KWAME NKRUMAH UNIVERSITY OF SCIENCE AND TECHNOLOGY

COMPARISON OF STABILITY OF SELECTED NUMERICAL METHODS IN SOLVING STIFF SEMI-LINEAR DIFFERENTIAL EQUATIONS

By

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DECLARATION

I hereby declare that this thesis is my own work towards the Master of Science and that, to the best of my knowledge, it contains no material previously published by another person nor material which has been accepted for the award of any other degree of the university or elsewhere, except where due acknowledgement has been made in the text.

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ABSTRACT

Many real-world applications involve situations where different physical phenomena acting on very different time scales occur simultaneously. The partial differential equations (PDEs) governing such situations are categorized as “stiff” PDEs. Stiffness is a challenging property of differential equations (DEs) that prevents conventional explicit numerical integrators from handling a problem efficiently. For such cases, stability (rather than accuracy) requirements dictate the choice of time step size to be very small. Considerable effort in coping with stiffness has gone into developing time-discretization methods to overcome many of the constraints of the conventional methods. Recently, there has been a renewed interest in exponential integrators that have emerged as a viable alternative for dealing effectively with stiffness of DEs.

Our attention has been focused on the explicit Exponential Time Differencing (ETD) integrators that are designed to solve stiff semi-linear problems. Semi-linear PDEs can be split into a linear part, which contains the stiffest part of the dynamics of the problem, and a nonlinear part, which varies more slowly than the linear part. The ETD methods solve the linear part exactly, and then explicitly approximate the remaining part by polynomial approximations.

The first part of this project involves a general study of the stiff semi-linear differential equations.

The second part of this project involves an analytical examination of the asymptotic stability properties of the Exponential Time Differencing Schemes in order to present the advantage of these methods in overcoming the stability constraints.

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LIST OF ABBREVIATIONS

DE	Differential Equation
ETD	Exponential Time Differencing Method
ETDRK	Exponential Time Differencing Runge Kutta Method
IF	Integrating Factor Method
IFEULER	Integrating Factor Euler Method
KNUST	Kwame Nkrumah University of Science and Technology
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation

DEDICATION

I dedicate this thesis to my beloved wife Cynthia Apuusiyine and my mother Maria Azure.

May God bless them.

ACKNOWLEDGEMENT

My ultimate thanks goes to God almighty for giving me the strength and making the completion of this thesis possible.

Early in this project, when I took the preliminary steps towards my thesis, I did not foresee how many individuals would contribute to its completion whom I owe my thanks and appreciation to. I am particularly grateful to my supervisor, Mr. K.F. Darkwah, for his ultimate support and guidance, thoughtful suggestions, objective comments, practical advice, and insightful direction. Without his knowledge and expertise this thesis would never have been completed.

My gratitude also goes to my beloved wife, Cynthia Apuusiyine, whose boundless love and firm belief in me have been a source of inspiration for me during my lengthy project.

I am extremely motivated to express my appreciation to my mother Maria Azure and my mother-in-law Hellen Apuusiyine for their continuous support and prayers for me, I love you all.

CHAPTER 1

INTRODUCTION

This chapter consists of background of the study, statement of the problem, objectives, methodology, justification and organization of the study.

1.0 Background of the Study

Various problems in the world can be solved when they are modeled and presented in the form of an ordinary differential equation or partial differential equation. However, there are times where different phenomena acting on very different time scales occur simultaneously introducing a parameter called stiff parameter which sometimes makes it difficult to solve. All differential equations with this property is said to be a stiff differential equation. Differential equations can be grouped into two type's namely Partial Differential equations (PDE) and Ordinary Differential Equations (ODE).

A partial differential equation (PDE) is a mathematical relation which involves functions of multiple variables and their partial derivatives. PDEs are used to formulate (and hence to aid in the solution of) problems involving functions of several variables, and they arise in a variety of important fields. For example, in physics, they are used to describe the propagation of sound or heat, electrostatics, electrodynamics, fluid flow and elasticity, whilst in finance; they have been used in the modeling of the pricing of financial options. Accordingly, the study of their properties and methods of solution has received a great deal of attention.

The earliest detection of stiffness in differential equations in the digital computer era, by Curtiss, et al (1952), was apparently far in advance of its time. They named the phenomenon and spotted the nature of stiffness (stability requirement dictates the choice of the step size to be very small).To resolve the problem they recommended possible methods such as the Backward Differentiation Formula for numerical integration. In 1963, Dahlquist defined the problem and demonstrated the difficulties that standard differential equation solvers have with stiff differential equations.

For a numerical method which makes use of derivative values, the fast component continues to influence the solution, and as a consequence, the selection of the step size in the numerical solution is problematic. This is because the required step size is governed not only by behavior of the solution as a whole, but also by that of the rapidly varying transient which does not persist in the solution that we are monitoring.

In reality, numerical values occurring in nature are frequently sure as to cause stiffness. Therefore, a realistic representation of a natural system using a differential equation is likely to encounter this phenomenon.

Practical application of stiff PDEs can be found in almost all technical disciplines. For example mathematical models of electrical circuits, mechanical systems, chemical processes, etc. are described by systems of PDEs.

1.1 Statement of the Problem

Various authors have looked at solutions of differential equations using the Exponential Time Differencing (ETD) and Exponential Time Differencing Runge-Kutta (ETDRK) methods without checking their stability. This study seeks to compare the asymptotic stability of some of these methods and to obtain stability expressions for these numerical schemes. 1.2 Objectives

1. To obtain stability expression for selected numerical methods.
2. To compare the stability of the selected numerical schemes using the asymptotic stability criteria.

1.3 Methodology

The problem is to determine the effectiveness of some Exponential Time Differencing Methods using the asymptotic stability criteria. Methods employed are ETD1, ETD2, ETD2RK1 and ETD2RK2. Computations leading to results will be carried out manually. The source of references is the internet and KNUST library.

1.4 Justification

The study would afford students the opportunity to be aware of some key numerical methods for solving stiff differential equations. Information gathered from the results would educate students about the stability of these methods and which one of these methods is much more preferred than the others. This would help fill the gap in the research carried out in Ghanaian Universities in this area.

In addition, it could pave the way for more comprehensive research on the comparison of these methods in relation to some specified complex functions which are very significant in drawing conclusions to research works.

The study would however be useful to researcher in the University. Researchers would be alerted of these important methods which play a very important role in obtaining accurate results when used to compute stiff differential equations.

The study would equally be helpful to chemist and physicist to understand which of these numerical schemes would be suitable to solve a modeled problem which turns out to be a stiff differential equation.

The University as a whole will find the study relevant in keeping tracks of numerical schemes with respect to their stability, and embark on further research on these schemes to find plausible solutions to the impending problems.

1.5 Organization of the Study

Chapter 1 is made up of introduction, which comprises the background of the study, statement of the problem, objectives of the study and justification. Chapter 2 highlights on review of literature of ideas of different authors whose findings have been defined in relation to the topic under study. Chapter 3 focuses on methodological review in the light of numerical methods that are relevant to solving stiff differential equations. Basically, the study seeks to use manual computation to for the methods. Chapter 4 deal with data analysis. In the same way, chapter five consists of summary, conclusion and recommendations.

The project report however ends with references and appendices in supportive to the researcher's investigation.

CHAPTER 2

LITERATURE REVIEW

2.0 Overview

In this section, there is a review of the work of several authors concerning concept definitions and various researches done to uncover different numerical methods used to solve stiff differential equations. Researches, empirical work and authors' opinion are looked at. Below are the focuses of the review.

- The Concept Definition of Stiff Differential Equation.
- History of Stiff Differential Equations.
- Solving Stiff Differential Equations with Exponential Time Differencing Methods.
- Stability of Exponential Time Differential Time Differencing Methods.
- Stability of Exponential Time Differential Time Differencing Runge-Kutta Methods.

2.1 The Concept Definition of Stiff Differential Equation

According to Lambers (assessed on 20/04/2013), differential equation of the form $y' = f(t, y)$ is said to be stiff if its exact solution $y(t)$ includes a term that decays exponentially to zero as t increases, but whose derivatives are much greater in magnitude than the term itself. An example of such a term is e^{-ct}, where c is a large, positive constant, because its *kth* derivative is $c^k e^{-ct}$. Because of the factor of c^k, this derivative decays to zero much more slowly than e^{-ct} as t increases. Garfinkel, et al (1977), described stiffness as a property of differential equation that makes it slow and expensive to solve by numerical methods. It is a result of the numerical coefficients in the differential equation (so that there is too wide a spread between the fastest and slowest elements).

According to Moler (assessed on 14/04/2013), stiffness is a subtle, difficult, and important - concept in the numerical solution of ordinary differential equations. It depends on the differential equation, the initial conditions and the numerical method. Dictionary definitions of the word “stiff” involve terms like “not easily bent”, “rigid”, and “stubborn”. We are concerned with a computational version of these properties.

An ordinary differential equation problem is stiff if the solution being sought is varying slowly, but there are nearby solutions that vary rapidly, so the numerical method must take small steps to obtain satisfactory results. Stiffness is an efficiency issue. If we weren't concerned with how much time a computation takes, we wouldn't be concerned about stiffness. Nonstiff methods can solve stiff problems; they just take a long time to do it.

Dahlquist et al (1973), defined a stiff system as one containing very fast components as well as very slow components. They represent coupled physical systems having components varying with very different time scales: that is they are systems having some components varying much more rapidly than the others. (Liniger, 1972).

