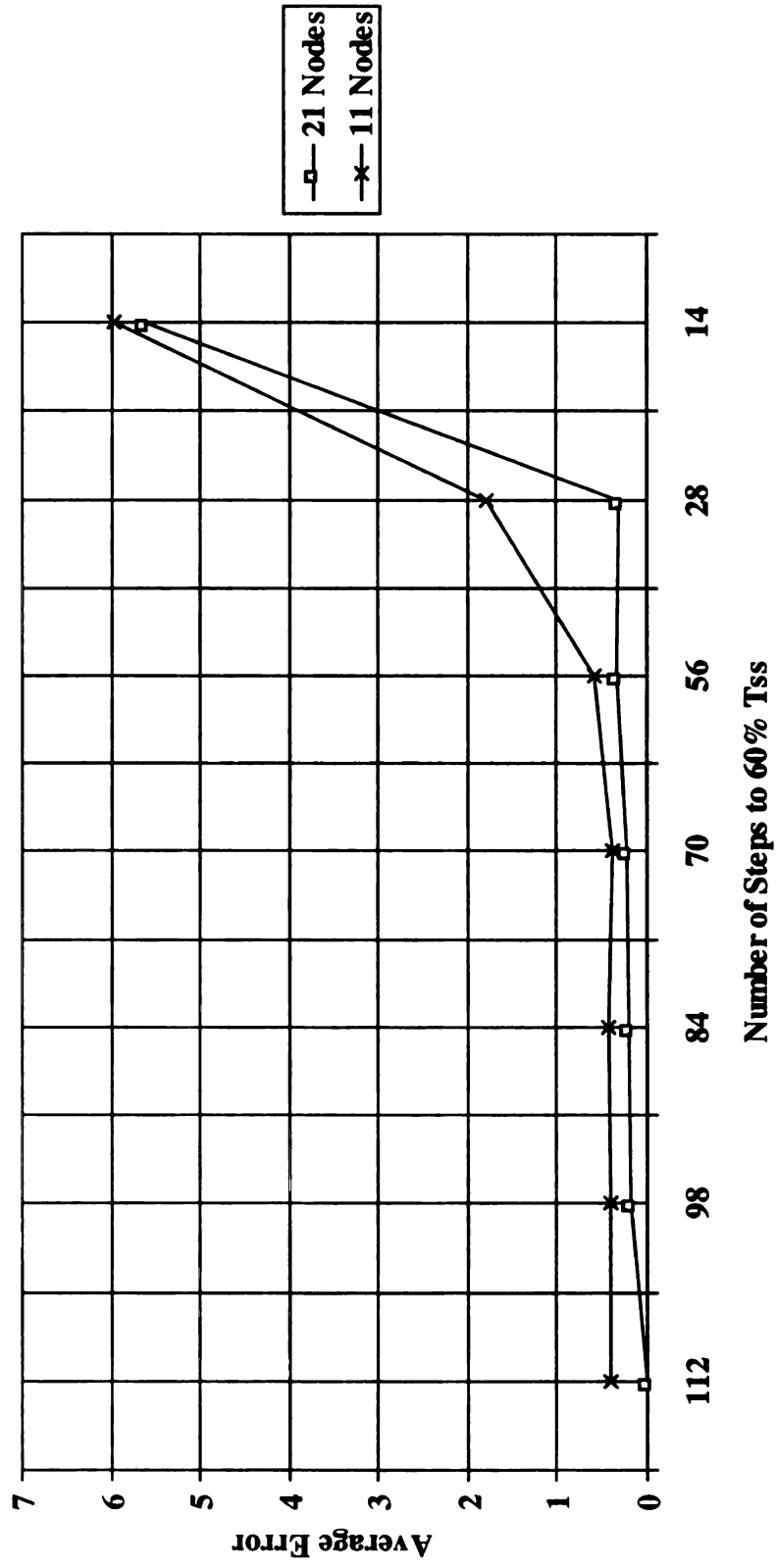


Figure 6.11

RADIAL UNIFORM GRID BACKWARD DIFFERENCE

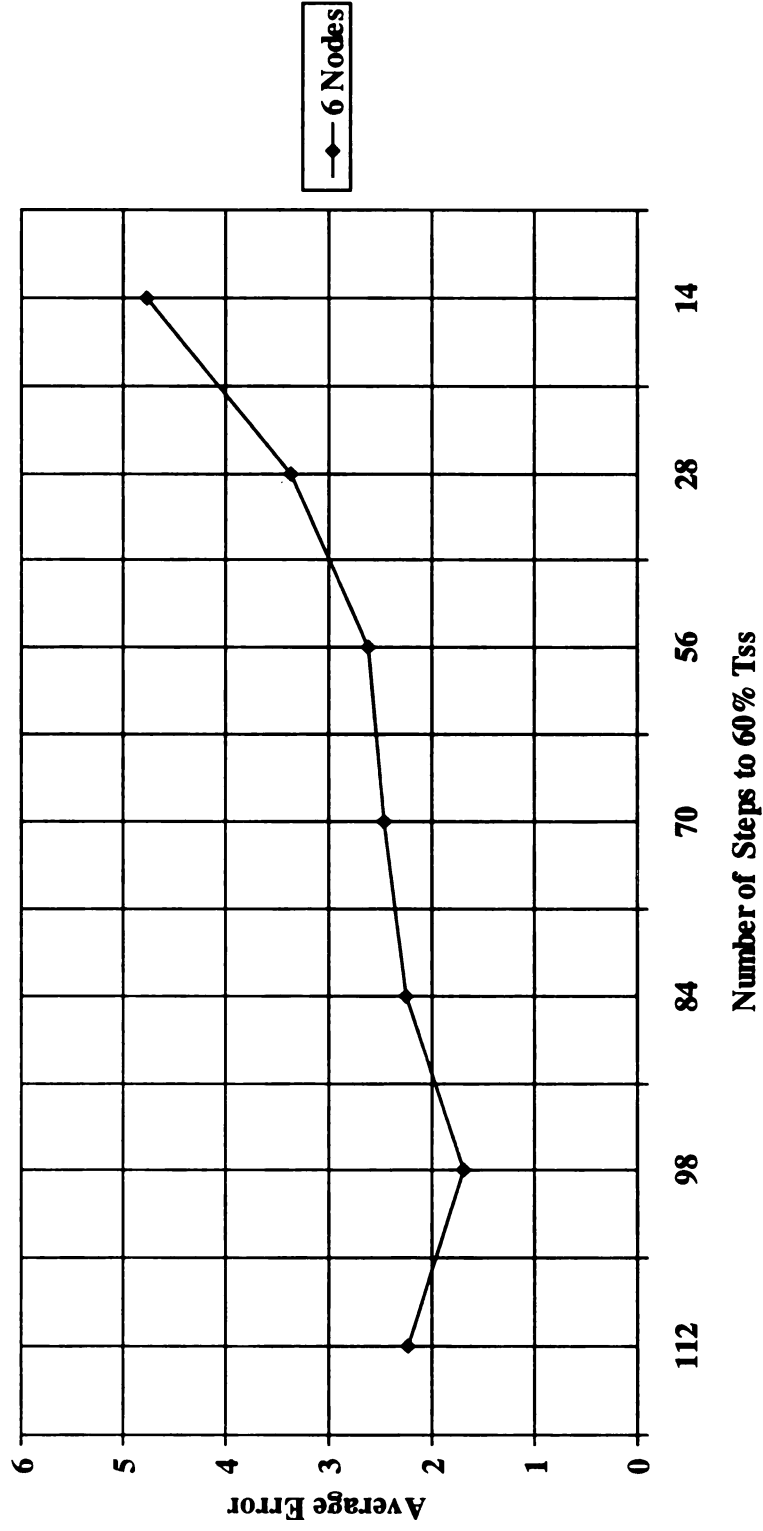


Figure 6.12

RADIAL UNIFORM GRID BACKWARD DIFFERENCE

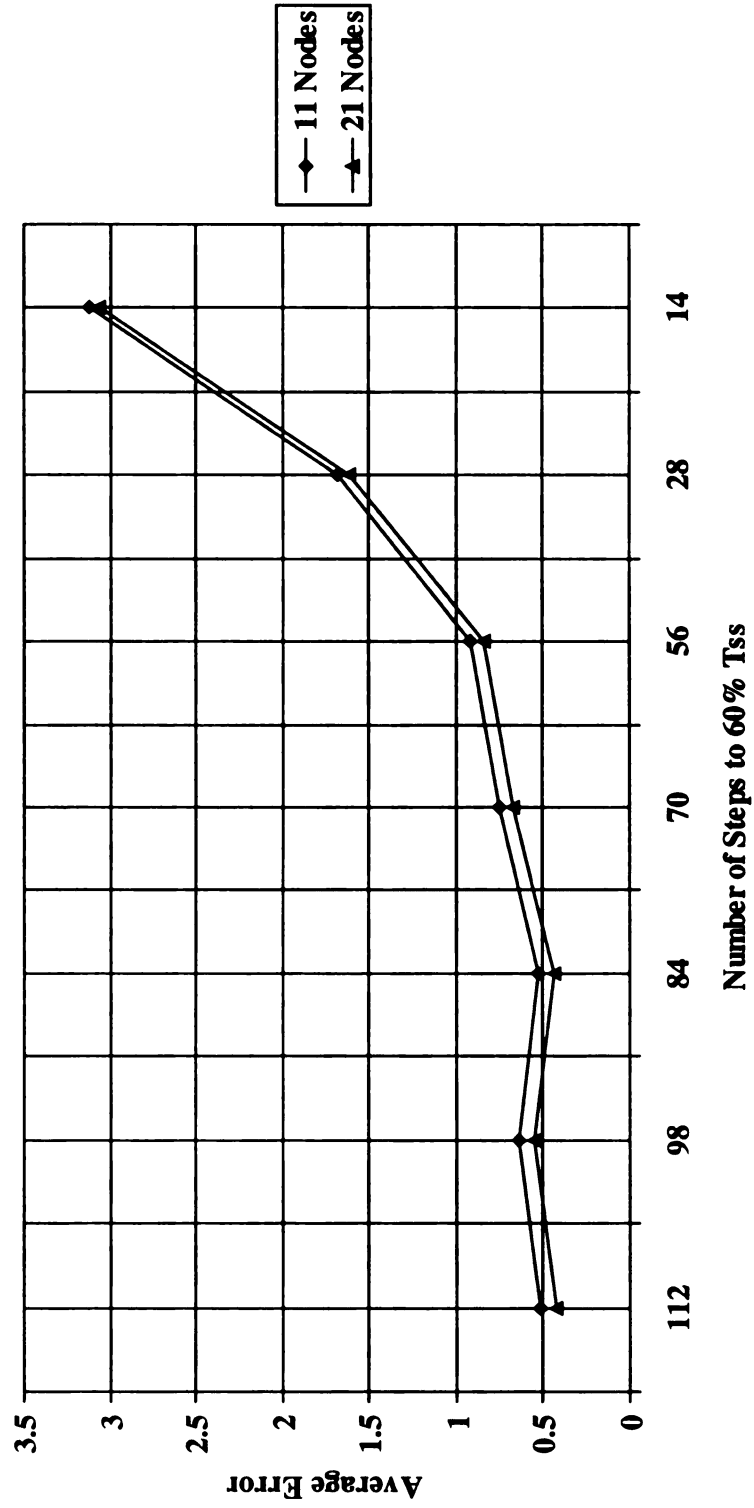


Figure 6.13

RADIAL UNIFORM GRID FORWARD DIFFERENCE

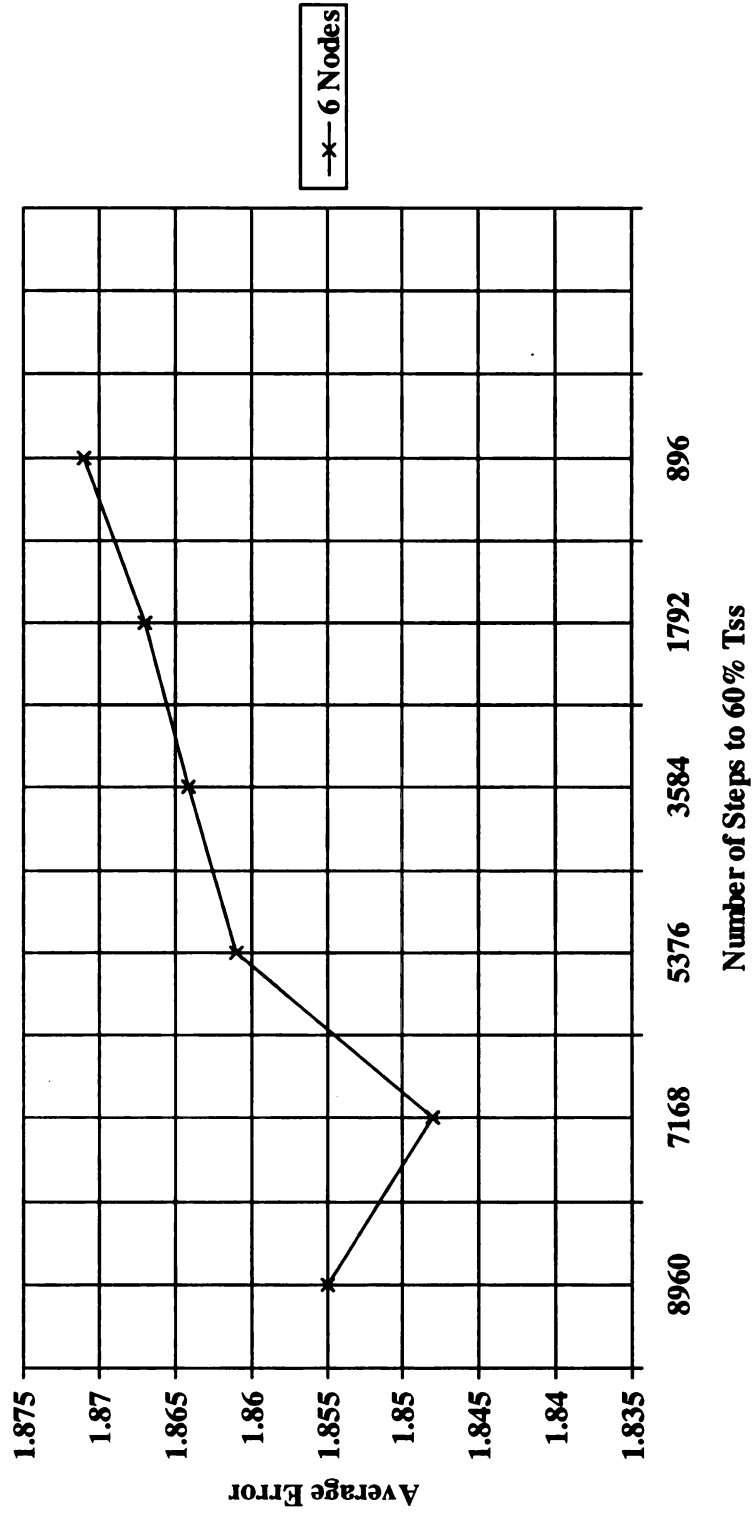


Figure 6.14

6.3.3.2 Eleven and Twenty-one Node Grid

Figure 6.15 represents the plot of the average results for the eleven and twenty one node grids. Average error remained below 0.5 percent for the smaller time steps but showed a sharp increase for the time steps larger than $0.6t_{ss}/3584$.