At the moment, even if the old intuitive definition relating stiffness to multi scale problems survives in most of the authors, the most successful definition seems to be the one based on particular effects of the phenomenon rather than on the phenomenon itself, such as for example, the following equivalent definitions. According to Curtiss, et al (1952), stiff equations are equations where certain implicit methods perform better, usually tremendous better, than explicit ones; while Hairer, et al (1996), defined stiff equations as problems for which explicit methods don't work.

As it usually happens, describing a phenomenon by means of its effects may not be enough to fully characterize the phenomenon itself. For example, saying that fire is what produces ash would oblige fire men to wait for until the end of a fire to see if the ash has been produced. In the same way, in order to recognize stiffness according to the previous definitions it would be necessary to apply first explicit methods and see if they work or not.

2.2 History of Stiff Differential Equations

Curtiss et al (1952), detected stiffness in differential equations. They named the phenomenon and spotted the nature of stiffness (stability requirement dictates the choice of the step size to be very small). To resolve the problem they recommended possible methods such as the Backward Differentiation Formula for numerical integration. In 1963, Dahlquist, defined the problem and demonstrated the difficulties that standard differential equation solvers have with stiff differential equations.

At about this time several authors participated in independent research for handling and evading the problems posed by stiff differential equations. For example, Gear (1968), became one of the most important names in this field. Considerable efforts have gone into developing numerical integration for stiff problems, and hence, the problem of stiffness was brought to the attention of the mathematical and computer science community for a comprehensive review of this phenomenon. Stiff differential equations are categorized as those whose solutions (or different components of a single solution) evolve on very different time scales occurring simultaneously, i.e. the rates of change of the various components of the solutions differ markedly. Consider, for example, if one component of the solution has a term of the form e^{ct}, where c is a large positive constant. This component, which is called the transient solution, decays to zero much more rapidly, as t increases, than other slower components of the solutions. Alternatively, consider a case where a component of the solution oscillates rapidly on a time scale much shorter than that associated with the other solution components. For a numerical method which makes use of derivative values, the fast component continues to influence the solution, and as a consequence, the selection of the step size in the numerical solution is problematic. This is because the required step size is governed not only by the behavior of the solution as a whole, but also by that of the rapidly varying transient which does not persist in the solution that we are monitoring.

In reality, the numerical values occurring in nature are frequently such as to cause stiffness. Therefore, a realistic representation of a natural system using a differential equation is likely to encounter this phenomenon. An example is the field of chemical kinetics, Curtiss, (1952). Here ordinary differential equations describe reactions of various chemical species to form other species. The stiffness in such systems is a consequence of the fact that different reactions take place on vastly different time scales.

2.3 Solving Stiff Differential Equations with Exponential Time Differencing Methods

Exponential Time Differencing (ETD) schemes are time integration methods that can be efficiently combined with special approximations to provide accurate smooth solutions for stiff or highly oscillatory semi-linear PDEs.

According to Du (2004), Exponential time differencing schemes are time integration methods that can be efficiently combined with spatial spectral approximations to provide very high resolution to the smooth solutions of some linear and nonlinear partial differential equations. We study in this paper the stability properties of some exponential time differencing schemes. We also present their application to the numerical solution of the scalar Allen-Cahn equation in two and three dimensional spaces.

Numerous time discretization methods that are designed to handle stiff systems have been developed. One example is the family of Exponential Time Differencing (ETD) schemes. This class of schemes is especially suited to semi-linear problems which can be split into a linear part, which contains the stiffest part of the dynamics of the problem, and a nonlinear part, which varies more slowly than the linear part. These schemes have been rediscovered several times in various forms and under various names, Calvo et al (2006). An example is the Exact Linear Part (ELP) schemes that were derived by Beylkin et al (1998) for arbitrary order. However, the authors Beylkin, and Vozovoi, did not give explicit formulas for the methods' coefficients. In a subsequent paper, Cox and Matthews gave an explicit derivation of the explicit ELP methods, for arbitrary order s, with explicit formulas for the methods' coefficients and referred to these methods as the Exponential Time Differencing (ETD) schemes (the term used arose originally in the field of computational electrodynamics. In addition, the authors Cox et al (2002) further constructed new explicit Runge-Kutta (ETD-RK) versions of these schemes up to fourth-order.

According to Livermore et al (2007), over the last decade there has been renewed interest in applying exponential time differencing (ETD) time stepping schemes to the solution of stiff systems. In this paper, we present an implementation of such a scheme to the fully spectral solution of the incompressible magneto hydrodynamic equations in a spherical shell. One problem associated with ETD schemes is the accurate calculation of the necessary matrices; we implement and discuss in detail a variety of different methods including direct computation, contour integration, spectral expansions and recurrence relations. We compare the accuracy of six different second-order methods in determining the evolution of a three-dimensional magnetic field under the action of a prescribed time-dependent flow of electrically conducting fluid, and find that for the time step restriction imposed by the nonlinear terms, ETD methods are no more accurate than linearly implicit methods which have the significant advantage of being easier to implement. However, ETD methods are more readily extendable than those which are linearly implicit and will become much more advantageous at higher order.

2.4 Stability of Exponential Time Differencing Methods

According to Hala (2008), the stability of a given method for solving a system of ODEs is a theoretical measure of the extent to which the method produces satisfactory approximations. Stability is related to the accuracy of the methods and refers to errors not growing in subsequent steps. Such methods are called numerically stable. The stability analysis determines the range of time step for which the method is numerically stable. The stability region is the subset of the complex plane consisting of those $\Delta t\lambda \in \mathbb{C}$ for which, with time step Δt, the numerical approximation produces bounded solutions when applied to the scalar linear model problem $du(t)/dt = \lambda u(t)$.

In general, the linear stability analysis of time discretization methods is valid for a linear autonomous system of ODEs, linearized about a fixed point. This analysis only gives an indicator as to how stable the numerical methods are. It cannot be directly applied to solutions of nonlinear time-dependent PDEs with large amplitude since convergence and stability are solution-dependent issues.

Beylkin, et al. (1998) studied the stability for a family of explicit and implicit ELP schemes, and showed that these schemes have significantly better stability properties when compared with known Implicit-Explicit schemes. In addition, Krogstad, et al (2005), analyzed the stability regions of various time integrating methods, including the fourth-order ETDRK4-B method and multi-step generalizations of the IF methods, all of which he proposed, and the ETD4RK method of Cox, et al (2002). He deduced that the ETDRK4-B method has the largest stability region. Cox and Matthews also studied the stability properties of the second-order ETD type schemes; the study was for the ETD-RK schemes of orders up to and including the fourth. All authors concluded that ETD type schemes maintain good stability properties and can be widely applicable to dissipative PDEs and nonlinear wave equations. The approach developed by Beylkin, et al. (1998), for the stability analysis of composite schemes, i.e. schemes that use different methods for the linear and nonlinear parts of the equation, computes the boundaries of the stability regions for a general test problem.

CHAPTER 3

METHODOLOGY

3.0 Overview

Numerical time discretization methods that are designed to handle stiff systems have been developed. One example is the family of Exponential Time Differencing (ETD) schemes. This class of schemes is especially suited to semi-linear problems which can be split into a linear part, which contains the stiffest part of the dynamics of the problem, and a nonlinear part, which varies more slowly than the linear part.

In this chapter, we will take a brief look at differential equations and understand the basic terminologies that go with it. We then take an in-depth look at the algorithm derivation of the Integration Factor Methods (IF schemes), the Exponential Time Differencing Methods (ETD) and the Exponential Time Differencing Runge-Kutta Methods (ETDRK).In addition to this, we will also analytically examine the methods stability properties, which determines the range of time step for which the method is numerically stable. The approach computes the boundaries of the stability regions for a general test problem for the explicit ETD methods of multi-step or RK type up to fourth-order.

3.1 Basic Concepts of Differential Equations

A differential equation is an equation that involves an unknown scalar function (the dependent variable) and one or more of its derivatives. For example

$$\frac{d^2y}{dx^2} - 5\frac{dy}{dx} + 3y = -3 \tag{3.1}$$

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial u^2} - \frac{\partial^2 u}{\partial y^2} + u = 0 \tag{3.2}$$

If the unknown function is a function in one single variable then the differential equation is called an ordinary differential equation. An example of an ordinary differential equation is equation (3.1). In contrast, when the unknown function is a function of two or more independent variables then the differential equation is called a partial differential equation, in short PDE. Equation (3.2) is an example of a partial differential equation.

3.1.1 Partial Differential Equations

Definition: A Partial Differential Equation (PDE) is an equation containing partial derivatives of the dependent variable.

For example, the following are PDEs

$$u_t + cu_x = 0 \tag{3.3}$$

$$u_{xx} + u_{yy} = f(x, y) \tag{3.4}$$

NOTE: We use subscript to mean differentiation with respect to the variables given, e.g. $u_t = \frac{\partial u}{\partial t}$. In general we may write a PDE as

$$F(x, y, \dots, u, u_x, u_y, \dots, u_{xx}, u_{yy}, \dots) = 0 \tag{3.5}$$

where $x, y, \dots$ are the independent variables and u is the unknown function of these variables. Of course, we are interested in solving the problem in a certain domain *D*. A solution is a function u satisfying equation (3.5). From these many solutions we will select the one satisfying certain conditions on the boundary of the domain *D*.

For example, the functions

$$u(x, t) = e^{x-ct}$$

$$u(x, t) = \cos(x - ct)$$

are solution of (3.3), as can be easily verified.

Definition: The order of a PDE is the order of the highest order derivative in the equation. For example, equation (3.3) is of first order and equation (3.4) is of second order

3.1.2 Types of PDEs

Linear PDE: A partial differential equation is called linear if it is linear in the unknown function and all its derivatives with coefficients depend only on the independent variables. . For example, a first order linear partial differential equation has the form

$$A(x,y)u_x + B(x,y)u_y + C(x,y)u = D(x,y)$$

where as a second order linear partial differential equation has the form

$$A(x,y)u_{xx} + B(x,y)u_{xy} + C(x,y)u_{yy} + D(x,y)u_x + E(x,y)u_y + F(x,y)u = G(x,y).$$

Quasi-linear PDE: A partial differential equation is called quasi-linear if the highest order derivatives which appear in the equation are of degree one (regardless of the manner in which lower-order derivatives and unknown functions occur in the equation). For example, a first order quasi-linear partial differential equation has the form

$$A(x,y,u)u_x + B(x,y,u)u_y = C(x,y,u)$$

whereas a second order quasi-linear partial differential equation has the form

$$A(x,y,u,u_x,u_y)u_{yy} + B(x,y,u,u_x,u_y)u_{xy} + C(x,y,u,u_x,u_y)u_{yy} = D(x,y,u,u_x,u_y)$$

Semi-linear PDE: A partial differential equation is semi-linear if it is quasi-linear and the coefficients of the highest-order derivatives are functions of independent variables only. For example, a first order semi-linear partial differential equation has the form

$$A(x,y)u_{xx} + B(x,y)u_{xy} + C(x,y)u_{yy} = D(x,y,u,u_x,u_y)$$

3.2 Derivation of Algorithm

We begin by giving briefly the main idea behind the Lawson Integrating Factor IF methods, Lawson et al. (2008), then give, in detail, the algorithm derivation for the explicit ETD scheme.

Consider stiff semi-linear PDEs that can be written in the form

$$\frac{\partial u(x,t)}{\partial t} = \mathcal{L}u(x,t) + \mathcal{F}(u(x,t),t), \qquad (3.1)$$

Where the linear operator $\mathcal{L}$ contains higher-order spatial derivatives than those contained in the nonlinear operator $\mathcal{F}$, and is mainly the term responsible for stiffness. For problems with spatially periodic boundary conditions, we use Fourier spectral methods to discretize the spatial derivations of (3.1), and hence obtain a stiff system of coupled ODEs in time t

$$\frac{du(t)}{dt} = Lu(t) + F(u(t),t) \qquad (3.2)$$

The linear part L of the system is represented by a diagonal matrix, and F represents the action of the nonlinear operator on u on the grid. For problems where the boundary conditions are not periodic, we use finite difference formulas or Chebyshev polynomials, and in this case, the linearized system is represented by a non-diagonal matrix. For dissipative PDEs, the eigenvalues of the matrix L are negative and real, whereas they are imaginary for dispersive PDEs. Dissipation in a dynamical system represents the concept of important mechanical modes, such as waves or oscillations, loosing energy over time. Such systems are called dissipative systems. On the order hand, a dispersive PDE represents a system in which waves of different frequencies propagate at different phase velocities (the phase velocity is the rate at which the phase of the wave propagates in space).

For the stiff system of ODEs (3.2), the eigenvalues of the matrix L vary widely in magnitude, and the stiffness is caused by the eigenvalues of large magnitude. A competitive time stepping method should be able to integrate the system (3.2) accurately without requiring very small time steps for the largest magnitude eigenvalue. Simultaneously it should be able to handle small eigenvalues. The nonlinear term F requires an explicit treatment since fully implicit methods are too costly for a large system of ODEs.

To derive the time discretization methods (Integrating Factor (IF) and ETD methods), we consider for simplicity a single model of a stiff ODE

$$\frac{du(t)}{dt} = cu(t) + F(u(t), t), \tag{3.3}$$

Where the stiffness parameter c is either large, negative and real, or large and imaginary, or complex with large, negative real part and $F(u(t), t)$ is the nonlinear forcing term.

3.2.1 Integrating Factor Methods

The main idea behind the IF schemes is to use a change variables

$$w(t) = u(t)e^{-ct},$$

So that when differentiating both sides of this equation we obtain

$$\frac{dw(t)}{dt} = \left(\frac{du(t)}{dt} - cu(t)\right)e^{-ct},$$

And then substituting from equation (3.3) we get

$$\frac{dw(t)}{dt} = F(u(t), t)e^{-ct},$$

$$= F(w(t)e^{ct}, t)e^{-ct} \qquad (3.4)$$

The main aim now is to use any numerical integrator (IF schemes can be generalizes to arbitrary order by applying any multi-step or Runge-Kutta methods) on the transformed nonlinear differential equation (3.4). The approximated solution is then transformed back to provide an approximate solution for the original u variable. For example, we can choose to apply the Euler method to the transformed differential equation as follows

$$w_{n+1} = w_n + \Delta t F(w_n e^{ct_n}, t_n)e^{-ct_n},$$

where Δt is the time step size and w_n denotes the numerical approximation to $w(t_n)$, and then transform back to the original variable to obtain the solution approximation. This yields the first-order Integrating Factor Euler (IFEULER) method

$$u_{n+1} = (u_n + \Delta t F_n)e^{c\Delta t}, \qquad (3.5)$$

Where u_n and F_n denote the numerical approximation to $u(t_n)$ and $F(u(t_n), t_n)$ respectively.

The purpose of transforming the differential equation (3.3) to equation (3.4), is to remove the explicit dependence in the differential equation on the operator *c*, except inside the exponential. Now the problem is no longer stiff since the linear "stiff" term of the differential equation (3.3), that contains the stability, is gone. Therefore, it can be solved exactly with the possibility of larger time steps. However, according to Wright (2004), for

PDEs with slowly varying nonlinear terms, the introduction of the fast decay time scale into the nonlinear term introduces large errors in the system.

3.2.2 Exponential Time Differencing Methods

To derive the s-step ETD schemes, we follow an approach similar to that of deriving the IF schemes, i.e. we multiply (3.3) through by the integrating factor e^{-ct}, and then integrate the equation over a single time step from $t = t_n$ to $t = t_{n+1} = t_n + \Delta t$ to get

$$u(t_{n+1}) = u(t_n)e^{c\Delta t} + e^{c\Delta t}\int_0^{\Delta t} e^{-c\tau}F(u(t_n+\tau), t_n+\tau)d\tau$$

(3.6)

This formula is exact, and the next step is to derive approximations to the integral in equation (3.6). This procedure does not introduce an unwanted fast time scale into the solution and the schemes can be generalized to arbitrary order.

If we apply the Newton Backward Difference Formula, using information about $F(u(t), t)$ at the nth and previous time steps, we can write a polynomial approximation to $F(u(t_n+\tau), t_n+\tau)$ in the form

$$F(u(t_n+\tau), t_n+\tau) \approx G_n(t_n+\tau) = \sum_{m=0}^{s-1}(-1)^m \binom{-\tau/\Delta t}{m} \nabla^m G_n(t_n),$$

(3.7)

where ∇ is the backward difference operator defined as follows

$$\nabla^m G_n(t_n) = \sum_{k=0}^{m}(-1)^k \binom{m}{k} G_{n-k}(t_{n-k}),$$

$$\approx \sum_{k=0}^{m} (-1)^k \binom{m}{k} F(u(t_{n-k}), t_{n-k}), \qquad (3.8)$$

and

$$m! \binom{-\Lambda}{m} = (-\Lambda)(-\Lambda - 1) \dots (-\Lambda - m + 1), m = 1, \dots\dots, s - 1$$

(note that $0! \binom{-\Lambda}{0} = 1$). If we substitute the approximation (3.7) in the integrand (3.6), we get

$$u(t_{n+1}) - u(t_n)e^{c\Delta t} \approx \Delta t \sum_{m=0}^{s-1} (-1)^m \int_0^1 e^{c\Delta t(1-\Lambda)} \binom{-\Lambda}{m} d\Lambda \nabla^m G_n(t_n) \qquad (3.9)$$

Where $\Lambda = \tau/\Delta t$.

We will indicate the integral in (3.9) by

$$g_m = (-1)^m \int_0^1 e^{c\Delta t(1-\Lambda)} \binom{-\Lambda}{m} d\Lambda, \qquad (3.10)$$

and then calculate the g_m by bringing in the generating function. For $z \in \mathbb{R}, |z| < 1$, we define the generating function

$$\Gamma(z) = \sum_{m=0}^{\infty} g_m z^m,$$

$$= \int_0^1 e^{c\Delta t(1-\Lambda)} \sum_{m=0}^{\infty} \binom{-\Lambda}{m} (-z)^m \, d\Lambda,$$

$$= \int_0^1 e^{c\Delta t(1-\Lambda)} (1-z)^{-\Lambda} d\Lambda,$$

$$= \frac{e^{c\Delta t}(1 - z - e^{-c\Delta t})}{(1-z)(c\Delta t + \log(1-z))} \qquad (3.11)$$

Rearranging (3.11) to form

$$(c\Delta t+\log(1-z))\Gamma(z)=e^{c\Delta t}-(1-z)^{-1},$$

and expanding as a power series in z

$$\left(c\Delta t-z-\frac{z^2}{2}-\frac{z^3}{3}-\cdots\right)(g_0+g_1z+g_2z^2+\cdots)=e^{c\Delta t}-1-z-z^2-z^3-\cdots,$$

we can find a recurrence relation for the g_m for $m\geq 0$ by equating like powers of z

$$c\Delta t g_o=e^{c\Delta t}-1, \qquad (3.11a)$$

$$c\Delta t g_{m+1}+1=g_m+\frac{1}{2}g_{m-1}+\frac{1}{3}g_{m-2}+\cdots+\frac{1}{m+1}g_0$$

$$=\sum_{k=0}^{m}\frac{1}{m+1-k}g_k \qquad (3.12)$$

Having determined the $g_{m,}$ the ETD schemes (3.9) then can be given in explicit forms. Substituting (3.8) and (3.10) in (3.9), we deduce the general generating formula of ETD schemes of order s

$$u_{n+1}=u_n e^{c\Delta t}+\Delta t\sum_{m=0}^{s-1}g_m\sum_{k=0}^{m}(-1)^k\binom{m}{k}F_{n-k} \qquad (3.13)$$

where u_n and F_n denote the numerical approximation to $\mathrm{u}(t_n)$ and $\mathrm{F}(\mathrm{u}(t_n),t_n)$ respectively, and the g_m are given by (3.12).