6.3 Analysis

After considering the individual details of each experiment, I summarized the results and developed the time step equations. The salient observations on the results are as follows:

1. The most common feature among all the calculated results is the fact that the error ratio decreases with decrease in the size of the time step, Δt . In other words, the accuracy of a numerical solution improves with the decrease in Δt . There is a Δt for some problems, however, where the error starts to increase.
2. In every scheme, there is a time step below which the improvement in accuracy is not significant and the reduction in the step size becomes counterproductive due to extra computational effort and possible round off errors.
3. There is definitely a region for Δt , where the solutions are within the desired accuracy range and show little shift with the variation of the step size. This region is between $\Delta t > 0.6t_{ss}/84$ and $\Delta t < 0.6t_{ss}/28$. This region was used to develop the a priori time step estimates.

6.4 Derivation of the A Priori Time Step Equations

The a priori time step estimate equations were developed using the numerical experiments conducted and analyzed in this chapter. Since the equations have been

RADIAL UNIFORM GRID FORWARD DIFFERENCE

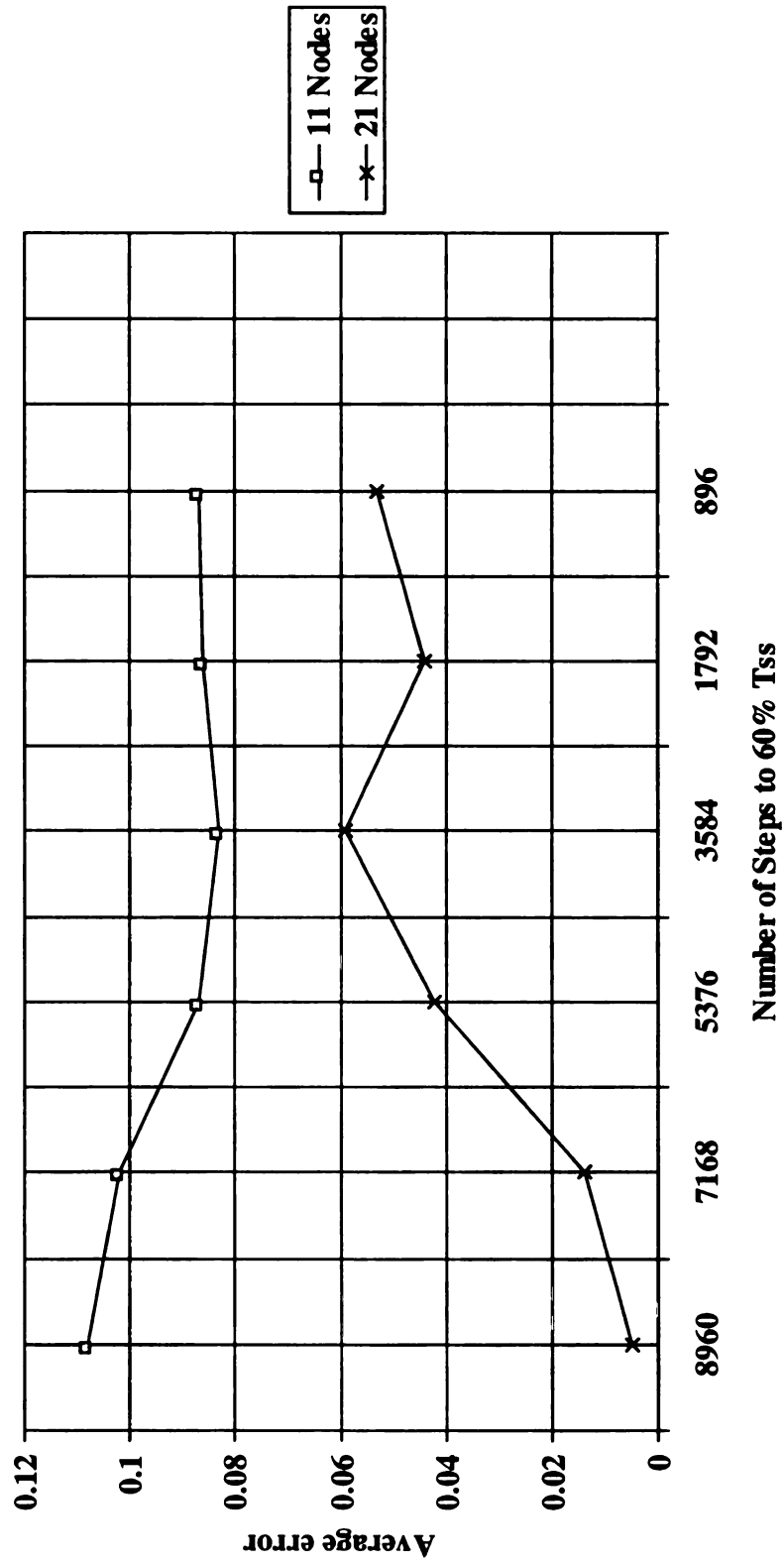


Figure 6.15

derived from step change problems, the hypothesis is that they can be used for problems with derivative boundary conditions.

Keeping in view the intricacies of the numerical schemes used, a separate equation has been developed for each scheme.

6.4.1 Central Difference

A large number of numerical experiments were conducted and analyzed. The analysis shows that accuracy level of less than one-percent has been obtained for all analysis up to a time step as larger as $0.6t_{ss}/28$. It has already been elaborated that t_{ss} has been obtained from the lowest eigenvalue λ_1 . Based on the relationship and results obtained during the numerical experiments the empirical equation deduced for the central difference time scheme is as follows:

$$\Delta t \lambda_1 = 0.025 \quad (6.1)$$

6.4.2 Backward Difference

The analysis indicates a lot of similarity between the backward difference and the central difference methods. However, it was observed that the average error remains within the limit of less than one-percent in the range of a time step around $0.6t_{ss}/56$. Therefore the empirical equation obtained for the backward difference time scheme is slightly different than the central difference:

$$\Delta t \lambda_1 = 0.05 \quad (6.2)$$

6.4.3 Forward Difference

Very small time steps were used in the forward difference scheme due to the problem of stability and oscillations associated with this scheme. Therefore, the results of forward difference method remain within the limit of desired accuracy. After deliberate

analysis it is has been found that the oscillation criteria for the forward difference method is also the accuracy criteria. The empirical equation is as follows:

$$\Delta t = \frac{1}{\lambda_{\max}} \quad (6.3)$$

These a priori time step estimation equations should provide a reasonable start point in numerical solution of the parabolic diffusion equations that approach to equilibrium. They should save considerable time by eliminating the present trial and error forecasting of Δt and eliminating the computationally expensive trials with very small time steps.

CHAPTER SEVEN

RESULTS: EQUAL VOLUME-GRID

This chapter discusses the solution of the spherical and the radial problems using an equal volume grid instead of a uniform grid. Details about the reference values, the error norm, and the solution procedures were identical to those discussed in Chapters Five and Six. Therefore, only the results of this study are presented in this chapter. A summary of the eigenvalues, time steps, average errors, maximum errors and other useful data is presented in Appendix B.

7.1 Constant Volume Spherical Grid

7.1.1 Central Difference Method in Time

Figure 7.1 graphically represents the average error for the central difference method and a six-node grid. The results were similar to the uniform grid. The average error remained above 1.4 percent for smaller time steps and showed a sharp increase for the step size larger than $0.6t_{ss}/28$. The average error for eleven and twenty-one node grids is presented in Figure 7.2. The average error remained below one percent for the time steps smaller than $0.6t_{ss}/56$, and increased rapidly after that.

7.1.2 Backward Difference Method in Time

The average error for the backward difference method and the six node grid is presented in Figure 7.3. The average error remains above 1.4 percent even for the smallest of the time step value. The average error for the eleven and twenty-one node grids is presented in Figure 7.4. Accurate results occur for Δt less than $0.6t_{ss}/56$ where the average error remained below 1 percent.