3.2.3 ETD Schemes

<u>ETD1 Scheme</u>

From equation (3.11a) above, g_0 can be written as

$$g_0=\frac{e^{c\Delta t}-1}{c\Delta t}$$

To obtain the ETD1 scheme, we set $s = 1$ in the explicit generating formula (3.13) to get

$$u_{n+1} = u_n e^{c\Delta t} + \Delta t g_0 F_n$$

$u_{n+1} = u_n e^{c\Delta t} + \Delta t \left(\frac{e^{c\Delta t}-1}{c\Delta t}\right) F_n$, hence the ETD1 scheme is given by;

$$u_{n+1} = u_n e^{c\Delta t} + (e^{c\Delta t} - 1)\, F_n/c, \tag{3.14}$$

<u>ETD2 Scheme</u>

In the same manner as was than for the ETD1, setting $s = 2$ in (3.13) gives us the second-order ETD2 scheme

$$u_{n+1} = u_n e^{c\Delta t} + \left\{\left((c\Delta t + 1)e^{c\Delta t} - 2c\Delta t - 1\right) F_n + (-e^{c\Delta t} + c\Delta t + 1)F_{n-1}\right\} /(c^2\Delta t) \quad (3.15)$$

<u>ETD3 Scheme</u>

If $s = 3$ in (3.13), we obtain the third-order ETD3 scheme

$$u_{n+1} = u_n e^{c\Delta t} + \left\{\left((2c^2\Delta t^2 + 3c\Delta t + 2)e^{c\Delta t} - 6c^2\Delta t^2 - 5c\Delta t - 2\right) F_n + (-(4c\Delta t + 4)e^{c\Delta t} + 6c^2\Delta t^2 + 8c\Delta t + 4)F_{n-1} + \left((c\Delta t + 2)e^{c\Delta t} - 2c^2\Delta t - 3c\Delta t - 2\right) F_{n-2}\right\} /(2c^3\Delta t^2) \quad (3.16)$$

<u>ETD4 Scheme</u>

Set $s = 4$ in (3.13) to achieve the fourth-order ETD4 scheme

$$u_{n+1} = u_n e^{c\Delta t} + (\Phi_1 F_n - \Phi_2 F_{n-1} + \Phi_3 F_{n-2} - \Phi_4 F_{n-3})/(6c^4\Delta t^3), \tag{3.17}$$

where

$\Phi_1 = (6c^3\Delta t^3 + 11c^2\Delta t^2 + 12c\Delta t + 6)e^{c\Delta t} - 24c^3\Delta t^3 - 26c^2\Delta t^2 - 18c\Delta t - 6,$

$\Phi_2 = (18c^2\Delta t^2 + 30c\Delta t + 18)e^{c\Delta t} - 36c^3\Delta t^3 - 57c^2\Delta t^2 - 48c\Delta t - 18,$

$\Phi_3 = (6c^2\Delta t^2 + 24c\Delta t + 18)e^{c\Delta t} - 24c^3\Delta t^3 - 42c^2\Delta t^2 - 42c\Delta t - 18,$

$\Phi_4 = (2c^2\Delta t^2 + 6c\Delta t + 6)e^{c\Delta t} - 6c^3\Delta t^3 - 11c^2\Delta t^2 - 12c\Delta t - 6.$

Note that as $c \to 0$ in the coefficients of the s-order ETD methods, the methods reduce to the corresponding order of the Adams-Bashforth schemes. For example, if we expand the exponential function, using Taylor series, in the first-order ETD1 method (3.14) as follows

$$u_{n+1} = u_n\left(1 + c\Delta t + \frac{(c\Delta t)^2}{2} + \frac{(c\Delta t)^3}{3!} + \cdots\right) + F_n\left(\Delta t + \frac{c\Delta t^2}{2} + \frac{c^2\Delta t^3}{3!} + \cdots\right),$$

and then take the limit as $c \to 0$, while keeping terms of $O(\Delta t)$, we obtain

$$u_{n+1} = u_n + \Delta t(cu_n + F_n) = u_n + \Delta t du(t)/dt,$$

which corresponds to the forward Euler method. In fact, in the case of $c = 0$, the explicit formulas of the coefficients involve division by zero, and for very small values of $|c|$, the coefficients suffer from rounding errors due to the large amount of cancellation in the formulas. To tackle this problem we can use the Taylor series instead of using the explicit formula of the coefficients.

3.2.4 Exponential Time Differencing Runge-Kutta Methods

Generally, for the one-step time-discretization methods and the Runge-Kutta (RK) methods, all the information required to start the integration is available. However, for the multi-step time-discretization methods this is not true. These methods require the evaluations of a certain number of starting values of the nonlinear term $F(u(t), t)$at the nth and previous time steps to build the history required for the calculations. Therefore, it is desirable to construct ETD methods that are based on RK methods.

ETD Runge-Kutta Schemes

Cox et al (2002), constructed a second-order ETD Runge-Kutta method, analogous to the "improved Euler" method given as follows.

ETDRK1 Scheme

Putting $s = 1$ in equation (3.13) gives

$$u_{n+1} = u_n e^{c\Delta t} + (e^{c\Delta t} - 1)F_n/c. \qquad (3.18$$

Let $a_n \approx u_{n+1}$, than it implies that

$$a_n = u_n e^{c\Delta t} + \frac{(e^{c\Delta t} - 1)F_n}{c} \qquad (3.18)$$

The term a_n approximates the value of u at $t_n + \Delta t$. The next step is to approximate F in the interval $t_n \leq t \leq t_{n+1}$, with

$$F = F_n + (t - t_n)(F(a_n, t_n + \Delta t) - F_n)/\Delta t + O(\Delta t^2)$$

and substitute into (3.6) to give the ETD2RK1 scheme

$$u_{n+1} = a_n + (e^{c\Delta t} - c\Delta t - 1)(F(a_n, t_n + \Delta t) - F_n)/(c^2 \Delta t). \qquad (3.19)$$

ETD2RK2 Scheme

In a similar way, we can also form an ETD2RK2 scheme analogous to the "modified Euler" method. The first step

$$a_n = u_n e^{c\Delta t/2} + \left(e^{\frac{c\Delta t}{2}} - 1\right) F_n/c,$$

is formed by taking half a step of (3.18); then use the approximation

$$F = F_n + \frac{(t - t_n)}{\Delta t/2}(F(a_n, t_n + \Delta t/2) - F_n) + O(\Delta t^2),$$

in the interval $[t_n, t_n + \Delta t]$ in (3.6) to deduce the ETD2RK2 scheme

$$u_{n+1} = u_n e^{c\Delta t} + \Big\{\Big((c\Delta t - 2)e^{c\Delta t} + c\Delta t + 2\Big)F_n + 2(e^{c\Delta t} - c\Delta t - 1)F(a_n, t_n +$$

$$\Delta t/2))/c2\Delta t \qquad (3.20)$$

In fact there is a one-parameter family of such $ETD2RK_J$ schemes. For $j \in \mathbb{R}^+$, one can start with any fraction $1/j$ of Δt for the first step (3.18) which gives

$$a_n = u_n e^{c\Delta t/j} + \left(e^{\frac{c\Delta t}{j}} - 1\right)F_n/c.$$

The term a_n approximate the value of u at $t_n + \Delta t/j$. Next use the approximation

$$F = F_n + \frac{(t - t_n)}{\Delta t/j}\left(F(a_n, t_n + \Delta t/j) - F_n\right) + O(\Delta t^2),$$

in the interval $[t_n, t_n + \Delta t]$ in (3.6) to deduce the general $ETD2RK_J$ schemes as follows

$$u_{n+1} = u_n e^{c\Delta t} + \Big\{\Big((c\Delta t - j)e^{c\Delta t} + (j-1)c\Delta t + j\Big)F_n + j(e^{c\Delta t} - c\Delta t - 1)F(a_n, t_n +$$

$$\Delta t/j))/(c2\Delta t).$$

<u>ETD3RK Scheme</u>

In a similar way, for different values of the fraction $1/j$ there are infinitely many third-order and fourth-order ETD-RK schemes. For example, the third-order ETD3RK scheme which is analogous to the classical third-order RK method is given by

$$a_n = u_n e^{c\Delta t/2} + (e^{c\Delta t/2} - 1)F_n/c,$$

$$b_n = u_n e^{c\Delta t} + (e^{c\Delta t} - 1)(2F(a_n, t_n + \Delta t/2) - F_n)/c,$$

$$u_{n+1} = u_n e^{c\Delta t} + \Big\{\Big((c^2\Delta t^2 - 3c\Delta t + 4)e^{c\Delta t} - c\Delta t - 4\Big)F_n + 4\Big((c\Delta t - 2)e^{c\Delta t} +$$

$$c2\Delta t2 - 3c\Delta t - 4Fbn,tn + \Delta t/(c3\Delta t2) \qquad (3.21)$$

The terms a_n and b_n approximate the values of u at $t_n + \Delta t/2$ and $t_n + \Delta t$ respectively. The formula (3.21) is the quadrature formula for (3.6) derived from quadratic interpolation through the points $t_n, t_n + \Delta t/2$ and $t_n + \Delta t$.

ETD4RK Scheme

Introducing a further parameter, a fourth-order scheme ETD4RK is obtained as follows:

$a_n = u_n e^{c\Delta t/2} + (e^{c\Delta t\Delta/2} - 1)F_n/c,$

$b_n = u_n e^{c\Delta t/2} + (e^{c\Delta t/2} - 1)F(a_n, t_n + \Delta t/2)/c,$

$c_n = a_n e^{c\Delta t/2} + (e^{c\Delta t/2} - 1)(2F(b_n, t_n + \Delta t/2) - F_n)/c,$

$u_{n+1} = u_n e^{c\Delta t} + \Big\{\Big((c^2\Delta t^2 - 3c\Delta t + 4)e^{c\Delta t} - c\Delta t - 4\Big) F_n + 2((c\Delta t - 2)e^{c\Delta t} + c\Delta t +$

2)(F(an,tn+Δt/2)+F(bn,tn+Δt/2))+−cΔt+4ecΔt−c2Δt2−3cΔt−4F(cn,tn+Δt)/(c3 Δt2). (3.22)

The terms a_n and b_n approximate the values of u at $t_n + \Delta t/2$ and the term c_n approximates the value of u at $t_n + \Delta t$. The formula (3.22) is the quadrature formula for (3.6) derived from quadratic interpolation through the points $t_n, t_n + \Delta t/2$ and $t_n + \Delta t$, using average values of F at a_n and b_n.

In general, the ETD4RK method (3.22) has classical order four, but Hochbruck .M. and Ostermann, .A. et al (2005), showed that this method suffers from an order reduction. This is due to not satisfying some of the stiff order conditions. These conditions were derived for explicit exponential Runge-Kutta methods applied to stiff semi-linear parabolic problems with homogeneous Dirichlet boundary condition and under appropriate temporal smoothness of the exact solution. They also presented numerical experiments which show that the order reduction, predicted by their theory, may in fact arise in practical examples. In the worst case, this leads to an order reduction to order three of the Cox and Matthews method (3.22) and gives order four for Krogstad's method.

Finally, we note that as $c \rightarrow 0$ in the coefficients of the s-order ETD-RK methods, the methods reduce to the corresponding order of the Runge-Kutta schemes.

3.3 Stability Analysis

The stability of a given method for solving a system of PDEs or ODEs is a theoretical measure of the extent to which the method produces satisfactory approximations. Stability is related to the accuracy of the methods and refers to errors not growing in subsequent steps. Such methods are called numerically stable methods.

3.3.1 Diagrammatic Representation of Stability Regions for ETD and ETDRK Schemes

Hala (2008), studied the stability of ETD and ETDRK schemes and came out with diagrams to represent their stability regions. These Diagrams give a clearer understanding of the stability of the schemes.

Stability Analysis of ETD1and ETD2 Schemes

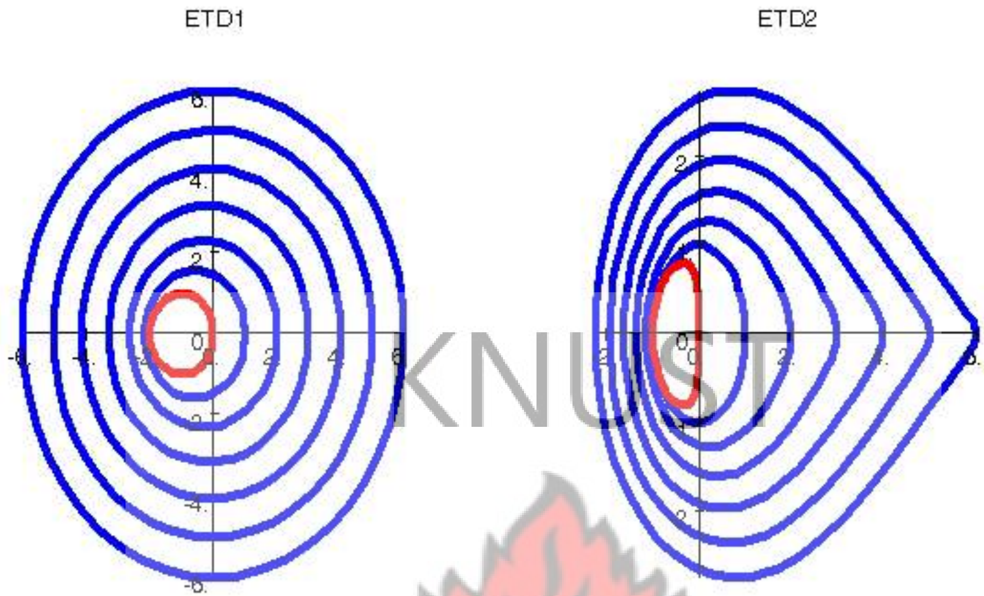

Figure 3.1: Stability region in the complex x plane for the ETD1 and the ETD2 schemes

As shown in figure 3.1, the boundary of the stability region for the ETD1 and the ETD2 schemes passes through the point $x = -y$ (this is true for any fixed value of y), which agrees with the result found for the ETD2 schemes. A view of these two diagrams above confirms that ETD1 is more stable than ETD2.

Stability Analysis of ETD2RK1 and ETD2RK2

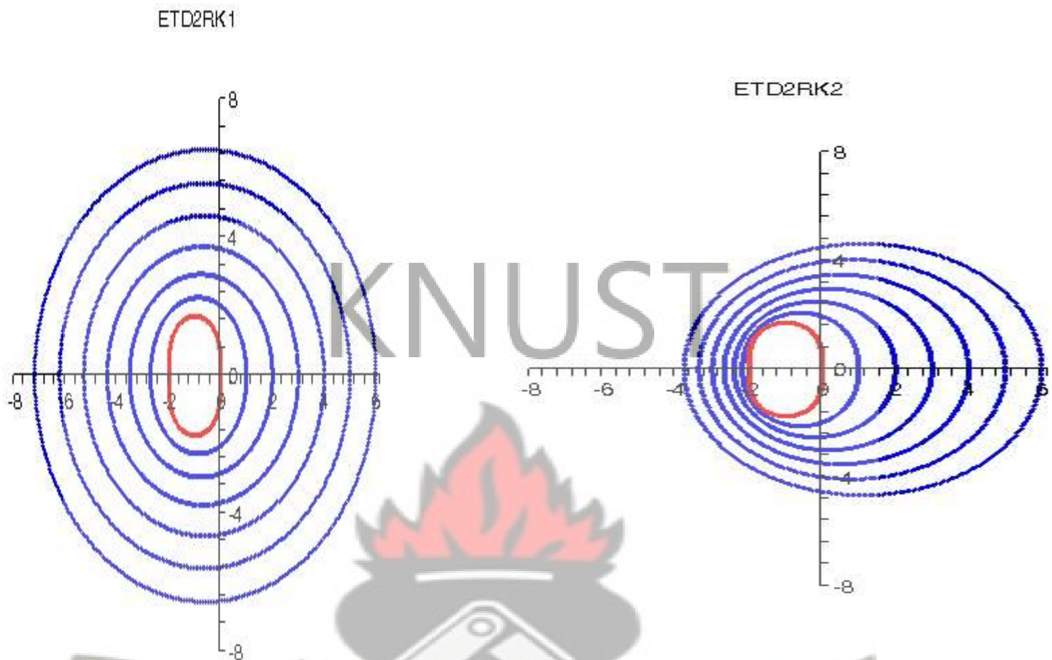

FIGURE 3.2: Stability Regions of ETD2RK1 and ETD2RK2 in the complex x plane.

From the two figures above, it can be seen that ETD2RK1 scheme is more accurate than the ETD2RK2. Generally, the stability regions of the ETD-RK schemes are larger than those of the explicit multi-step ETD schemes making the ETD schemes more stable than the ETDRK schemes.

The approach developed for the stability analysis of composite schemes, i.e. schemes that use different methods for the linear and nonlinear parts of the equation, computes the boundaries of the stability regions for a general test problem. That is to analyze the stability of the ETD schemes, we linearize the autonomous ODE

$$\frac{du(t)}{dt} = cu(t) + F\big(u(t)\big), \tag{3.23}$$

about a fixed point u_0 (so that $cu_0 + F(u_0) = 0$), to obtain

$$\frac{du(t)}{dt} = cu(t) + \lambda u(t) = (c + \lambda)u(t), \tag{3.24}$$

where $u(t)$ is the perturbation to u_0 and

$$\lambda = \frac{dF(u(t))}{du}|u(t) = u_0$$

Again $F(u_0) - F(u_n) = \lambda(u_0) - \lambda(u_n)$

But $u_0 = 0$

Therefore, $\mathrm{F}(u_n) = \lambda u_n$ $(3.24a)$

In order to keep the fixed point u_0 stable, we require $Re(c + \lambda) < 0$ (note that the fixed points of the ETD methods are the same as those of the ODE (3.23), in contrast to the IF methods which do not preserve the fixed points for the ODE that they discretize. It seems desirable for a numerical method to fulfill this property with respect to capturing as much of the dynamics of the system as possible).

If both c and λ are complex, the stability region is four-dimensional. But if both c and λ are purely imaginary or purely real, or if λ is complex and c is fixed and real then the stability region is two-dimensional.

This study concentrates on two cases to determine whether the schemes are asymptotically stable. The conditions are as follows;

- λ is complex and c is fixed, negative and purely real.
- c is negative and both c and λ are purely real.

Algorithm

To determine whether an exponential time differencing method is asymptotically stable, considering the problem

$$\frac{du(t)}{dt} = cu(t) + \lambda u(t)$$

Step 1: Solve the problem using any one of the ETD1, ETD2, ETD2RK2 and ETD2RK2 methods.