SPHERICAL EQUAL VOLUME GRID CENTRAL DIFFERENCE

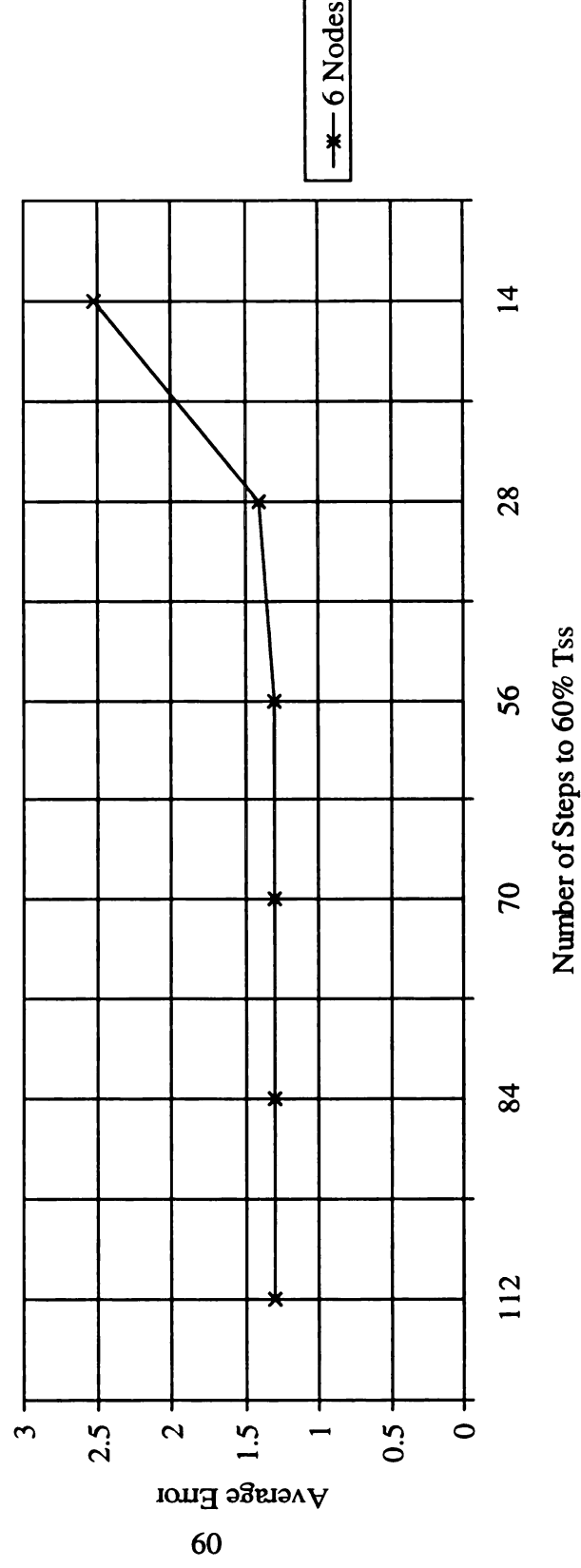


Figure 7.1

SPHERICAL EQUAL VOLUME GRID CENTRAL DIFFERENCE

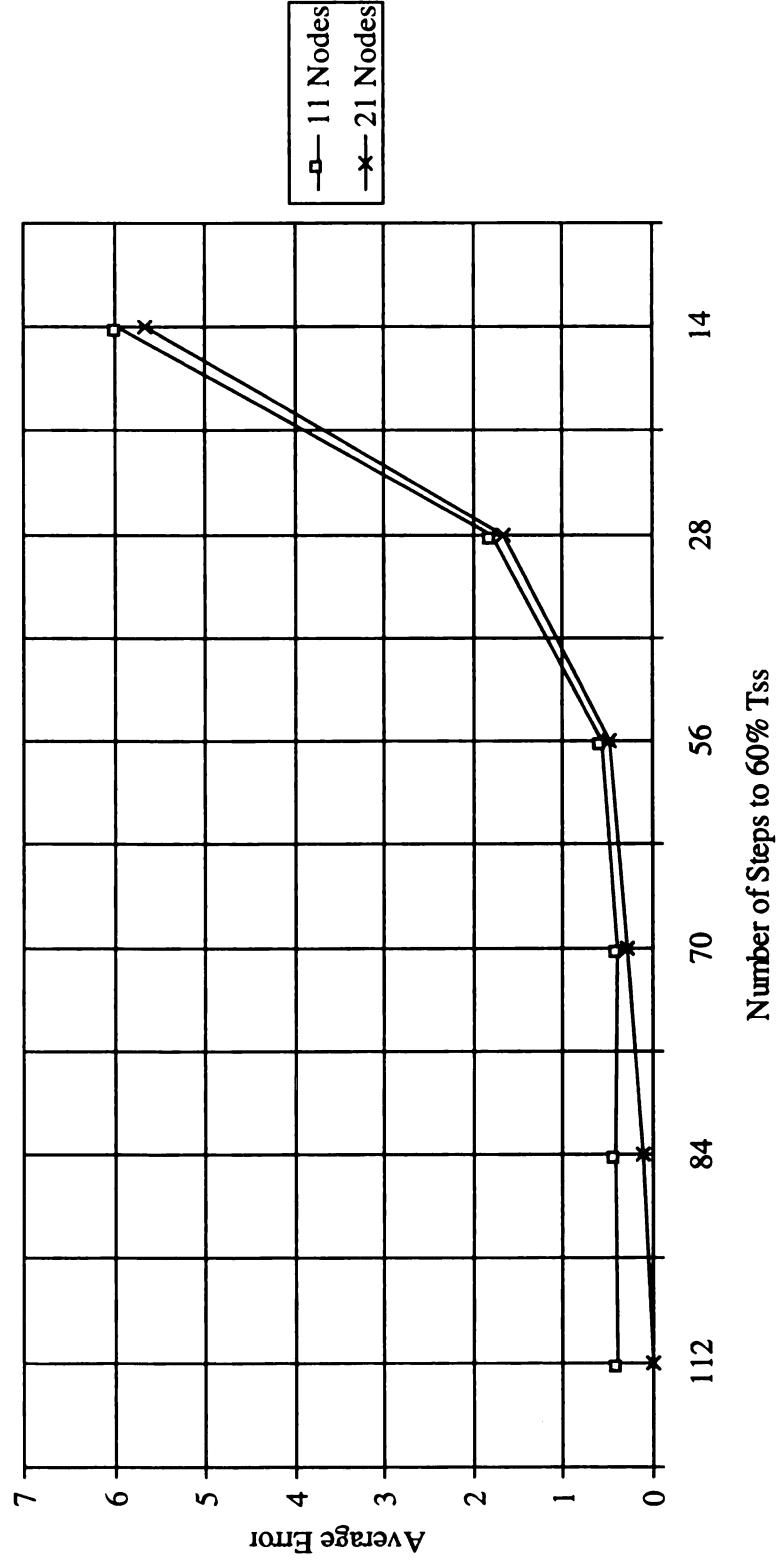


Figure 7.2

SPHERICAL EQUAL VOLUME GRID BACKWARD DIFFERENCE

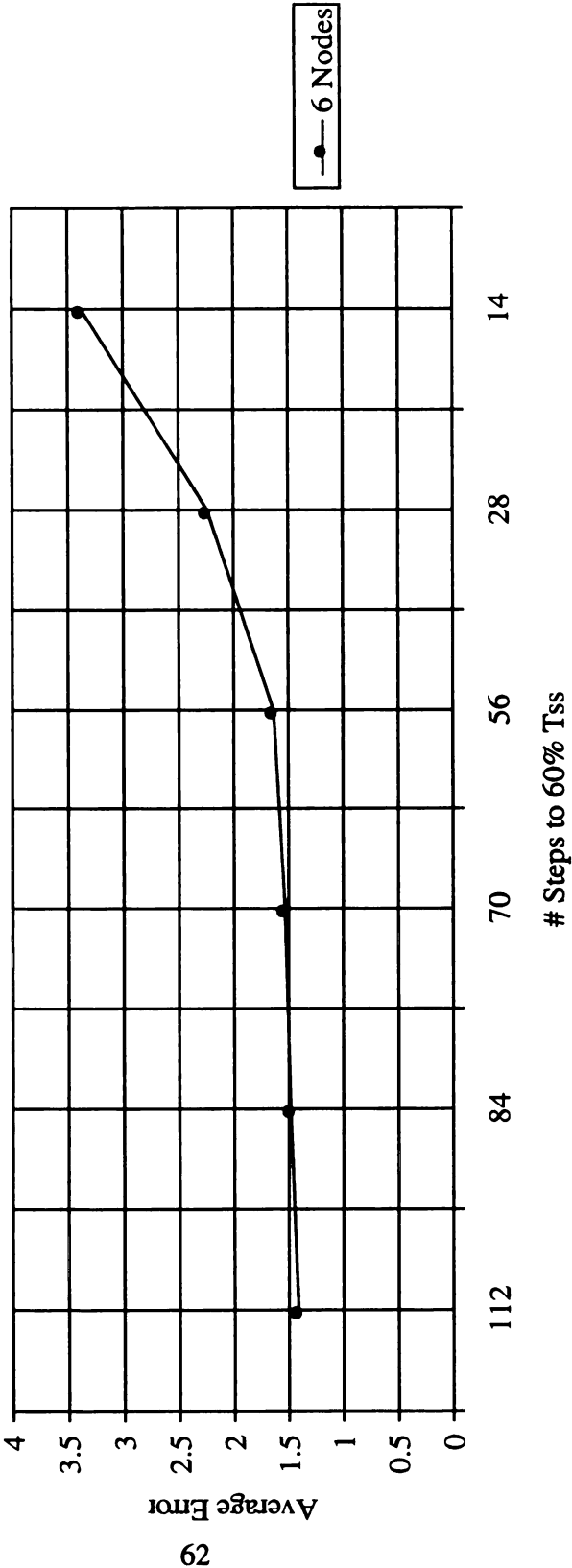


Figure 7.3

SPHERICAL EQUAL VOLUME GRID BACKWARD DIFFERENCE

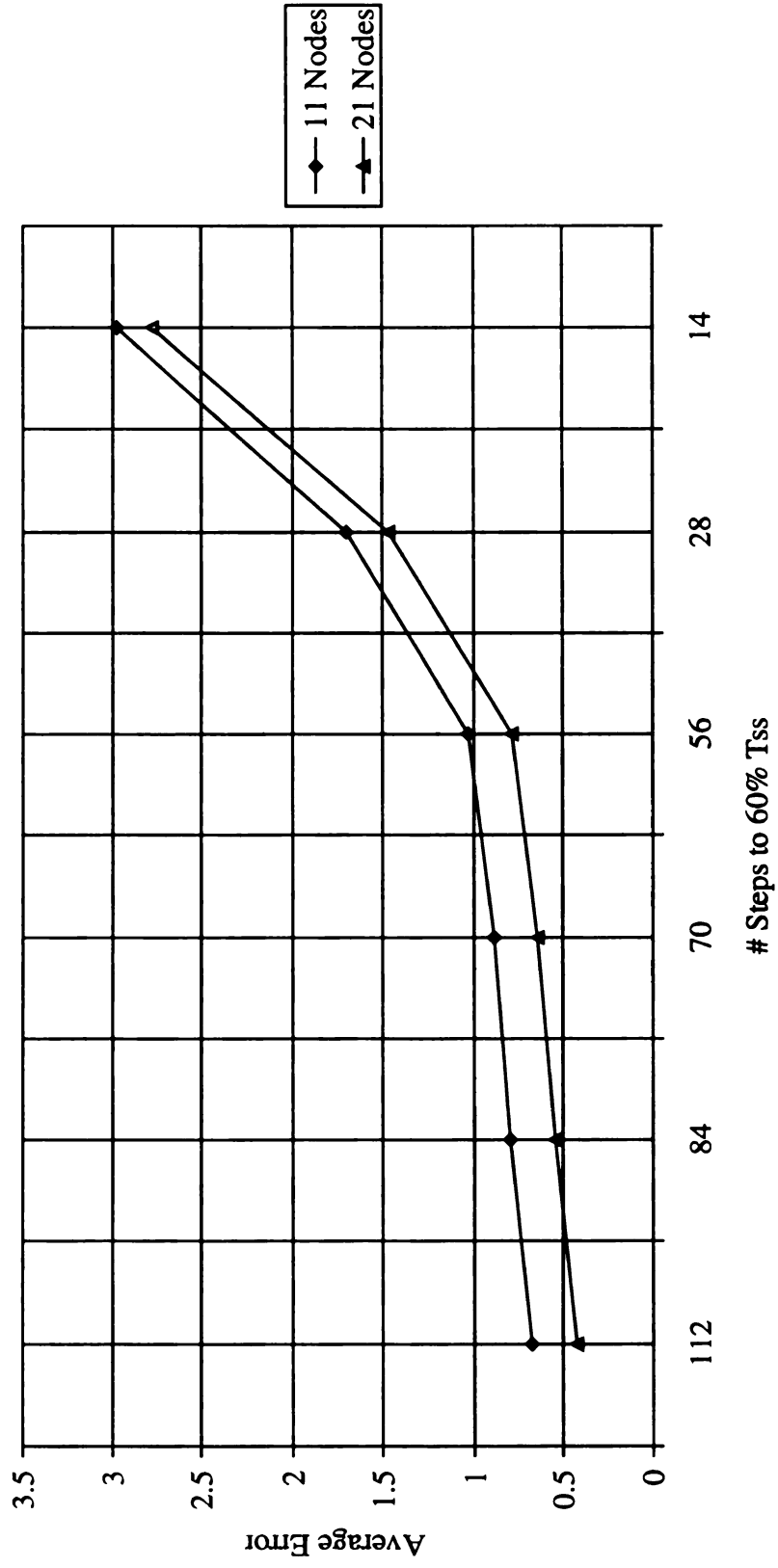


Figure 7.4

7.1.3 Forward Difference Method in Time

The time steps had to be kept very small due to an increase in $\lambda_{\max}$, for the system of differential equations. The stability and oscillation criteria depend upon the $\lambda_{\max}$.

The average error for the six node grid is presented in Figure 7.5. The average error remained above one-percent even for all time steps. The average errors for the eleven and twenty one node grid are displayed in Figure 7.6. The results were accurate and the average error remained below one percent for smaller time steps but increased rapidly for time steps larger than $0.6t_{ss}/3584$.

7.3 Radial Shapes

7.3.1 Central Difference Method in Time

Figure 7.7 exhibits the average error for central difference method six node grid, the error remained beyond two-percent. Figure 7.8 displays the plot of average error for eleven and twenty one-node grids. The results for the time steps up to $0.6t_{ss}/56$ are accurate with the average error remaining below 0.5 percent. However, the error suddenly went to 3 percent for the time steps larger than $0.6t_{ss}/28$.

7.3.2 Backward Difference Method in Time

Figure 7.9 graphically displays the average error for six node grid and. Figure 7.10 represents the average error for the eleven and twenty-one node grid. The results were accurate with the average error remaining below 0.5 percent for several time steps. The error had a sudden increase at time steps larger than $0.6t_{ss}/56$.