Step 2: Divide through the u_{n+1} solution with u_n to obtain an equation for $\frac{u_{n+1}}{u_n}$

Step 3: Set $r = \frac{u_{n+1}}{u_n}$, $x = \lambda\Delta t$ and $y = c\Delta t$, where c and λ are parameters in the given problem and Δt is the time step.

Step 4: For a scheme to be asymptotically stable then;

$$r = \frac{u_{n+1}}{u_n} \leq 1$$

Given the problem above, the asymptotic stability of the schemes can be determined as follows;

3.3.2 Stability of ETD1 Scheme

Equation (3.14) can be written in the form;

$$\frac{u_{n+1}}{u_n} = e^{c\Delta t} + \frac{(e^{c\Delta t} - 1)}{cu_n}F_n \tag{3.25}$$

From equation (3.24a), F_n can be written as;

$$F_n = \lambda u_n \tag{3.26}$$

Putting (3.26) in to (3.25), gives;

$$\frac{u_{n+1}}{u_n} = e^{c\Delta t} + \frac{(e^{c\Delta t} - 1)}{cu_n}\lambda u_n$$

$$\frac{u_{n+1}}{u_n} = e^{c\Delta t} + \frac{(e^{c\Delta t} - 1)}{c}\lambda \qquad (3.26a)$$

putting $x = \lambda\Delta t, y = c\Delta t$ and $r = \frac{u_{n+1}}{u_n}$ in to the above equation gives;

$$r = e^y + \frac{x}{y}(e^y - 1) \qquad (3.27)$$

If

$$r = e^y + \frac{x}{y}(e^y - 1) \leq 1 \qquad (3.27a)$$

then ETD1 is asymptotically stable.

3.3.3Stability of ETD2 Scheme

Equation (3.15) can be written in the form;

$$\frac{u_{n+1}}{u_n} = e^{c\Delta t} + \frac{\left\{\left((c\Delta t + 1)e^{c\Delta t} - 2c\Delta t - 1\right)F_n + (-e^{c\Delta t} + c\Delta t + 1)F_{n-1}\right\}}{c^2\Delta t u_n}$$

Substituting equation (3.26) in to the above equation gives;

$$\frac{u_{n+1}}{u_n} = e^{c\Delta t} + \frac{\left\{\left((c\Delta t + 1)e^{c\Delta t} - 2c\Delta t - 1\right)\lambda u_n + (-e^{c\Delta t} + c\Delta t + 1)F_{n-1}\right\}}{c^2\Delta t u_n} \qquad (3.28)$$

putting $x = \lambda\Delta t, y = c\Delta t$ and $r = \frac{u_{n+1}}{u_n}$ in to the above equation gives;

$$y^2r^2 - (y^2e^y + [(y+1)e^y - 2y - 1]x)r + (e^y - y - 1)x = 0$$

$$r = e^y + \left(\frac{e^y - 1}{y}\right)x + \left(\frac{(e^y - y - 1)}{y^2}\right)x^2 \qquad (3.28a)$$

If

$$r = e^{y} + \left(\frac{e^{y}-1}{y}\right)x + \left(\frac{(e^{y}-y-1)}{y^{2}}\right)x^{2} \leq 1 \qquad (3.28b)$$

then ETD2 is asymptotically stable.

3.3.4 Stability of ETD2RK1 Scheme

Equation (3.19) can be written as;

$$\frac{u_{n+1}}{u_n} = e^{c\Delta t} + \frac{(e^{c\Delta t}-1)F_n}{cu_n} + (e^{c\Delta t} - c\Delta t - 1)(F(a_n, t_n + \Delta t)/c^{2}\Delta t u_n$$

Substituting $F_n = \lambda u_n$ in to the above equation gives

$$\frac{u_{n+1}}{u_n} = e^{c\Delta t} + \frac{(e^{c\Delta t}-1)\lambda u_n}{cu_n} + \left((e^{c\Delta t} - c\Delta t - 1)\frac{F(a_n, t_n + \Delta t)}{c^{2}\Delta t u_n}\right) \quad (3.29)$$

Putting $x = \lambda\Delta t, y = c\Delta t$ and $r = \frac{u_{n+1}}{u_n}$ in to the above equation, we get

$$r = e^{y} + (e^{y}-1)\frac{\lambda u_n}{cu_n} + \left(\frac{(e^{y}-y-1)(e^{y}-1)}{y^{2}}\right)x^{2}$$

$$r = e^{y} + (e^{y}-1)\frac{x}{y} + \left(\frac{(e^{y}-y-1)(e^{y}-1)}{y^{2}}\right)x^{2}$$

$$r = e^{y} + \left(\frac{e^{y}-1}{y}\right)x + \left(\frac{(e^{y}-y-1)(e^{y}-1)}{y^{2}}\right)x^{2} \qquad (3.29a)$$

If

$$r = e^{y} + \left(\frac{e^{y}-1}{y}\right)x + \left(\frac{(e^{y}-y-1)(e^{y}-1)}{y^{2}}\right)x^{2} \leq 1 \qquad (3.29b)$$

then ETD2RK2 is asymptotically stable.

3.3.5 ETD2RK2 Scheme

Equation (3.20) can be written as

$$\frac{u_{n+1}}{u_n} = e^{c\Delta t} + \frac{\left\{\left((c\Delta t-2)e^{c\Delta t}+c\Delta t+2\right)F_n+2\left(e^{c\Delta t}-c\Delta t-1\right)F(a_n,t_n+\Delta t)+\Delta t/2)\right\}}{u_n c^2\Delta t} \qquad (3.30)$$

Let $r = \frac{u_{n+1}}{u_n}$, $x = \lambda\Delta t$ and $y = c\Delta t$

$$r = e^y + \left(\frac{2(e^y - y - 1)e^{y/2} + (y-2)e^y + y + 2}{y^2}\right)x + \left(\frac{2(e^y - y - 1)(e^{y/2} - 1)}{y^3}\right)x^2 \qquad (3.30a)$$

If

$$r = e^y + \left(\frac{2(e^y - y - 1)e^{y/2} + (y-2)e^y + y + 2}{y^2}\right)x + \left(\frac{2(e^y - y - 1)(e^{y/2} - 1)}{y^3}\right)x^2 \leq 1 \qquad (3.30b)$$

then ETD2RK2 is asymptotically stable.

CHAPTER 4

ANALYSIS AND RESULTS

4.0 Overview

This chapter presents manual computational results for the *r* values of ETD1, ETD2, ETD2RK1 and ETD2RK2 schemes which will be used later to determine the stability of each of the schemes. A brief discussion of the manual computational results is used to end this chapter.

4.1 Computational Results of Stability of ETD Schemes

Du et al (2009), gave the parameter values for c, λ and Δt. These values were adopted in this study to compute the values of x and y given that $x = \lambda\Delta t \; and \; y = c\Delta t$.

Following the first condition in section (3.3), where λ is complex and c is fixed, negative and both $\lambda \; and \; c$ are purely real; the values of x and y were computed using the adopted values for the parameters $c, \lambda \; and \; \Delta t$ and represented in a tabular form below.

Table 4.1: x and y Values Given that c is Fixed and Negative and λ is Complex and both are Purely Real.

Δt	c	λ	x	y
1×10^{-3}	-0.1	1×10^{-4}	1×10^{-7}	-1×10^{-4}
2×10^{-3}	-0.1	1×10^{-5}	2×10^{-8}	-2×10^{-4}
3×10^{-3}	-0.1	1×10^{-6}	3×10^{-9}	-3×10^{-4}
4×10^{-3}	-0.1	1×10^{-7}	4×10^{-10}	-4×10^{-4}
5×10^{-3}	-0.1	1×10^{-8}	5×10^{-11}	-5×10^{-4}
6×10^{-3}	-0.1	1×10^{-9}	6×10^{-12}	-6×10^{-4}

It can be observed from Table 4.1 above that as the values of Δt and λ increase and c remain constant values of x and y decreases accordingly. Because of the negative values of c, all values obtained for y were also negative.

Considering the second condition in section (3.3), where λ is complex and c is changing and negative and both λ *and* c are purely real; the values of x and y were computed using the adopted values for the parameters c, λ *and* Δt and represented in a tabular form below.

Table 4.2: x and y Values Given c is Changing and Negative and λ is Complex and both c and λ are Real

Δt	c	λ	x	y
1×10^{-3}	-0.1	1×10^{-4}	1×10^{-7}	-1×10^{-4}
2×10^{-3}	-0.2	1×10^{-5}	2×10^{-8}	-4×10^{-4}
3×10^{-3}	-0.3	1×10^{-6}	3×10^{-9}	-9×10^{-4}
4×10^{-3}	-0.4	1×10^{-7}	4×10^{-10}	-1.6×10^{-3}
5×10^{-3}	-0.5	1×10^{-8}	5×10^{-11}	-2.5×10^{-3}
6×10^{-3}	-0.6	1×10^{-9}	6×10^{-12}	-3.6×10^{-3}

Values from Table 4.2 show that given the condition that c is changing and negative and λ is complex and both c *and* λ are real, both values of x and y decrease as Δt increases.

4.2 Computations of the r Values of the ETD and ETDRK Schemes

From tables (4.1) and (4.2), the computed values of x and y were used to carry out the computations for the r values of ETDI, ETD2, ETD2RK1 and ETD2RK2.

Considering the condition that λ is complex and c is fixed and negative and both λ and c are purely real, equations(3.24),(3.26a) and (3.27) computes the r values for ETD1, in a similar way, equations(3.24), (3.28) and (3.28a) computes the r values for ETD2, while equations (3.24), (3.29) and 93.29a) computes the r values for ETD2RK1. Finally equations (3.24), (3.30) and (3.30a) computes the *r* values for ETD2RK2. Below is a summary of the computed values of *r* for the schemes.

Table 4.3: The *r* Values of the Schemes when Parameter c is Fixed and Negative and λ is Complex

$\|r\|$ *VALUES OF SCHEMES*			
$ETD1$	$ETD2$	$ETD2RK1$	$ETD2RK2$
0.9999	0.9999	0.9999	0.9999
0.9998	0.9998	0.9998	0.9998
0.9997	0.9997	0.9997	0.9997
0.9996	0.9996	0.9996	0.9996
0.9995	0.9995	0.9995	0.9995
0.9994	0.9994	0.9994	0.9994

From Table 4.3, all values corresponding to the ETD and ETDRK schemes are less than one indicating that all schemes are asymptotically stable at these points studied. It can also be observed that at each Δt all schemes have the same values and this is true for all values of Δt. Hence none of the schemes can be said to be more asymptotically stable than the other. Again descending down the table, the values of *r* corresponding to the schemes decreases, hence making the schemes more stable.

Considering the condition that λ is complex and c is changing and negative and both λ and c are purely real, equations (3.24), (3.26a) and (3.27) computes the r values for ETD1, in a similar way, equations (3.24), (3.28) and (3.28a) computes the r values for ETD2, while equations (3.24), (3.29) and (3.29a) computes the r values for ETD2RK1. Finally equations (3.24), (3.30) and (3.30a) computes the r values for ETD2RK2. Below is a summary of the computed values of r for the schemes.

Table 4.4: The *r* Values of the Schemes when Parameter c is changing and Negative and λ is Complex.

$\lvert r \rvert$ *VALUES OF SCHEMES*			
$ETD1$	$ETD2$	$ETD2RK1$	$ETD2RK2$
0.9999	0.9999	0.9999	0.9999
0.9996	0.9996	0.9996	0.9996
0.9991	0.9991	0.9991	0.9991
0.9980401	0.9980401	0.9980401	0.9980401
0.997503	0.997503	0.997503	0.997503
0.996406	0.996406	0.996406	0.996406

Again in Table 4.4, all values corresponding to ETD and ETDRK schemes are less than one, indicating that all schemes are asymptotically stable at these points. It can also be observed that at each Δt all the schemes have the same values suggesting that none of the schemes studied is better in terms of asymptotic stability than the other. Descending down the table, the r values of the schemes are decreasing, hence suggesting that the schemes are becoming more asymptotically stable.

4.3 Discussion

From Table 4.1, given that $1 \times 10^{-3} \leq \Delta t \leq 6 \times 10^{-3}$, c is fixed and negative and λ is complex, results obtained for $x = \lambda\Delta t$ and $y = c\Delta t$ showed that both values of x and y increased for every increase in Δt, however all values of y were negative.

In Table 4.2, if c is changing and negative and λ is complex, the values of remained the same while y values were found to be changing.

From Table 4.3, all values corresponding to the various ETD and ETDRK schemes are less than one indicating that all schemes are asymptotically stable at these points studied. It can also be observed that at each Δt all schemes have the same values and this is true for all values of Δt. Hence none of the schemes can be said to more asymptotically stable than the order. Again descending down the table, the values of r corresponding to the schemes decreases, hence making the schemes more stable.

Again in Table 4.4, all values corresponding to ETD and ETDRK schemes are less than one, indicating that all schemes are asymptotically stable at these points. It can also be observed that at each Δt all the schemes have the same values suggesting that none of the schemes studied is better in terms of asymptotic stability than the other. Descending down the table, the r values of the schemes are decreasing, hence suggesting that the schemes are becoming more asymptotically stable.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

5.1 Conclusion

This research suggest that the comparison of the asymptotic stability of ETD1, ETD2, ETD2RK2 and ETD2RK2 schemes in solving the stiff semi-linear differential equation (3.24) was properly executed. This was made possible when some parameters $c,\ \lambda\ and\ \Delta$t were adopted and used for computations.

To ensure that the first objective was met, ETD1, ETD2, ETD2RK1 and ETD2RK2 schemes were used to solve the stiff semi-linear differential equation (3.24) to obtain the asymptotic stability expressions (3.27a), (3.28a), (3.29b) and (3.30b).

The second objective suggested the following conclusions;

- When the parameter c is negative and changing, and λ is complex, all the schemes are asymptotically stable, however as Δt increases and the parameter c is changing, the corresponding $|r|$ values of the schemes decreases accordingly making them more asymptotically stable.
- When the parameter c is negative and fixed and λ is complex and both are real, all the schemes studied are asymptotically stable, however as Δt increases, corresponding $|r|$ values of the schemes decreases accordingly making them more stable.
- At each Δt, the $|r|$ values of all the schemes are the same, that is; at $\Delta t = 0.001$, $|r|$ value of ETD1 is 0.9999, ETD2 is 0.9999, ETD2RK1 is 0.9999 and ETD2RK2 is 0.9999. Hence as far as asymptotic stability is concern, none of the schemes

studied is more stable than the other, therefore ETD1, ETD2, ETD2RK and ETD2RK2 are efficient schemes for solving stiff semi-linear differential equations.

- It will take several Δt values to make the schemes more stable when c is fixed and negative and λ is complex than when c is changing and negative and λ is complex.

5.2 Recommendations

The conclusions drawn in this research were based on the values of the parameters used in this work and may not have the same observations when different values are used for the similar study.

This study serves as the basis for more detailed analysis in to the stability properties of other numerical methods to be carried out in future. It is hoped that future research should look at how stability affects each of these schemes studied and come out with different methods to improve on the stability of these methods.

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APPENDIX

Fourier Analysis of Steady State Solution of Kuramoto- Sivashinsky (K-S) Equation

The Kuramoto-Sivashinsky equation, which will be refered to as K-S equation, is one of the simplest semi-linear PDEs capable of describing complex (chaotic) behavior in both time and space. This equation has been of mathematical interest because of its rich dynamical properties. In physical terms, this equation describes reaction diffusion problems, and the dynamics of viscous-fluid films flowing along walls, and was introduced by Sivashinsky as a model of laminar flame-front instabilities and by Kuramoto as a model of phase turbulence in chemical oscillations. A fairly large number of numerical and theoretical studies have been devoted to the K-S equation;

The K-S equation in one space dimension can be written in "derivative" form

$$\frac{\partial w(x,t)}{\partial t} = -w(x,t)\frac{\partial w(x,t)}{\partial x} - \frac{\partial^2 w(x,t)}{\partial x^2} - \frac{\partial^4 (x,t)}{\partial x^4}, \qquad (4.1)$$

Or in "integral" form, putting $w(x,t) = \partial u(x,t)/\partial x\partial$ in equation (4.1), we have

$$\frac{\partial}{\partial t}\left[\frac{\partial u(x,t)}{\partial x}\right] = -\frac{\partial u(x,t)}{\partial x}\frac{\partial}{\partial x}\left[\frac{\partial u(x,t)}{\partial x}\right] - \frac{\partial^2}{\partial x^2}\left[\frac{\partial u(x,t)}{\partial x}\right] - \frac{\partial^4}{\partial x^4}\left[\frac{\partial u(x,t)}{\partial x}\right]$$

This reduces to;

$$\frac{\partial (x,t)}{\partial t} = -\frac{1}{2}\left(\frac{\partial u(x,t)}{\partial x}\right)^2 - \frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial^4 u(x,t)}{\partial x^4}, \qquad (4.2)$$

or in a more simpler form as;

$$u_t + uu_x + u_{xx} + u_{xxxx} = 0 \qquad (4.3)$$

where the subscript denote differentiation of the state variable u with respect to time and space, respectively. Here we seek steady state standing wave solution ($u_t = 0$) to the equation in an infinite spacial domain using Fourier analysis.

For a start, consider the simplest model consisting of a single sine wave;

$$u = asinkx \tag{4.3a}$$

Taking derivatives of (4.3a), the following are obtained;

$u_x = akcoskx$

$u_{xx} = -ak^2sinkx$

$u_{xxx} = -ak^3coskx$

$u_{xxxx} = ak^4sinkx$

The nonlinear term of the K-S equation is

$uu_x = a^2ksinkxcoskx$

Simplify using the following trigonometric identities;

$sinAcosB = \frac{1}{2}[\sin(A+B) + \sin(A-B)]$

To obtain the following:

$uu_x = \frac{1}{2}a^2ksin2kx$

Steady state of K-S equation

$$uu_x + u_{xx} + u_{xxxx} = 0$$

Equating term by term, we have

$$-ak^2 + ak^4 = 0$$

$$\frac{1}{2}a^2k = 0$$

Clearly there is no solution except for $a = 0$ or $k = 0$. However, the first equation has a second solution given by $k = 0$, which is not very different from the value observed numerically at $k = 26\pi/100 = 0.816814$.