SPHERICAL EQUAL VOLUME GRID FORWARD DIFFERENCE

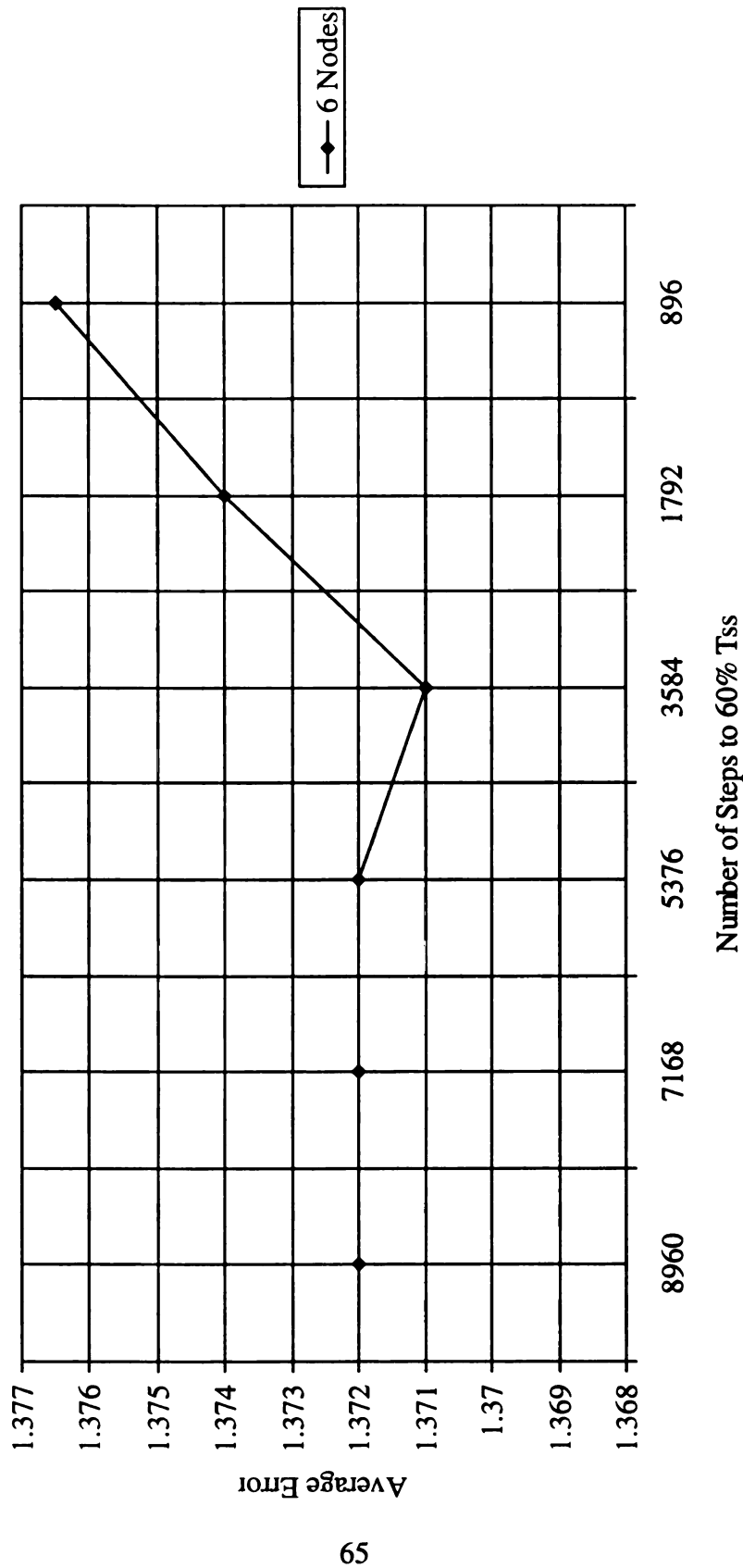


Figure 7.5

SPHERICAL EQUAL VOLUME GRID FORWARD DIFFERENCE

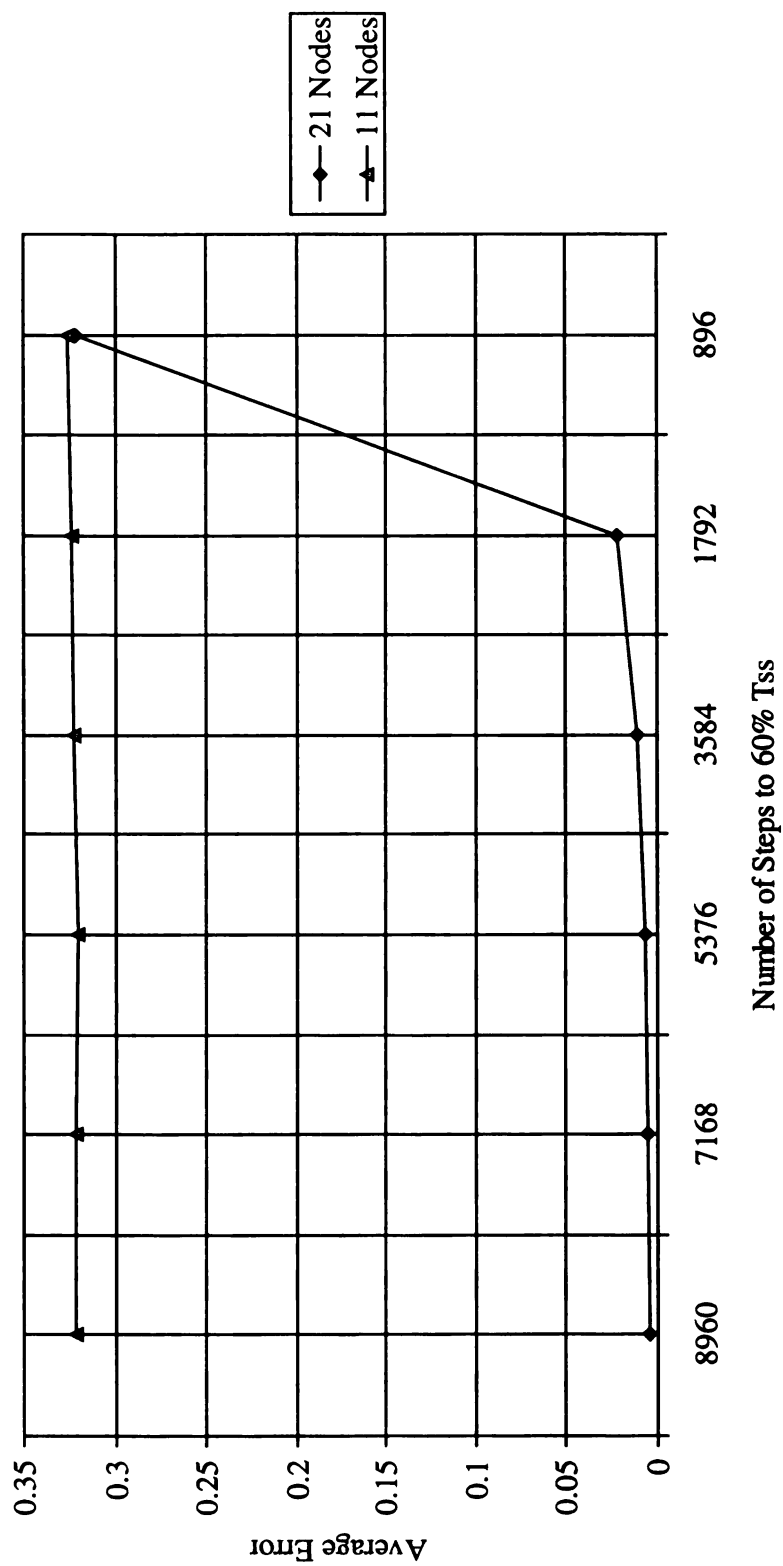


Figure 7.6

RADIAL CONSTANT VOLUME GRID CENTRAL DIFFERENCE

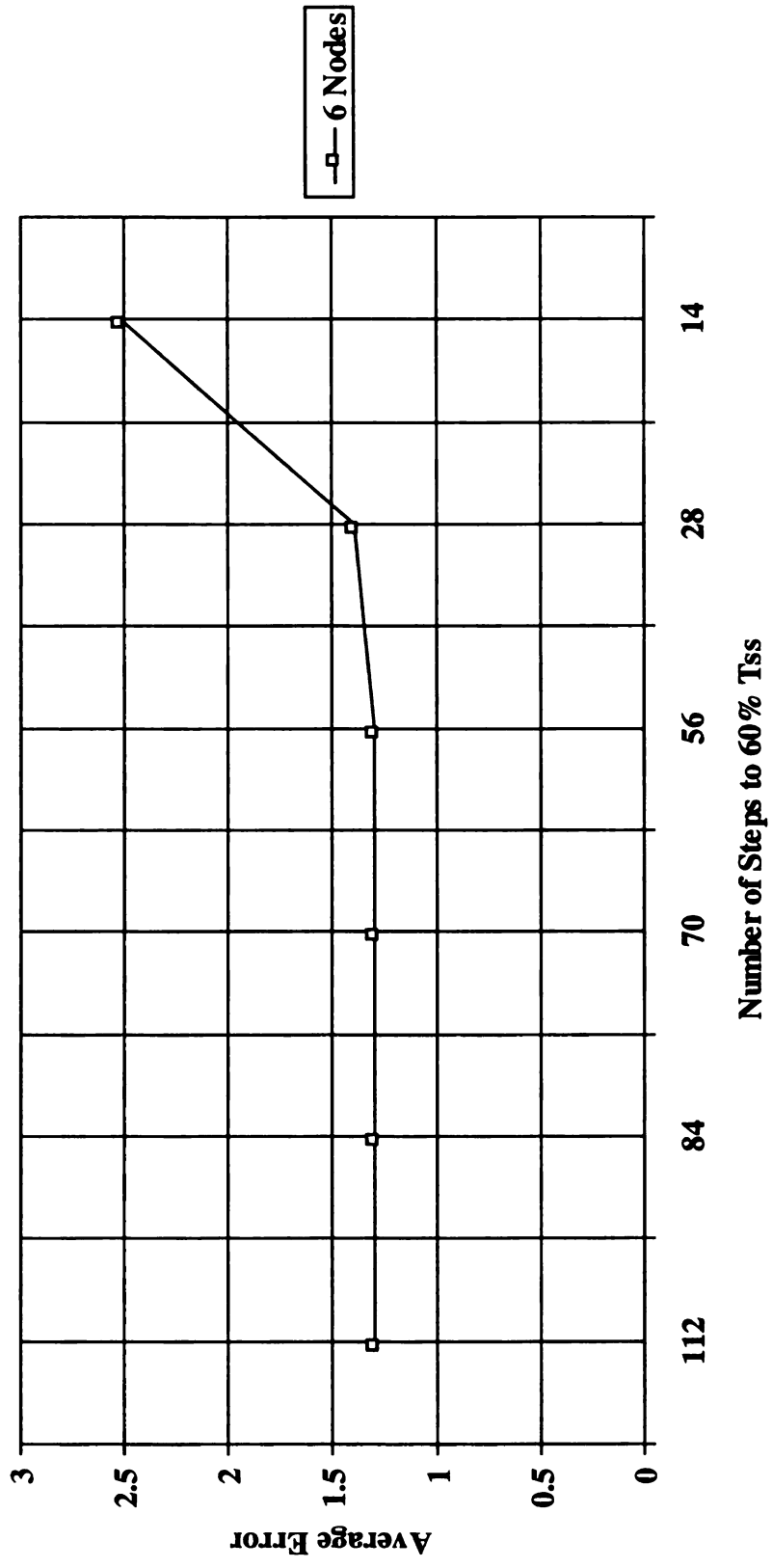


Figure 7.7

RADIAL CONSTANT VOLUME GRID CENTRAL DIFFERENCE

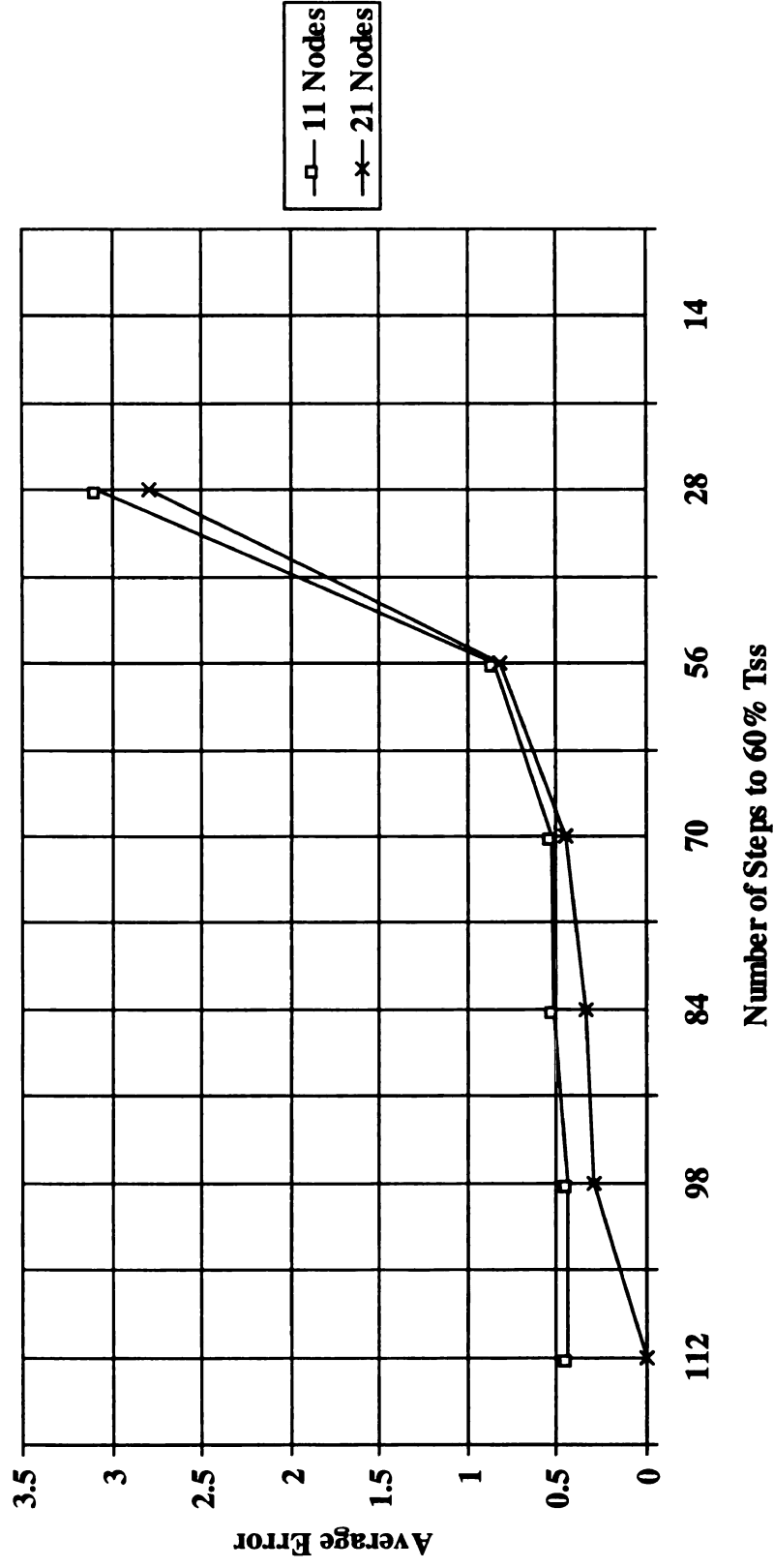


Figure 7.8

RADIAL CONSTANT VOLUME GRID BACKWARD
DIFFERENCE

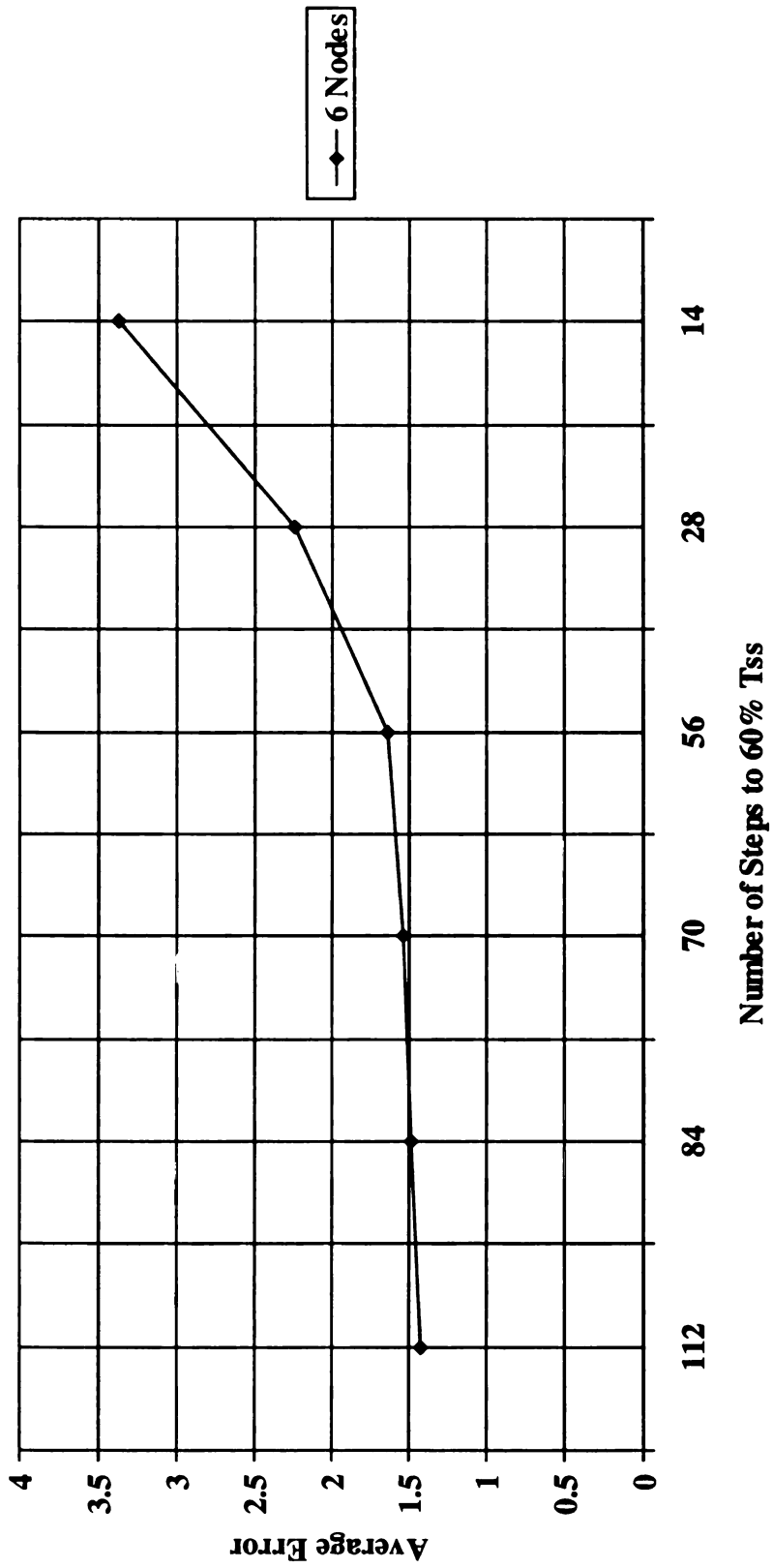


Figure 7.9

RADIAL CONSTANT VOLUME GRID BACKWARD DIFFERENCE

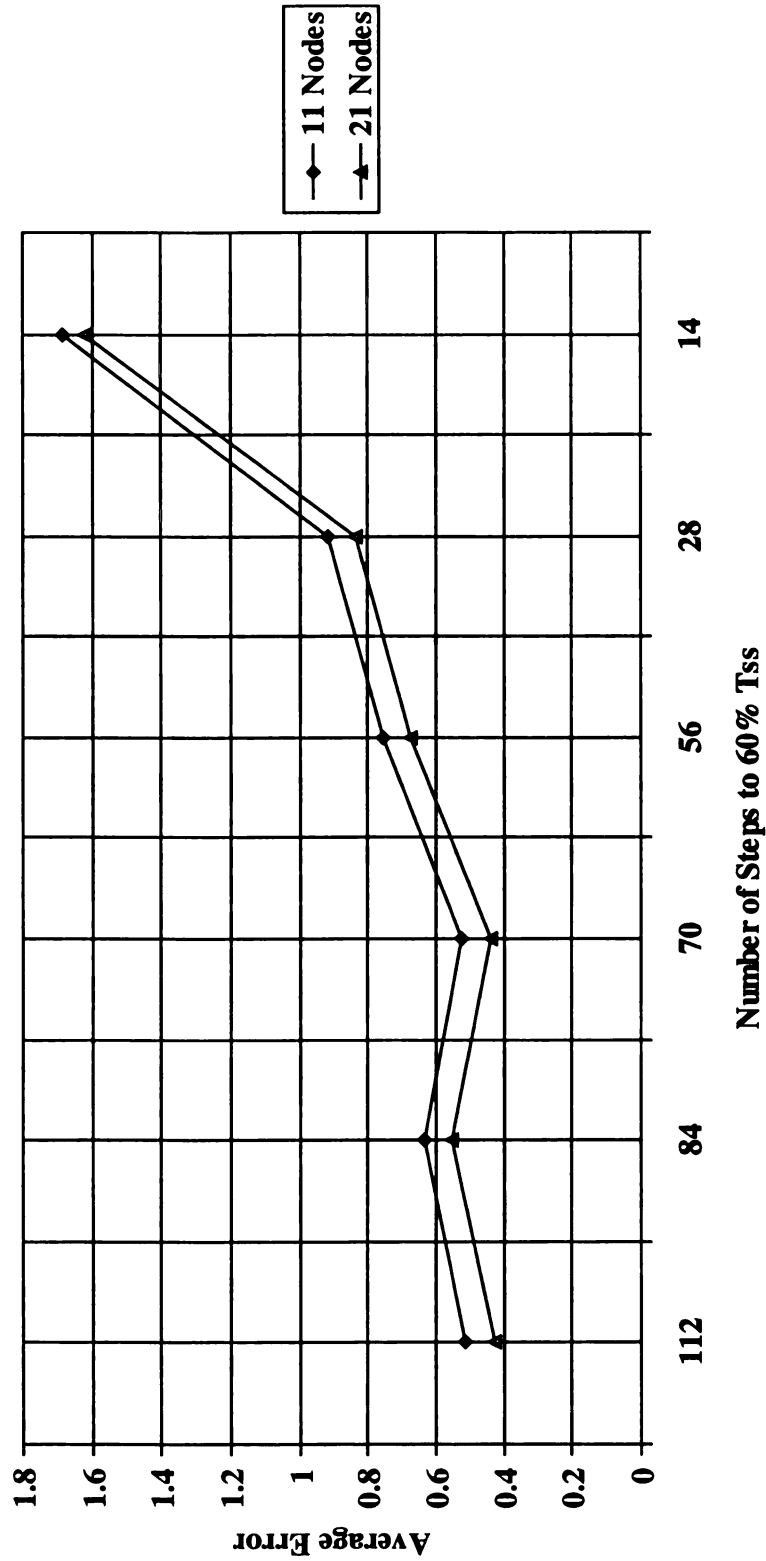


Figure 7.10

7.3.3 Forward Difference Method in Time

Figure 7.11 displays the average error for forward difference method in six node grid. The results remain inaccurate. Figure 7.12 represents the plot of the average results for eleven and twenty one node grids. Average error remained below 0.5 percent for the smaller time steps but shows a sharp increase for the time steps larger than $0.6t_{ss}/3584$.

7.4 Analysis

A large number of experiments were carried out on the problems already solved by using the equal volume grid instead of the uniform grid. Radial length of the elements was varied in such a manner that the volume of each element was kept equal. Review of the analysis of these experiments is as follows:

1. There are no perceptible advantages associated with the equal volume grid.
2. However, the major disadvantage noticed during the study was a noteworthy increase in the maximum eigenvalues of the system of equations generated by using the equal volume grid. This phenomenon was observed in both, the spherical as well as the radial problems.
3. Figure 7.13 presents a graphical comparison of the maximum eigenvalues of the equal volume grids with uniform grid for spherical problems. Similarly, Figure 7.14 gives the comparison of maximum eigenvalues associated with radial problems.
4. The variance in the minimum eigenvalues of the system of equations using equal volume grid as compared to uniform grid was not significant.
5. Figure 7.15 displays the comparison of the lowest eigenvalues of the equal volume grid with the uniform grid for spherical problems. Figure 7.16 gives a similar comparison for the lower eigenvalues associated with radial problems.

RADIAL EQUAL VOLUME GRID FORWARD DIFFERENCE

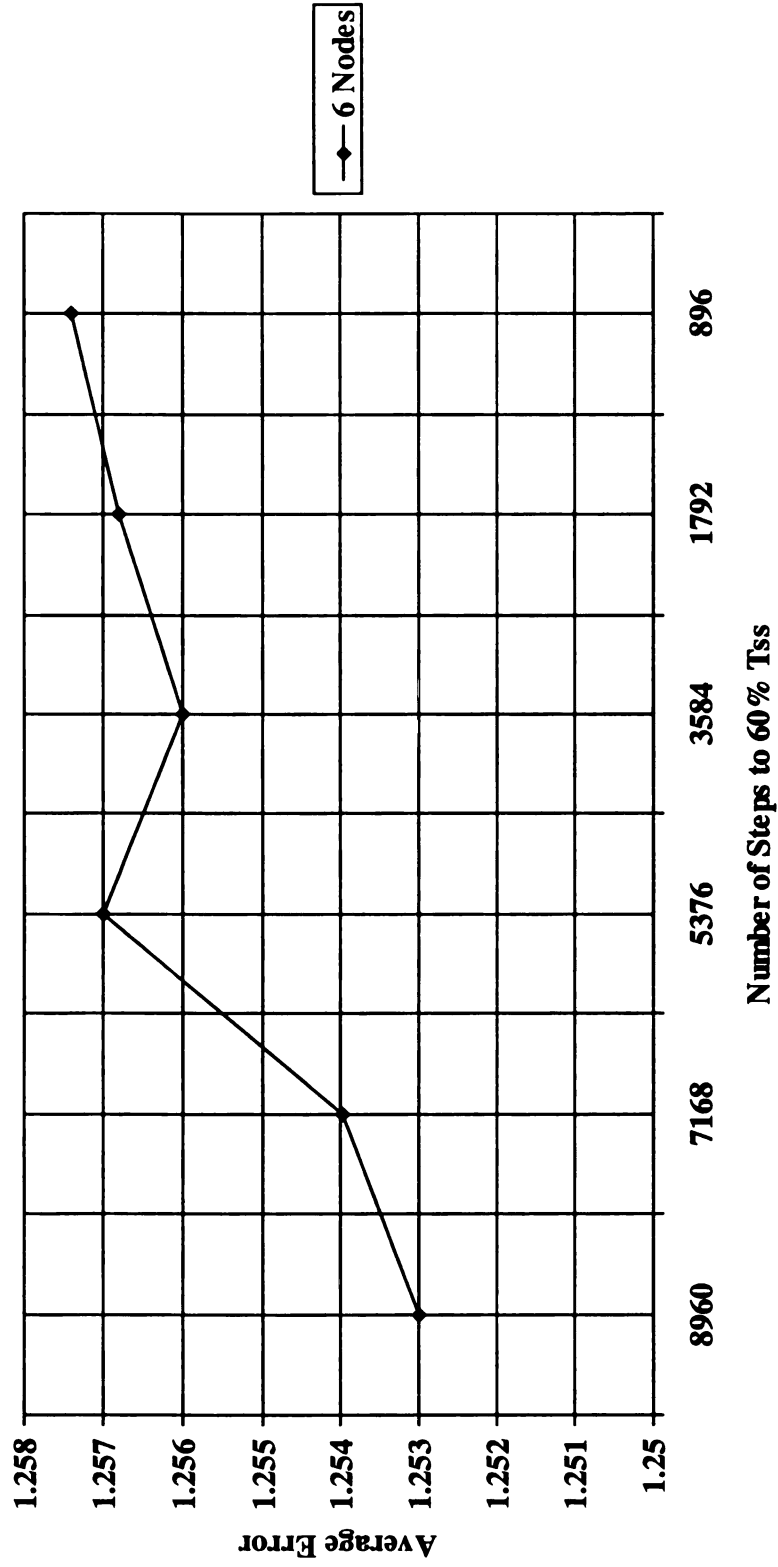


Figure 7.11

RADIAL EQUAL VOLUME GRID FORWARD DIFFERENCE

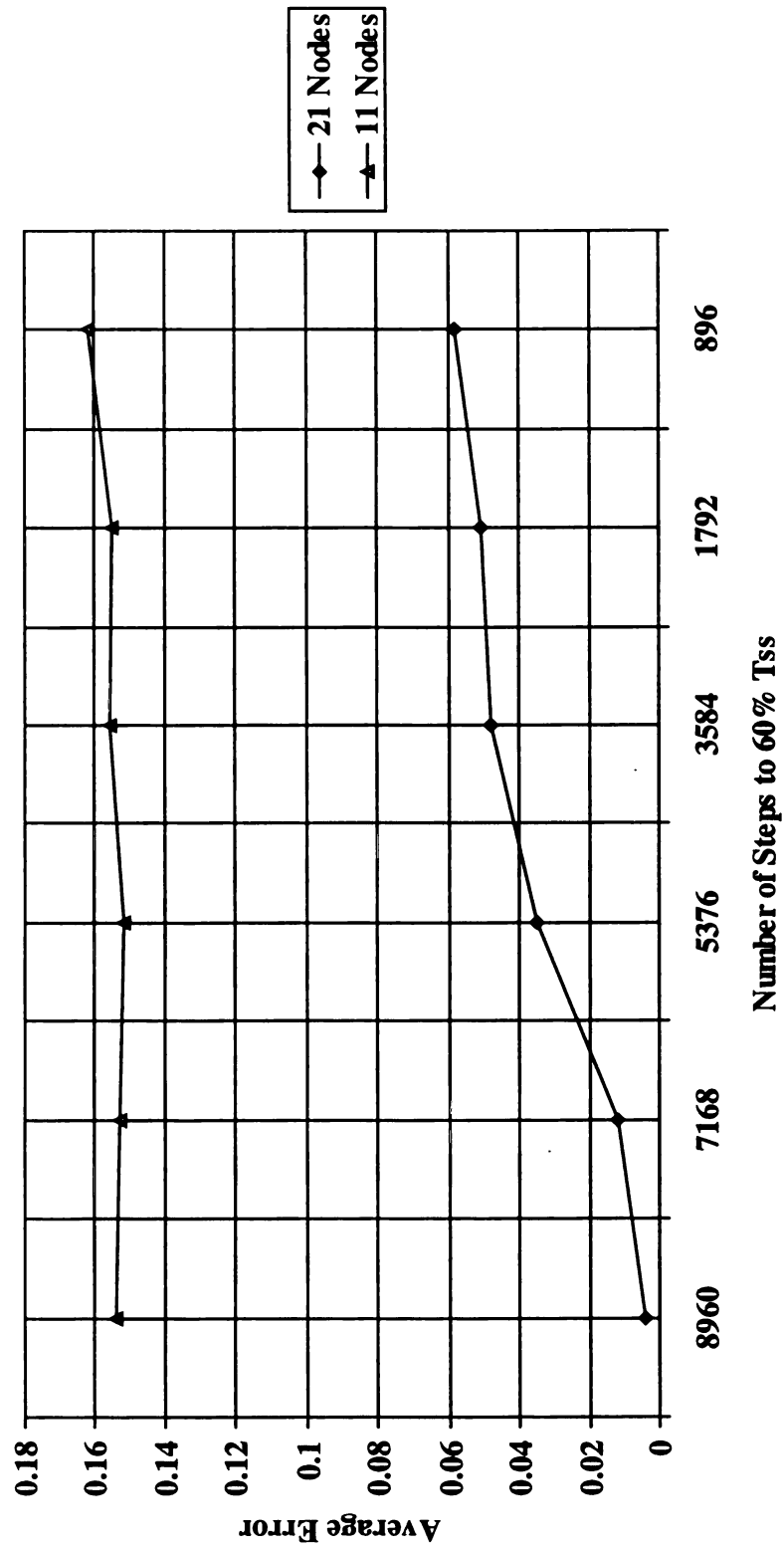


Figure 7.12

SPHERICAL PROBLEM MAXIMUM EIGENVALUES

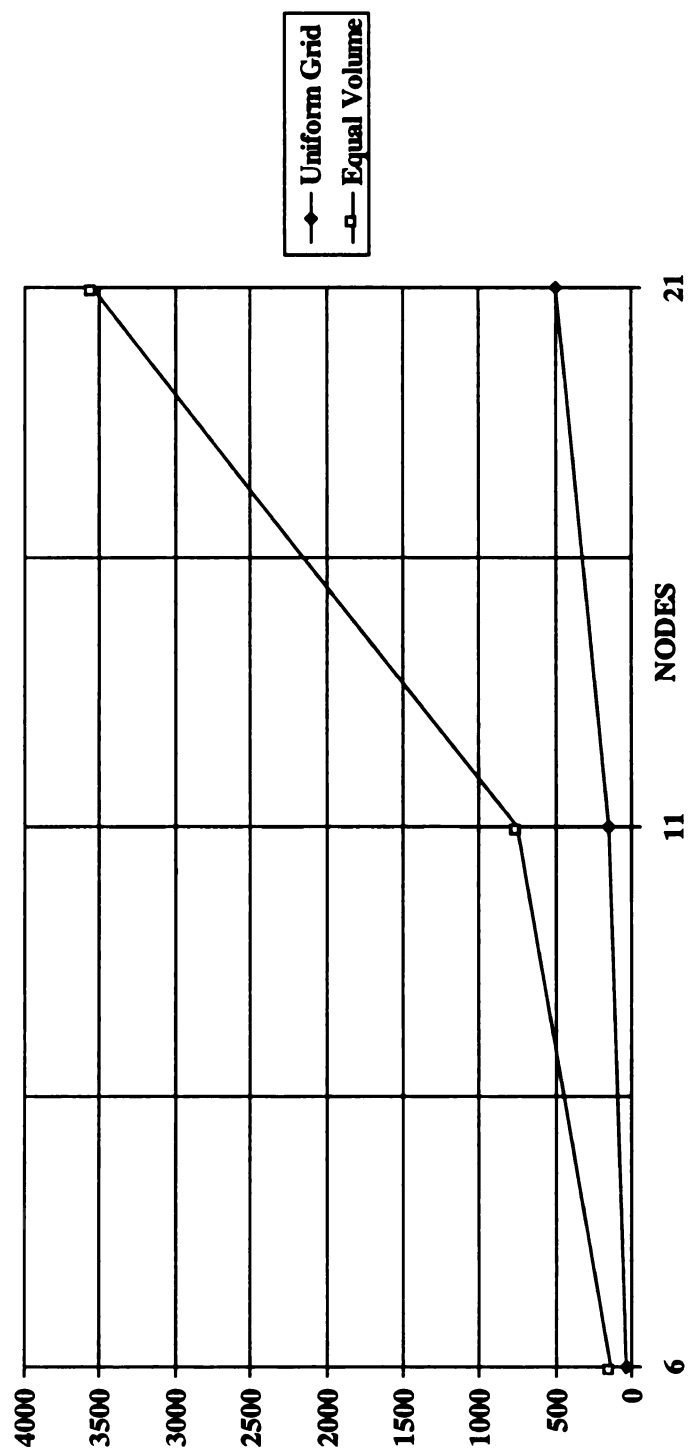


Figure 7.13

SPHERICAL PROBLEM MINIMUM EIGENVALUES

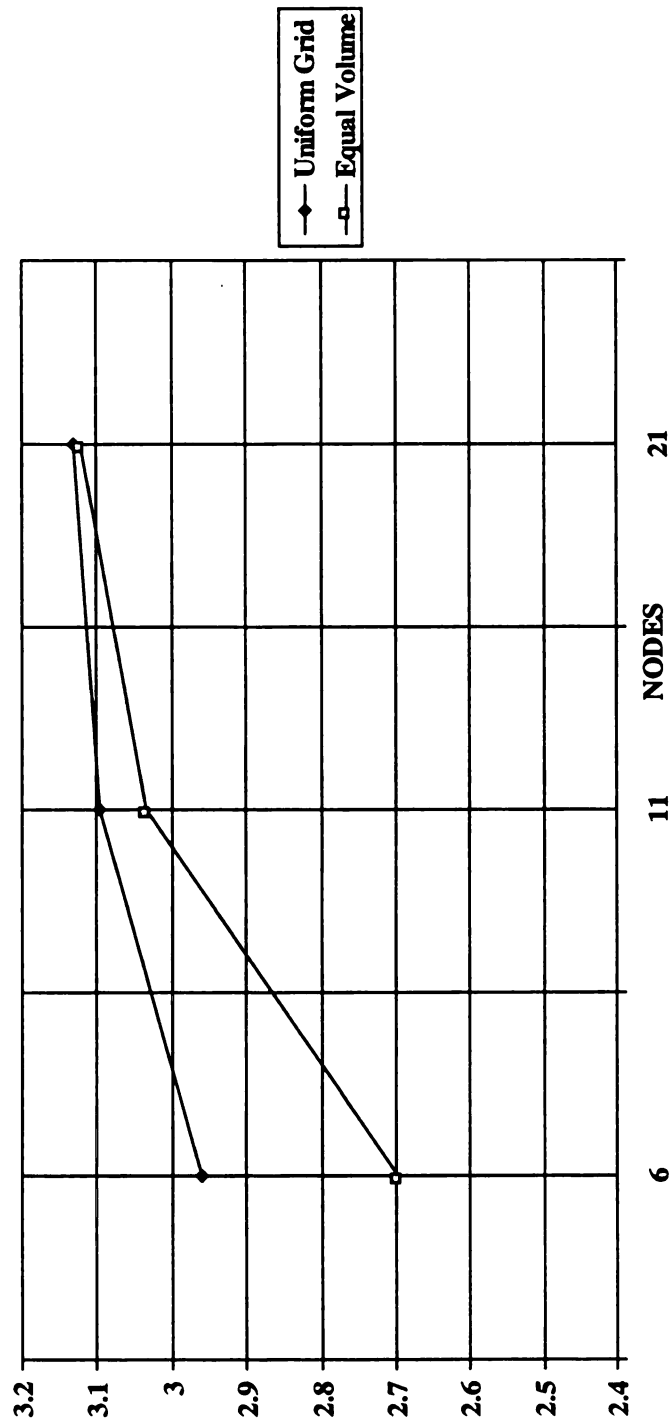


Figure 7.14

RADIAL PROBLEM MAXIMUM EIGENVALUES

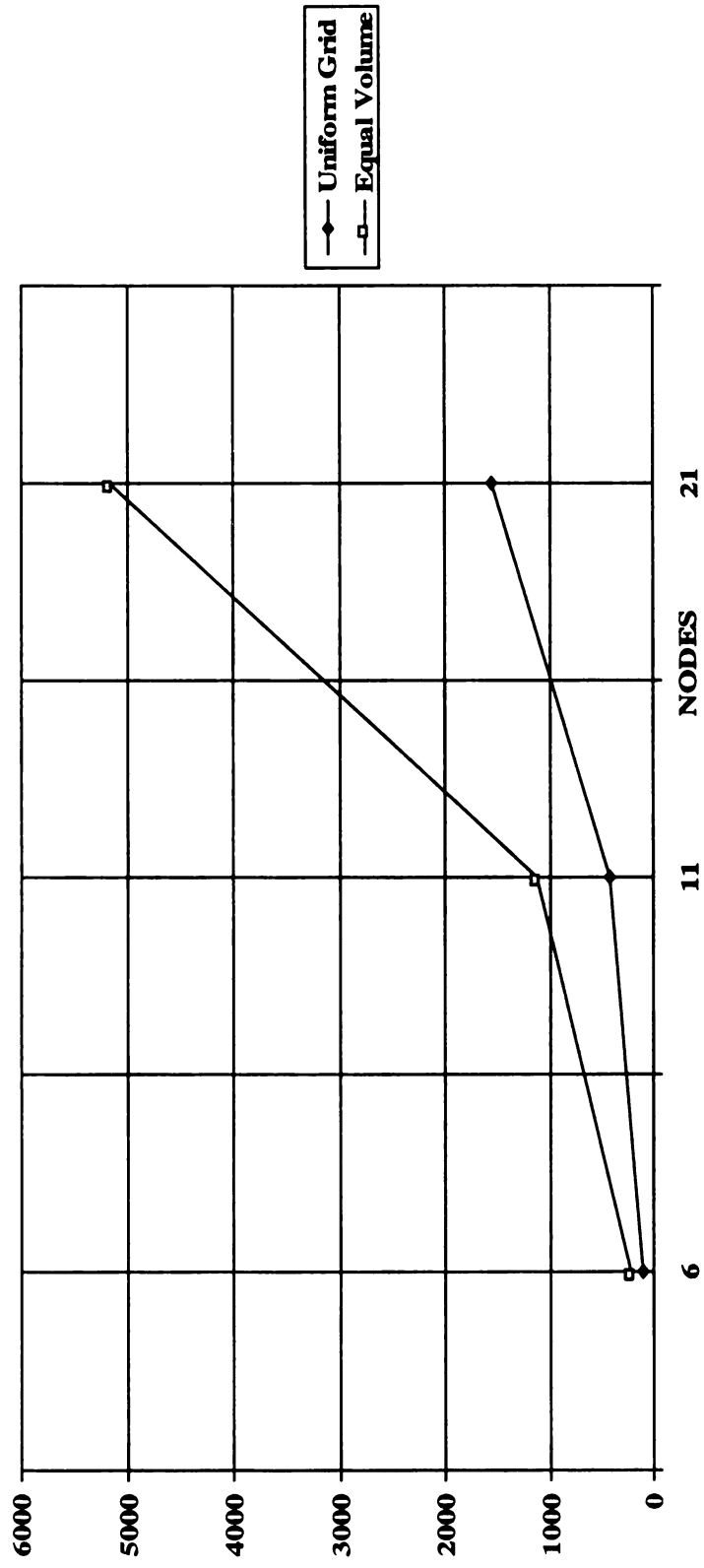


Figure 7.15

RADIAL PROBLEM MINIMUM EIGENVALUES

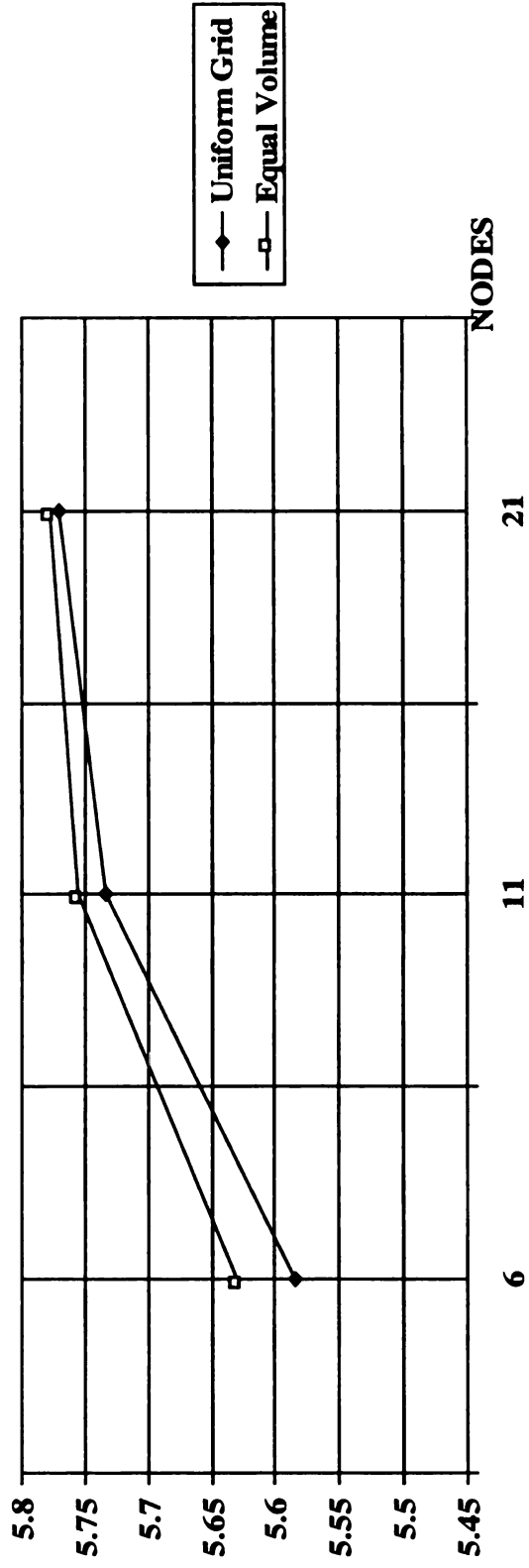


Figure 7.16

CHAPTER EIGHT

EVALUATION OF THE TIME STEP ESTIMATES

This chapter recommends a procedure to apply the empirical time step equations for the solution of spherical and radial field problems. This chapter also deals with the verification of the time step estimates by applying them to the numerical solution of problems different than what were used during the numerical experimentation.

8.1 A Priori Procedure

The recommended procedure for handling the numerical solution in the light of the prepriorri time step equations is as follows:

1. Calculate λ_1 and $\lambda_{\max}$ for the system of ordinary differential equations developed using the finite element method or finite difference method in space.
2. Calculate Δt for the intended numerical scheme using equations 6.1, 6.2 or 6.3.
3. Round Δt to a convenient value. Round the value down for step change boundary conditions. The value can be rounded up for convection boundary conditions.
4. Solve the problem using the numerical scheme selected, printing the calculated values as desired.

8.2 Evaluation

The time step estimates presented in Chapter Six were developed using the step change problem on a solid sphere and solid cylinder of radius one and assuming $Dr=Dt=1$. The ability of these equations to predict the time step for real problems was evaluated using different materials and other boundary conditions.

The comparison problems were chosen with real values of the material properties and realistic dimensions with the convection boundary conditions. The results

proved that the empirical a priori time step estimate equations produce reasonable results and maintain the desired level of accuracy. A number of experiments were conducted to verify the developed a priori equations. However, for the purpose of clarity results of a radial problem with convection boundary conditions and actual physical properties are displayed in the form of graphs and analyzed.

The Figure 8.1 presents the average error for eleven and twenty-one node central difference method. It is clearly evident that the desired accuracy level of less than one percent is available for the value of Δt lesser than $0.6t_{ss}/28$. Similarly Figure 8.2 displays the average error for eleven and twenty-one node grid using backward difference scheme and verifies our a priori time step estimate equation.

Figures 8.3 and 8.4 present the plot of maximum error for central difference and forward difference methods. It is indicated by the graphs that the maximum error remains within the specified range for both the schemes.