Considering a more realistic model, motivated by a numerical solution of the K-S equation is

$$u = asinkx + bsin2kx \qquad (4.3b)$$

Taking the derivatives of (4.3b), we have

$$u_x = akcoskx + 2bkcos2kx$$

$$u_{xx} = -ak^2 sinkx - 4bk^2 sin2kx$$

$$u_{xxx} = -ak^3 coskx - 8bk^3 cos3kx$$

$$u_{xxxx} = ak^4 sinkx + 16bk^4 sin2kx$$

The nonlinear term of the equation will be

$$uu_x = a^2 kxcoskx + 2absinkxcos2kx + abksin2kxcoskx + 2b^2 ksin2kxcos2kx$$

Simplify using the following trigonometric identity

$$sinAcosB = \frac{1}{2}[\sin(A+B) + \sin(A-B)]$$

to obtain the following;

$$uu_x = \frac{1}{2}a^2 ksin2kx + abk[sin3kx - sinkx] + \frac{1}{2}abk[sin3kx + sinkx] + b^2 ksin4kx$$

Steady state of K-S equation

$$uu_x + u_{xx} + u_{xxxx} = 0$$

Equating term by term, we have

$$-abk + \frac{1}{2}abk - ak^2 + ak^4 = 0$$

$$\frac{1}{2}a^2 k - 4bk^2 + 16bk^4 = 0$$

$$b^2 k = 0$$

This system is over specified since there are four equations for three unknowns. However, the last two equations are only approximations since they are inconsistent with the assumption that only terms in $sinkx$ and $sin2kx$ are present.

The first two equations are exact and can be simplified (for *k, a* and *b* nonzero) to;

$$2k(k^2 - 1) = b$$

$$8bk(1 - 4k^2) = a^2$$

From the numerical solution of the K-S equation, we have

$$k = 26\pi/100 = 0.816814$$

from which we can determine *a* and *b*.

$$b = 2k(k^2 - 1) = -0.5436957$$

$$a = \sqrt{8bk(1 - 4k^2)} = 2.4348874$$

There values are in reasonable agreement with numerical results. Hence;

$$u = 2.4348874 sin 0.816814x - 0.5436957 sin 0.816814x$$

Solving a more involving equation in the form

$$u = a + bsinkx + csin2kx + dcos2kx + esin3kx + fcos3kx \qquad (4.3c)$$

Its derivatives will be

$$u_x = bkcoskx + 2ckcos2kx - 2dksin2kx + 3ekcos3kx - 3fksin3kx$$

$$u_{xx} = -bk^2sinkx - 4ck^2sin2kx - 4dk^2cos2kx - 9ek^2sin3kx - 9fk^2coskx$$

$$u_{xxx} = -bk^3coskx - 8ck^3cos2kx + 8dk^3sin2kx - 27ek^3cos3kx + 27fk^3sin3kx$$

$$u_{xxxx} = bk^2sinkx + 16ck^2sin2kx + 16dk^4cos2kx + 81ek^4sin3kx + 81fk^4cos3kx$$

Therefore the nonlinear term will be

$$
\begin{aligned}
uu_x = {} & abkcoskx + 2ackcos2kx - 2adksin2kx + 3aekcoskx - 3afksin3kx \\
& + b^2ksinkxcoskx + 2bcksinkxcos2kx - 2bdksin2kxsinkx \\
& + 3beksinkxcos3kx - 3cfksin3kxsin2kx + bcksin2kxcoskx \\
& + 2c^2ksin2kxcos2kx - 2cdksin^2 2kx + 3ceksin2kxcoskx \\
& - 3cfksin3kxsin2kx + bdkcos2kxcoskx + 2cdkcos2kx \\
& - 2d^2ksin2kxcos2kx + 3dekcos3kxcos2kx - 3dfksin3kxcos2kx \\
& + beksin3kxcoskx + 2ceksin3kxcos2kx - 2deksin2kxsin2kx \\
& + 3e^2ksin3kxcos3kx - 3efksin^2 3kx + bfkcos3kxcoskx \\
& + 2cfkcos3kxcoskx - 2dfksin2kxcos3kx + 3efkcos^2 3kx \\
& - 3f^2ksin3kxcoskx
\end{aligned}
$$

Simplify using the following trigonometric identities;

$$sinAsinB = \frac{1}{2}[\cos(A-B) - \cos(A+B)]$$

$$cosAcosB = \frac{1}{2}[cos(A+B) + \cos(A-B)]$$

$$sinAcosB = \frac{1}{2}[\sin(A+B) + \sin\,(A-B)$$

to obtain the following;

$$uu_x = abkcoskx + 2ackcos2kx - 2adksin2kx + 3aekcos3kx - 3afksin3kx$$

$$+ \frac{1}{2}b^2ksin2kx + bck[sin3kx - sinkx] - bdk[coskx - cos3kx]$$

$$+ \frac{3}{2}bek[sin4kx - sin2kx] - \frac{3}{2}bfk[coskx - cos4kx]$$

$$+ \frac{1}{2}bck[sin3kx + sinkx] + c^2ksin4kx - cdk[1 - cos4kx]$$

$$+ \frac{3}{2}cef[sin5kx - sinkx] - \frac{3}{2}cfk[coskx - cos5kx]$$

$$+ \frac{1}{2}bdk[cos3kx + coskx] + cdk[cos4kx + 1] - d^2ksin4kx$$

$$+ \frac{3}{2}dek[cos5kx + coskx] - \frac{3}{2}dfk[sin5kx + sinkx]$$

$$+ \frac{1}{2}bek[sin4kx + sin2kx] + cef[sin5kx + sinkx]$$

$$- dek[coskx - cos5kx] + \frac{3}{2}[e^2ksin6kx] - \frac{3}{2}efk(1 - cos6kx)$$

$$+ \frac{1}{2}bfk[cos4kx + cos2kx] + cfk[cos5kx + coskx]$$

$$- dfk[sin5x - sinkx] + \frac{3}{2}efk[cos6kx + 1] - \frac{3}{2}f^2ksin6kx$$

Steady state of K-S equation

$$uu_x + u_{xx} + u_{xxxx} = 0$$

Equating term by term, we have

$$\frac{1}{2}bk - \frac{1}{2}cek - \frac{1}{2}dfk - bk^2 + bk^4 = 0$$

$$-2adk + \frac{1}{2}b^2k - bek - 4ck^2 + 16ck^4 = 0$$

$2ack - bfk - 4dk^2 + 16dk^4 = 0$

$$-3afk + \frac{3}{2}bdk - 9fk^2 + 81fk^4 = 0$$

$$3aek + \frac{3}{2}bdk - 9fk^2 + 81fk^4 = 0$$

$$2bfk + 2cdk = 0$$

$$\frac{5}{2}cek - \frac{5}{2}dfk = 0$$

$$\frac{5}{2}cfk + \frac{5}{2}dek$$

The $sin6kx$ and $cos6kx$ terms are ignored since they would require $e = f = 0$

Similarly;

$$2[2bk(k^2 - 1) + bc - ce - df] = 0$$

$$2[8ck(4k^2 - 1) - 4ad + b^2 - 2be] = 0$$

$$4dk(4k^2 - 1) + 2ac - bf = 0$$

$$3[6ek(9k^2 - 1) - 2af + bc]/2 = 0$$

$$3[6fk(9k^2 - 1) + 2ae + bd]/2 = 0$$

$$(c^2 - d^2)k + 2be = 0$$

$$2[bf + cd] = 0$$

$$5[ce - df]/2 = 0$$

$$5[cf - de]/2 = 0$$

This system is over-determined since there are nine equations for seven unknowns. Using only the first seven equations (ignoring the $sin5kx$ and $cos5kx$ terms), gives the following exact numerical results (may not be unique);

$$k = 0.4463$$

$a = 0$

$$b = 0.5172$$

$$c = 0.5646$$

$$d = 0$$

$$e = -0.3176$$

$$f = 0$$

Hence

$$u = 0.5172sin0.4463x + 0.5646sin0.8926x - 0.3176sin1.3389x$$

However, we can perform a numerical least-square fit to the entire system of nine equations with the following results (mean square error $\sim 7 \times 10^{-5}$)

$$k = 1.0267$$

$$a = 0.4469$$

$$b = 1.7029$$

$$c = -0.1111$$

$$d = 0.0075$$

$$e = 0.0036$$

$$f = -0.0003$$

Hence

$$u = 0.4469 + 1.7209sin1.0267x - 0.1111sin2.0534x + 0.0075cos2.0534x$$
$$+ 0.0036sin3.0801x - 0.0003cos3.0801x$$

In summary, the table below shows the numerical results of the Kuramoto-Sivashinsky equation when using M Fourier terms.

Numerical Results of K-S Equation Using M Fourier terms

M	K	a_1	a_2	a_3	a_4	a_5	a_6	a_7
1	1.0000	0						
2	1.0000	0.0111	-0					
3	0.9973	0.5038	-0.0107	0.0001				
4	0.9801	1.3141	-0.0772	0.0023	-0.0001			
5	0.9033	2.3439	-0.3294	0.0224	-0.0012	0.0001		
6	0.8214	2.4704	-0.5237	0.0514	-0.0041	0.0003	-0	
7	0.8433	2.5042	-0.4856	0.0442	-0.0033	0.0002	-0	0

These are the values obtained by Fourier analysis of the steady state numerical solution of the Kuramoto-Sivashinsky equation.

When $k = 0.8168$

Fourier Analysis of the Steady State Numerical Solution of the K-S Equation.

n	$Real\ Part$	$Imaginary\ Part$	$Amplitude$	$Phase$
1	-0.02678	-2.913	2.913	89.5
2	0.01649	0.8968	-0.897	88.9
3	-0.004718	-0.1711	0.1711	88.9
4	0.001284	0.03491	-0.03493	87.9
5	-0.0003761	0.008161	0.008169	-87.4

The table above shows the trend in the numerical results of the Kuramoto-Sivashinsky Equation when using M Fourier terms. From the table it can be observed that as the value of M increases, the K value decreases and the terms in the terms in the K-S equation increases.

An analysis of the steady state numerical solution of the K-S equation using the Fourier analysis summarized in Table(4.3) show the trend of values of the real, imaginary, amplitude and phase when $K = 0.8168$. From the table, values representing the phase decreases as the n values increase.