RADIAL VARIFICATION PROBLEM CENTRAL DIFFERENCE

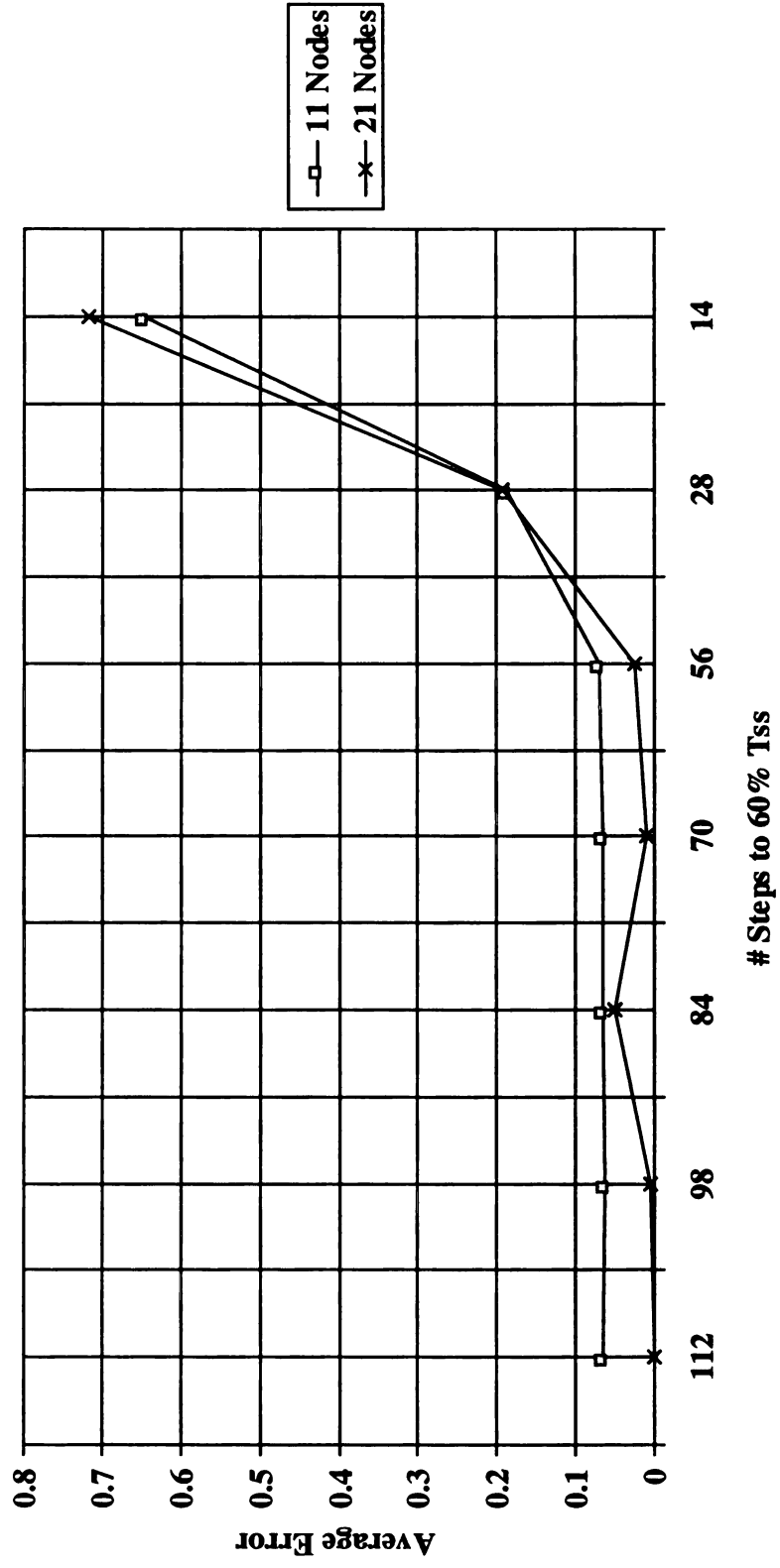


Figure 8.1

RADIAL VARIFICATION PROBLEM BACKWARD DIFFERENCE

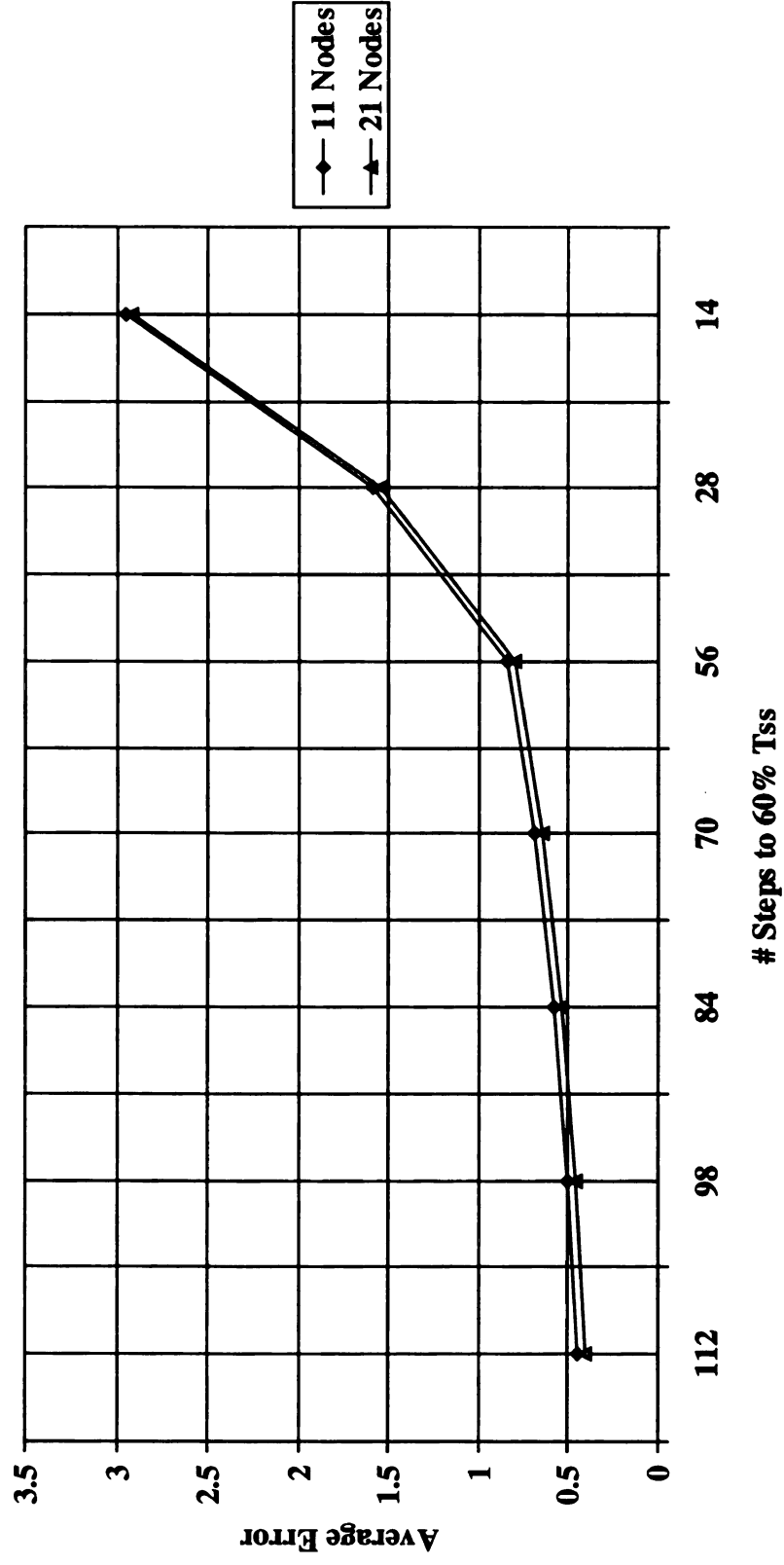


Figure 8.2

RADIAL VARIFICATION PROBLEM CENTRAL DIFFERENCE

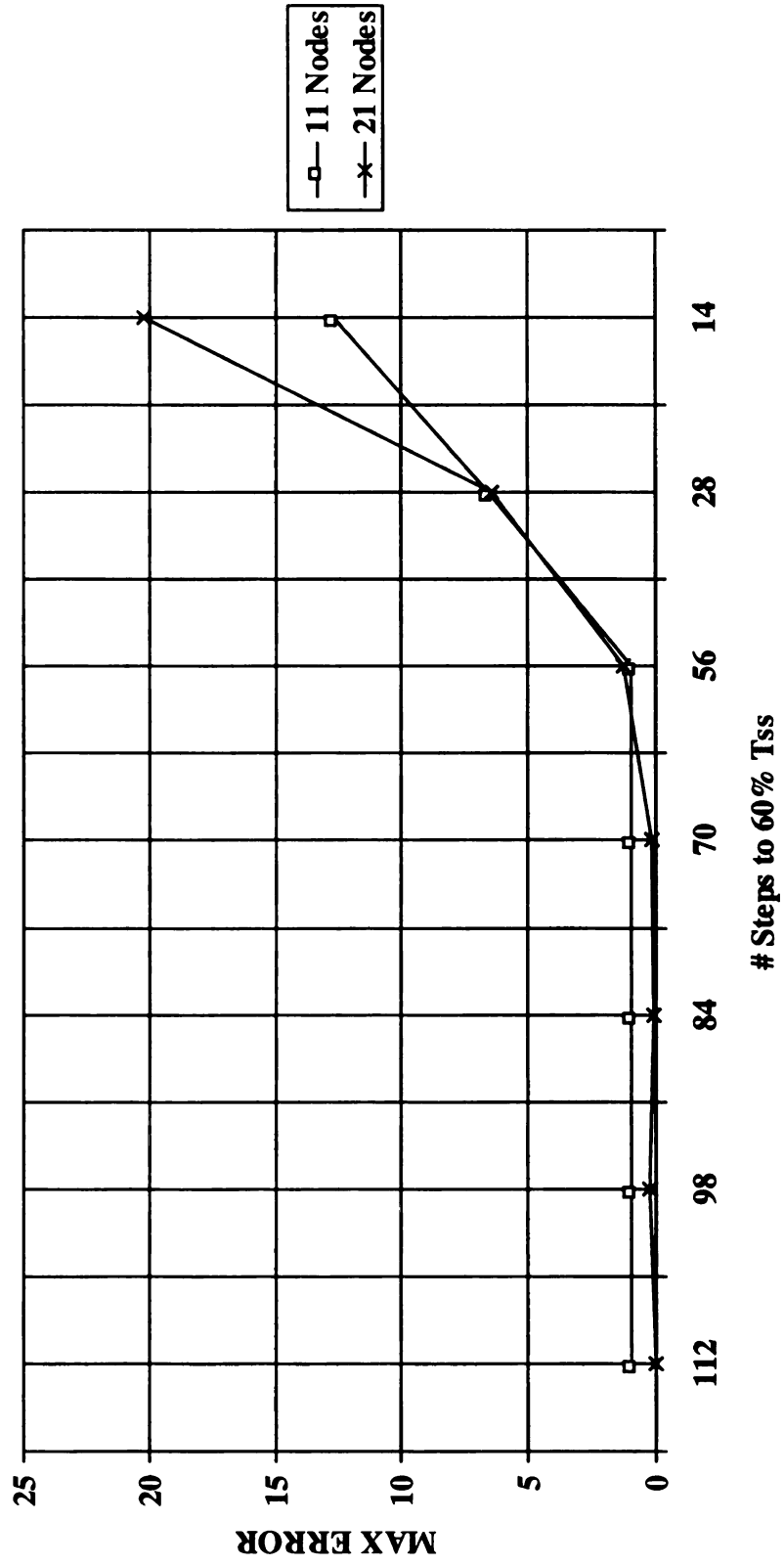


Figure 8.3

RADIAL VARIFICATION PROBLEM BACKWARD DIFFERENCE

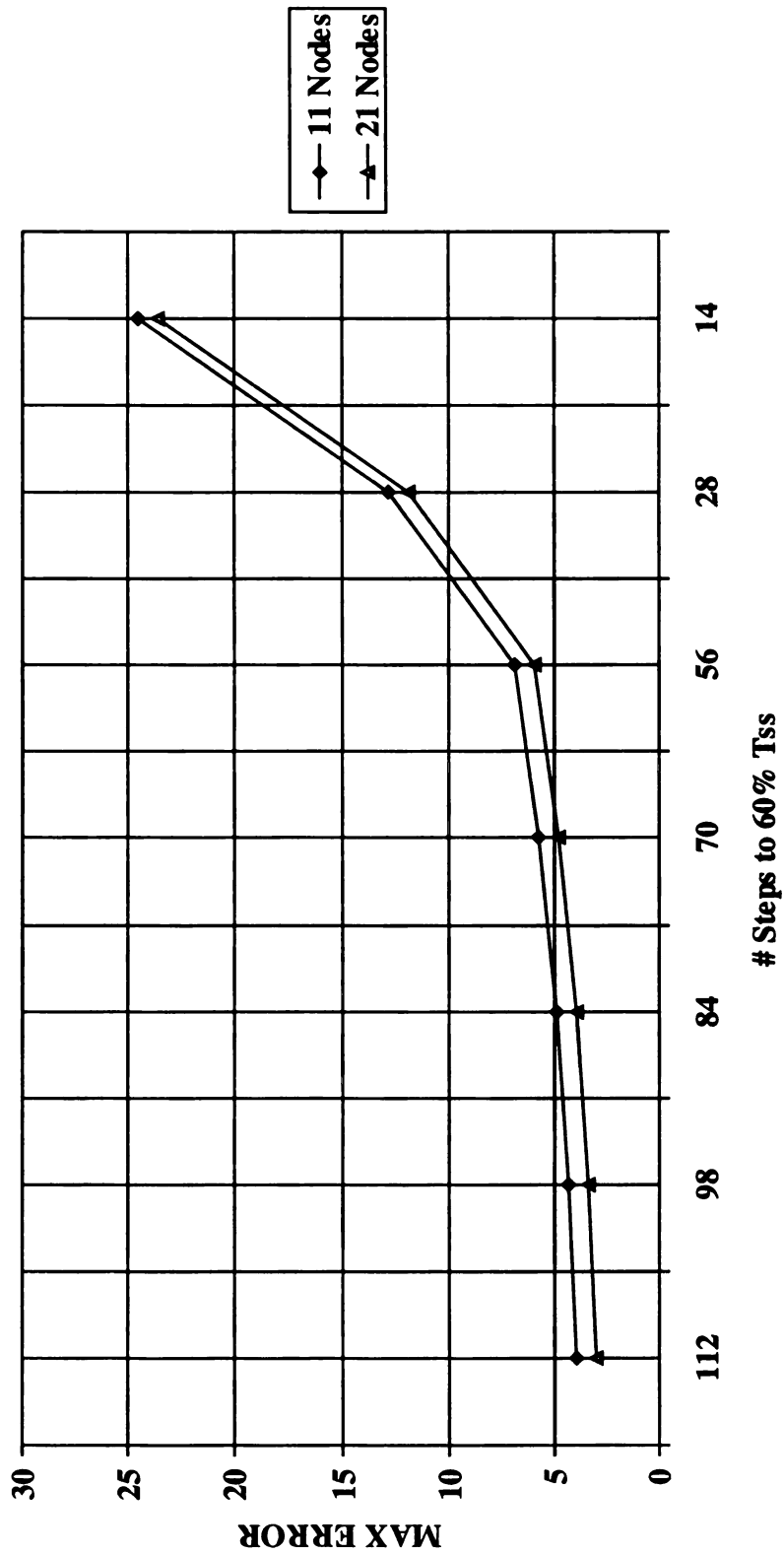


Figure 8.4

CHAPTER NINE

DISCUSSION AND CONCLUSION

The empirical equations for calculating the prepriorri time step estimate to solve the system of ordinary differential equations for spherical and radial field problems have been successfully accomplished and verified. The prepriorri time step estimates, meet all accuracy criteria or the stability requirements (equations 6.1, 6.2 and 6.3).

The forward difference method is conditionally stable; therefore, both λ_1 and $\lambda_{\max}$ must be evaluated, λ_1 is utilized to acquire the t_{ss} and $\lambda_{\max}$ is used for estimating the prepriorri time step. Time step value calculated for forward difference method should be rounded down because of the stability and oscillation criteria. The time step values for the central and backward difference schemes can be rounded up or down, to a suitable value for easy division by integers and displaying the results.

The prepriorri time step estimate equations define a time step that will give overall accurate results and not at any particular time. It has been observed that the error distribution is not linear through out the time domain. The error is highest at small time values and dies out as time increases. The distribution also changes with the integration scheme. Some schemes are more accurate than others at the same point in the time domain. The fact that the error is highest at small time values might explain why in the central difference scheme increasing the time step did not reduce the accuracy. In the later scheme, the inaccuracies present at small time values will not be included for large values of the time step. On the other hand smaller time steps capture the numerical error present at small time values.

10.1 Future Study

1. It is recommended that two and three-dimensional problems be studied in details and validity of the existing empirical equations should be observed on them and prospect of evolving new empirical equations may also be carefully thought about.
2. Application of the empirical prepriorri time step equations to composite materials and materials with multiple layers of insulation should also be studied.

APPENDIX A

Radial	Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
<i>Uniform Grid</i>							
0	6						
	8960	0.5012	5.5938E-05	1.855	3.58	5.5856	102.6
	7168	0.5012	6.9922E-05	1.848	6.77	5.5856	102.6
	5376	0.5012	9.3229E-05	1.861	5.86	5.5856	102.6
	3584	0.5012	0.00013984	1.864	11.47	5.5856	102.6
	1792	0.5012	0.00027969	1.867	12.667	5.5856	102.6
	896	0.5012	0.00055938	1.871	14.324	5.5856	102.6
	0.5						
	112	0.5012	0.00447500	1.86	118.352	5.5856	102.6
	98	0.5012	0.00511429	1.97	120.056	5.5856	102.6
1	84	0.5012	0.00596667	1.766	114.936	5.5856	102.6
	70	0.5012	0.00716000	1.853	118.301	5.5856	102.6
	56	0.5012	0.00895000	1.847	118.255	5.5856	102.6
	28	0.5012	0.01790000	1.815	117.872	5.5856	102.6
	14	0.5012	0.03580000	1.766	116.34	5.5856	102.6
	1						
	112	0.5012	0.00447500	2.234	126.033	5.5856	102.6
	98	0.5012	0.00511429	1.692	128.861	5.5856	102.6

	Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
0	84	0.5012	0.00596667	2.244	125.153	5.5856	102.6
	70	0.5012	0.00716000	2.465	130.63	5.5856	102.6
	56	0.5012	0.00895000	2.616	133.698	5.5856	102.6
	28	0.5012	0.01790000	3.372	149.06	5.5856	102.6
	14	0.5012	0.03580000	4.769	179.908	5.5856	102.6
	8960	0.5012	5.5938E-05	0.108	1.4	5.7329	410.31
	7168	0.5012	6.9922E-05	0.102	2.47	5.7329	410.31
	5376	0.5012	9.3229E-05	0.087	2.68	5.7329	410.31
	3584	0.5012	0.00013984	0.083	3.014	5.7329	410.31
0.5	1792	0.5012	0.00027969	0.086	3.694	5.7329	410.31
	896	0.5012	0.00055938	0.087	4.574	5.7329	410.31
	112	0.5012	0.00447500	0.112	1.865	5.7329	410.31
	98	0.5012	0.00511429	0.167	2.681	5.7329	410.31
	84	0.5012	0.00596667	0.114	0.543	5.7329	410.31
	70	0.5012	0.00716000	0.106	1.84	5.7329	410.31
	56	0.5012	0.00895000	0.105	1.817	5.7329	410.31
	28	0.5012	0.01790000	0.228	12.917	5.7329	410.31
	14	0.5012	0.03580000	1.346	106.991	5.7329	410.31
1							
	112	0.5012	0.00447500	0.514	6.457	5.7329	410.31
	98	0.5012	0.00511429	0.635	7.469	5.7329	410.31

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	Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
0	84	0.5012	0.00596667	0.526	8.074	5.7329	410.31
	70	0.5012	0.00716000	0.757	10.025	5.7329	410.31
	56	0.5012	0.00895000	0.917	12.467	5.7329	410.31
	28	0.5012	0.01790000	1.687	25.01	5.7329	410.31
	14	0.5012	0.03580000	3.113	49.018	5.7329	410.31
	8960	0.5012	5.5938E-05	0.005	1.57	5.7706	1558.3
	7168	0.5012	6.9922E-05	0.014	1.364	5.7706	1558.3
	5376	0.5012	9.3229E-05	0.042	1.95	5.7706	1558.3
	3584	0.5012	0.00013984	0.059	2.56	5.7706	1558.3
	1792	0.5012	0.00027969	0.044	3.12	5.7706	1558.3
0.5	896	0.5012	0.00055938	0.053	4.01	5.7706	1558.3
	112	0.5012	0.00447500	0	6.05	5.7706	1558.3
	98	0.5012	0.00511429	0.079	0.954	5.7706	1558.3
	84	0.5012	0.00596667	0.16	2.565	5.7706	1558.3
	70	0.5012	0.00716000	0.033	5.511	5.7706	1558.3
	56	0.5012	0.00895000	0.075	12.427	5.7706	1558.3
	28	0.5012	0.01790000	0.441	31.54	5.7706	1558.3
	14	0.5012	0.03580000	1.572	287.102	5.7706	1558.3
	112	0.5012	0.00447500	0.428	5.973	5.7706	1558.3
	98	0.5012	0.00511429	0.554	6.977	5.7706	1558.3
1	84	0.5012	0.00596667	0.526	8.074	5.7329	410.31
	70	0.5012	0.00716000	0.757	10.025	5.7329	410.31
	56	0.5012	0.00895000	0.917	12.467	5.7329	410.31
	28	0.5012	0.01790000	1.687	25.01	5.7329	410.31
	14	0.5012	0.03580000	3.113	49.018	5.7329	410.31
	8960	0.5012	5.5938E-05	0.005	1.57	5.7706	1558.3
	7168	0.5012	6.9922E-05	0.014	1.364	5.7706	1558.3
	5376	0.5012	9.3229E-05	0.042	1.95	5.7706	1558.3
	3584	0.5012	0.00013984	0.059	2.56	5.7706	1558.3
	1792	0.5012	0.00027969	0.044	3.12	5.7706	1558.3

21

Spherical

Uniform Grid

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Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
84	0.5012	0.00596667	0.439	7.582	5.7706	1558.3
70	0.5012	0.00716000	0.675	9.529	5.7706	1558.3
56	0.5012	0.00895000	0.837	11.987	5.7706	1558.3
28	0.5012	0.01790000	1.62	24.888	5.7706	1558.3
14	0.5012	0.03580000	3.067	50.174	5.7706	1558.3
8960	0.896	0.00010000	2.74	0	2.96	36.847
7168	0.896	0.00012500	2.873	0	2.96	36.847
5376	0.896	0.00016667	2.842	0	2.96	36.847
3584	0.896	0.00025000	2.924	0	2.96	36.847
1792	0.896	0.00050000	3.046	0	2.96	36.847
896	0.896	0.00100000	3.634	0	2.96	36.847
112	0.896	0.00800000	2.471	0	2.96	36.847
98	0.896	0.00914286	2.545	0	2.96	36.847
84	0.896	0.01066667	2.47	0	2.96	36.847
70	0.896	0.01280000	2.469	0	2.96	36.847
56	0.896	0.01600000	2.466	0	2.96	36.847
28	0.896	0.03200000	2.446	0	2.96	36.847
14	0.896	0.06400000	2.402	0	2.96	36.847

	Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
1	112	0.896	0.00800000	2.74	0	2.96	36.847
	98	0.896	0.00914286	2.873	100	2.96	36.847
	84	0.896	0.01066667	2.842	100	2.96	36.847
	70	0.896	0.01280000	2.924	0	2.96	36.847
	56	0.896	0.01600000	3.046	0	2.96	36.847
	28	0.896	0.03200000	3.634	0	2.96	36.847
	14	0.896	0.06400000	4.74	0	2.96	36.847
0	8960	0.896	0.00010000	0.212	0	3.0955	147.24
	7168	0.896	0.00012500	0.211	0	3.0955	147.24
	5376	0.896	0.00016667	0.209	0	3.0955	147.24
	3584	0.896	0.00025000	0.20799	0	3.0955	147.24
	1792	0.896	0.00050000	0.208	0	3.0955	147.24
	896	0.896	0.00100000	0.209	0	3.0955	147.24
0.5	112	0.896	0.00800000	0.217	3.226	3.0955	147.24
	98	0.896	0.00914286	0.318	4.571	3.0955	147.24
	84	0.896	0.01066667	0.214	3.205	3.0955	147.24
	70	0.896	0.01280000	0.212	3.204	3.0955	147.24
	56	0.896	0.01600000	0.208	3.182	3.0955	147.24
	28	0.896	0.03200000	0.215	3.075	3.0955	147.24
	14	0.896	0.06400000	0.772	53.785	3.0955	147.24

11

	Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
1	112	0.896	0.00800000	0.638	6.767	3.0955	147.24
	98	0.896	0.00914286	0.807	8.633	3.0955	147.24
	84	0.896	0.01066667	0.778	8.375	3.0955	147.24
	70	0.896	0.01280000	0.89	9.873	3.0955	147.24
	56	0.896	0.01600000	1.056	12.109	3.0955	147.24
	28	0.896	0.03200000	1.848	22.943	3.0955	147.24
	14	0.896	0.06400000	3.285	41.911	3.0955	147.24
	8960	0.896	0.00010000	0.005	0	3.1312	496.53
	7168	0.896	0.00012500	0.007	0	3.1312	496.53
	5376	0.896	0.00016667	0.001	0	3.1312	496.53
0	3584	0.896	0.00025000	0.014	0	3.1312	496.53
	1792	0.896	0.00050000	0.028	0	3.1312	496.53
	896	0.896	0.00100000	0.057	0	3.1312	496.53
	112	0.896	0.00800000	0	7	3.1312	496.53
	98	0.896	0.00914286	35.412	112.594	3.1312	496.53
	84	0.896	0.01066667	0.006	0.335	3.1312	496.53
	70	0.896	0.01280000	0.01	0.46	3.1312	496.53
	56	0.896	0.01600000	0.035	4.329	3.1312	496.53
	28	0.896	0.03200000	0.29	19.669	3.1312	496.53
	14	0.896	0.06400000	1.13	121.423	3.1312	496.53
0.5	8960	0.896	0.00010000	0.005	0	3.1312	496.53
	7168	0.896	0.00012500	0.007	0	3.1312	496.53
	5376	0.896	0.00016667	0.001	0	3.1312	496.53
	3584	0.896	0.00025000	0.014	0	3.1312	496.53
	1792	0.896	0.00050000	0.028	0	3.1312	496.53
	896	0.896	0.00100000	0.057	0	3.1312	496.53
	112	0.896	0.00800000	0	7	3.1312	496.53
	98	0.896	0.00914286	35.412	112.594	3.1312	496.53
	84	0.896	0.01066667	0.006	0.335	3.1312	496.53
	70	0.896	0.01280000	0.01	0.46	3.1312	496.53

21

	Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
1	112	0.896	0.00800000	0.453	5.839	3.1312	496.53
	98	0.896	0.00914286	34.945	100	3.1312	496.53
	84	0.896	0.01066667	0.598	7.762	3.1312	496.53
	70	0.896	0.01280000	0.714	9.319	3.1312	496.53
	56	0.896	0.01600000	0.884	11.666	3.1312	496.53
	28	0.896	0.03200000	1.699	23.28	3.1312	496.53
	14	0.896	0.06400000	3.174	43.752	3.1312	496.53

Verification P

Uniform Grid

11

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8960	0.896	0.00010000	0.0254	0	.16114	17.2
7168	0.896	0.00012500	0.089	0	.16114	17.2
5376	0.896	0.00016667	0.098	0	.16114	17.2
3584	0.896	0.00025000	0.1458	0	.16114	17.2
1792	0.896	0.00050000	0.157	0	.16114	17.2
896	0.896	0.00100000	0.1664	0	.16114	17.2
112	16.002	0.14287500	0.064	0.941	.16114	17.2
98	16.002	0.16328572	0.063	0.915	.16114	17.2
84	16.002	0.19050001	0.064	0.932	.16114	17.2
70	16.002	0.22860001	0.064	0.923	.16114	17.2

0.5

	Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
1	56	16.002	0.28575000	0.069	0.907	.16114	17.2
	28	16.002	0.57150000	0.188	6.545	.16114	17.2
	14	16.002	1.14300001	0.646	12.705	.16114	17.2
	112	16.002	0.14287500	0.45	3.929	.16114	17.2
	98	16.002	0.16328572	0.505	4.331	.16114	17.2
	84	16.002	0.19050001	0.582	4.92	.16114	17.2
	70	16.002	0.22860001	0.686	5.713	.16114	17.2
	56	16.002	0.28575000	0.841	6.901	.16114	17.2
	28	16.002	0.57150000	1.586	12.829	.16114	17.2
	14	16.002	1.14300001	2.95	24.585	.16114	17.2
	8960	0.896	0.00010000	0	0	.16114	65.373
	7168	0.896	0.00012500	0	0	.16114	65.373
0	5376	0.896	0.00016667	0	0	.16114	65.373
	3584	0.896	0.00025000	0	0	.16114	65.373
	1792	0.896	0.00050000	0	0	.16114	65.373
	896	0.896	0.00100000	0	0	.16114	65.373
	112	16.002	0.14287500	0	0	.16114	65.373
	98	16.002	0.16328572	0.005	0.273	.16114	65.373
	84	16.002	0.19050001	0.051	0.051	.16114	65.373
	70	16.002	0.22860001	0.009	0.168	.16114	65.373
	8960	0.896	0.00010000	0	0	.16114	65.373
	7168	0.896	0.00012500	0	0	.16114	65.373
	5376	0.896	0.00016667	0	0	.16114	65.373
	3584	0.896	0.00025000	0	0	.16114	65.373
0.5	1792	0.896	0.00050000	0	0	.16114	65.373
	896	0.896	0.00100000	0	0	.16114	65.373
	112	16.002	0.14287500	0	0	.16114	65.373
	98	16.002	0.16328572	0.005	0.273	.16114	65.373
	84	16.002	0.19050001	0.051	0.051	.16114	65.373
	70	16.002	0.22860001	0.009	0.168	.16114	65.373
	8960	0.896	0.00010000	0	0	.16114	65.373
	7168	0.896	0.00012500	0	0	.16114	65.373
	5376	0.896	0.00016667	0	0	.16114	65.373
	3584	0.896	0.00025000	0	0	.16114	65.373
	1792	0.896	0.00050000	0	0	.16114	65.373
	896	0.896	0.00100000	0	0	.16114	65.373

Steps		Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
1	56	16.002	0.28575000	0.024	1.297	.16114	65.373
	28	16.002	0.57150000	0.194	6.462	.16114	65.373
	14	16.002	1.14300001	0.718	20.256	.16114	65.373
	112	16.002	0.14287500	0.408	2.981	.16114	65.373
	98	16.002	0.16328572	0.462	3.308	.16114	65.373
	84	16.002	0.19050001	0.54	3.968	.16114	65.373
	70	16.002	0.22860001	0.644	4.758	.16114	65.373
	56	16.002	0.28575000	0.799	5.944	.16114	65.373
	28	16.002	0.57150000	1.546	11.862	.16114	65.373
	14	16.002	1.14300001	2.915	23.645	.16114	65.373

APPENDIX B

Radial

Equal Volume

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Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
8960	0.5012	5.5938E-05	1.253	4.51	5.629	217.87
7168	0.5012	6.9922E-05	1.254	4.65	5.629	217.87
5376	0.5012	9.3229E-05	1.257	5.031	5.629	217.87
3584	0.5012	0.00013984	1.256	4.15	5.629	217.87
1792	0.5012	0.00027969	1.2568	6.7	5.629	217.87
896	0.5012	0.00055938	1.2574	7.8	5.629	217.87

0.5

112	0.5012	0.00447500	1.301	100	5.629	217.87
98	0.5012	0.00511429	23.042	105.653	5.629	217.87
84	0.5012	0.00596667	1.3	100	5.629	217.87
70	0.5012	0.00716000	1.3	100	5.629	217.87
56	0.5012	0.00895000	1.3	100	5.629	217.87
28	0.5012	0.01790000	1.399	100	5.629	217.87
14	0.5012	0.03580000	2.522	128.681	5.629	217.87

1

112	0.5012	0.00447500	1.422	100	5.629	217.87
98	0.5012	0.00511429	22.721	100	5.629	217.87

	Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
0	84	0.5012	0.00596667	1.482	100	5.629	217.87
	70	0.5012	0.00716000	1.538	100	5.629	217.87
	56	0.5012	0.00895000	1.64	100	5.629	217.87
	28	0.5012	0.01790000	2.244	100	5.629	217.87
	14	0.5012	0.03580000	3.376	100	5.629	217.87
	8960	0.5012	5.5938E-05	0.154	2.24	5.756	1123.2
	7168	0.5012	6.9922E-05	0.153	3.146	5.756	1123.2
	5376	0.5012	9.3229E-05	0.152	3.547	5.756	1123.2
	3584	0.5012	0.00013984	0.156	3.664	5.756	1123.2
0.5	1792	0.5012	0.00027969	0.155	3.945	5.756	1123.2
	896	0.5012	0.00055938	0.162	5.124	5.756	1123.2
	112	0.5012	0.00447500	0.404	49.16	5.756	1123.2
	98	0.5012	0.00511429	23.557	451.923	5.756	1123.2
	84	0.5012	0.00596667	0.422	58.743	5.756	1123.2
	70	0.5012	0.00716000	0.388	27.431	5.756	1123.2
	56	0.5012	0.00895000	0.573	130.794	5.756	1123.2
	28	0.5012	0.01790000	1.801	457.787	5.756	1123.2
	14	0.5012	0.03580000	5.971	1815.385	5.756	1123.2
1							
	112	0.5012	0.00447500	0.685	58.693	5.756	1123.2
	98	0.5012	0.00511429	22.774	100	5.756	1123.2

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Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
84	0.5012	0.00596667	0.799	62.262	5.756	1123.2
70	0.5012	0.00716000	0.892	65.237	5.756	1123.2
56	0.5012	0.00895000	1.028	69.894	5.756	1123.2
28	0.5012	0.01790000	1.697	98.868	5.756	1123.2
14	0.5012	0.03580000	2.974	164.465	5.756	1123.2
21						
0						
8960	0.5012	5.5938E-05	0.004	0	5.7785	5160.1
7168	0.5012	6.9922E-05	0.012	0	5.7785	5160.1
5376	0.5012	9.3229E-05	0.035	0	5.7785	5160.1
3584	0.5012	0.00013984	0.048	0	5.7785	5160.1
1792	0.5012	0.00027969	0.051	0	5.7785	5160.1
896	0.5012	0.00055938	0.058	0	5.7785	5160.1
0.5						
112	0.5012	0.00447500	0	5.871	5.7785	5160.1
98	0.5012	0.00511429	0.176	847.74	5.7785	5160.1
84	0.5012	0.00596667	0.195	35.729	5.7785	5160.1
70	0.5012	0.00716000	0.222	78.516	5.7785	5160.1
56	0.5012	0.00895000	0.345	98.982	5.7785	5160.1
28	0.5012	0.01790000	0.32	859.767	5.7785	5160.1
14	0.5012	0.03580000	5.653	1114.973	5.7785	5160.1
1						
112	0.5012	0.00447500	0.432	58.4	5.7785	5160.1
98	0.5012	0.00511429	22.821	22.821	5.7785	5160.1

Spherical

Equal Volume

6

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0.5

Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
84	0.5012	0.00596667	0.55	61.942	5.7785	5160.1
70	0.5012	0.00716000	0.645	64.894	5.7785	5160.1
56	0.5012	0.00895000	0.785	69.511	5.7785	5160.1
28	0.5012	0.01790000	1.473	96.291	5.7785	5160.1
14	0.5012	0.03580000	2.779	164.511	5.7785	5160.1
8960	0.896	0.00010000	1.372	0	2.6985	138.58
7168	0.896	0.00012500	1.372	0	2.6985	138.58
5376	0.896	0.00016667	1.372	0	2.6985	138.58
3584	0.896	0.00025000	1.371	0	2.6985	138.58
1792	0.896	0.00050000	1.374	0	2.6985	138.58
896	0.896	0.00100000	1.3765	0	2.6985	138.58
112	0.896	0.00800000	1.301	100	2.6985	138.58
98	0.896	0.00914286	23.042	100	2.6985	138.58
84	0.896	0.01066667	1.3	100	2.6985	138.58
70	0.896	0.01280000	1.3	100	2.6985	138.58
56	0.896	0.01600000	1.3	100	2.6985	138.58
28	0.896	0.03200000	1.399	100	2.6985	138.58
14	0.896	0.06400000	2.522	100	2.6985	138.58

	Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
1	112	0.896	0.00800000	1.422	100	2.6985	138.58
	98	0.896	0.00914286	22.721	100	2.6985	138.58
	84	0.896	0.01066667	1.482	100	2.6985	138.58
	70	0.896	0.01280000	1.538	100	2.6985	138.58
	56	0.896	0.01600000	1.64	100	2.6985	138.58
	28	0.896	0.03200000	2.244	100	2.6985	138.58
11							
0	8960	0.896	0.00010000	0.322	0	3.0349	
	7168	0.896	0.00012500	0.321	0	3.0349	
	5376	0.896	0.00016667	0.32	0	3.0349	
	3584	0.896	0.00025000	0.3235	0	3.0349	
	1792	0.896	0.00050000	0.326	0	3.0349	
	896	0.896	0.00100000	0.327	0	3.0349	
0.5	112	0.896	0.00800000	0.404	49.16	3.0349	748.77
	98	0.896	0.00914286	23.557	451.923	3.0349	748.77
	84	0.896	0.01066667	0.422	58.743	3.0349	748.77
	70	0.896	0.01280000	0.388	27.431	3.0349	748.77
	56	0.896	0.01600000	0.573	130.794	3.0349	748.77
	28	0.896	0.03200000	1.801	457.787	3.0349	748.77
	14	0.896	0.06400000	5.971	1815.385	3.0349	748.77

	Steps	Tss	Delta T	AveError	MaxError	Lam_Min	Lam_
1	112	0.896	0.00800000	0.685	58.693	3.0349	748.77
	98	0.896	0.00914286	22.774	100	3.0349	748.77
	84	0.896	0.01066667	0.799	62.262	3.0349	748.77
	70	0.896	0.01280000	0.892	65.237	3.0349	748.77
	56	0.896	0.01600000	1.028	69.894	3.0349	748.77
	28	0.896	0.03200000	1.697	96.868	3.0349	748.77
	14	0.896	0.06400000	3.376	100	3.1213	3547.5
	14	0.896	0.06400000	2.974	164.465	3.0349	748.77
0	8960	0.896	0.00010000	0.004	0		
	7168	0.896	0.00012500	0.005	0		
	5376	0.896	0.00016667	0.0011	0		
	3584	0.896	0.00025000	0.022	0		
	1792	0.896	0.00050000	0.032	0		
	896	0.896	0.00100000	0.041	0		
0.5	112	0.896	0.00800000	0	0	3.1213	3547.5
	98	0.896	0.00914286	23.741	847.74	3.1213	3547.5
	84	0.896	0.01066667	0.102	35.729	3.1213	3547.5
	70	0.896	0.01280000	0.278	78.51	3.1213	3547.5
	56	0.896	0.01600000	0.476	98.982	3.1213	3547.5
	28	0.896	0.03200000	1.666	859.767	3.1213	3547.5

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