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Stability of Exponential Time Differencing Runge-Kutta Method for Solving Stiff Semi-linear Differential Equations

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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. Our attention has been focused on the explicit Exponential Time Differencing (ETD) integrators that are designed to solve stiff semi-linear problems, we employ asymptotic stability criteria to confirm the efficiency of Exponential Time Differencing Runge-Kutta method with necessary approximations.*

Keywords: Stability, Exponential Time Differencing, Stiff Semi-linear.

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INTRODUCTION

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 are said to be a stiff differential equation. Differential equations can be grouped into two types 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 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.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 e^{-ct}, 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).
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.

Azure (2013), Derived the various algorithms and stability expressions for ETD and ETDRK, and asymptotic stability criteria was used to establish the stability of the selected ETD schemes.

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 non-linear 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.

THE GOVERNING EQUATION

We begin by giving in detail, the algorithm derivation for the explicit ETD scheme.

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

$$\frac{\partial u(x,t)}{\partial t} = Lu(t) + F(u(t),t) \qquad (2.0.6)$$

Where the linear operator L contains higher-order spatial derivatives than those contained in the nonlinear operator F, and is mainly the term responsible for stiffness. For problems of spatially periodic boundary conditions, we use Fourier spectral methods to discretize the spatial derivations of (2.0.6), and hence obtain a stiff system of coupled ODEs in time *t*

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

The linear part *L* of the system is represented by a diagonal matrix, and *F* represents the action of te nonlinear operator on *u* on the grid.

To derive ETD methods, we consider for simplicity a single model of a stiff ODE.

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

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.

Exponential Time Differencing Methods

To derive the step ETD schemes, we multiply (2.0.3) through by the integrating factor e^{-ct} and then integrate the equation over a single time step from

$t = t_n \ to \ t = t_{n+1} = t_n + \Delta t$,

$$u(t_{n+1}) = u(t_n)e^{c\Delta t} \int_0^{\Delta t} e^{-c\tau} F(u(t_n + \tau), t_n + \tau)d\tau \qquad (2.0.9)$$

This formula is exact, and the next step is to derive approximations to the integral in equation (2.0.9). 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 $F(u(t_n + \tau), t_n + \tau)\ in\ the\ form$

$$F(u(t_n) + \tau), t_n + \tau) \approx G_n(t_n + \tau) = \sum_{m=0}^{s-1} (-1)^m \left(-\frac{\tau}{\Delta t}\right)^{\nabla m} G_n(t_n), \qquad (2.1.0)$$

Where ∇ is the backward difference operator defined as follows

$$\nabla^m G_n(t_n) = \sum_{k=0}^{m} (-1)^k \binom{m}{k} G_{n-k}(t_{n-k}) \quad (2.0.8)$$

$$\approx \sum_{k=0}^{m} (-1)^k \binom{m}{k} F(u(t_{n-k}), \qquad (2.1.1)$$

And

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

(Note that $0!\binom{-\Lambda}{0} = 1$). If we substitute the approximation (2.1.0) in the integrand (2.0.9), we get

$$u(t_{n+1}) - u(t_n)e^{c\Delta t} \approx \Delta t \sum_{m=0}^{s-1} (-1)^m \int_0^1 e^{c\Delta t(1-\wedge)} \binom{-\wedge}{m} d\wedge\, \nabla^m G_n(t_n) \qquad (2.1.2)$$

Where $\Lambda = \frac{\tau}{\Delta t}$. we will indicate the integral in (2.1.2) by

$$g_m = (-1)^m \int_0^1 e^{c\Delta t(1-\wedge)} \binom{-\wedge}{m} d\wedge, \qquad (2.1.3)$$

And then calculate the g_m by bringing in the generating function. For $z \epsilon R, |z| < 1$, we define the generating function

$$\Gamma(z) = \sum_{m=0}^{\infty} g_m z^m = \int_0^1 e^{c\Delta t(1-\wedge)} \sum_{m=o}^{\infty} \binom{-\wedge}{m} (-z)^m d\wedge = \int_0^1 e^{c\triangle t(1-\wedge)} (1-z)^{-\wedge}\, d\wedge \quad ,$$

$$= \frac{e^{c\Delta t}(1-z-e^{-c\Delta t})}{(1-z)(c\Delta t+\log(1-z))}$$
(2.1.4)

Rearranging (3.9) 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

$$\left(c\Delta t - z - \frac{z^2}{2} - \frac{z^2}{3} - \cdots\right)(g_o + g_1 z + g_2 z^2 \ldots) = e^{c\Delta t} - 1 - z - z^2 - z^3 - \cdots,$$

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

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

$$c\Delta t g_{m+1} + 1 = g_m + \frac{1}{2} g_{m-1} + \frac{1}{3} g_{m-2} + \cdots \frac{1}{m+1} g_0 = \sum_{k=0}^{m} \frac{1}{m+1-k} \qquad (2.1.5)$$

Having determined g_m, the ETD schemes (2.1.1) then can be given in explicit forms. Substituting (2.1.0) and (2.1.3) in (2.1.2), we deduce the general generating formula of ETD schemes or orders.

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

Where u_n and F_n denote the numerical approximation to $u(t_n)$ *and* $F(u(t_n), t_n)$ respectively, and the g_m are given by (2.1.5)

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.

ETD2RK1 Scheme

Putting $s = 1$ in equation (2.1.6) give

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

let $a_n \approx u_{n+1,}$ *then it implies that*

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

The term a_n approximate 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 (2.1.4a)

$$F = F_n + \frac{(t-t_n)}{\Delta t/j}\left(F\left(a_n, t_n + \frac{\Delta t}{j}\right) - F_n\right) + 0(\Delta t^2),$$

And substitute into (2.1.1) to give the ETD2RK1 scheme

$$u_{n+1} = a_n + (e^{c\Delta t} - c\Delta t - 1)(F(a_n, t_n + \Delta t) - F_n)/(c^2\Delta t) \qquad (2.1.9)$$

ETD2RK2 scheme

In a similar way, we can also form an ETD2RK2 scheme analogous to the "modified Euler" method. The first step (2.1.6)

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

Is formed by taking half a step of (2.1.8); then use the approximation

$$F = F_n + \frac{(t-t_n)}{\Delta t/j}\left(F\left(a_n, t_n + \frac{\Delta t}{j}\right) - F_n\right) + 0(\Delta t^2),$$

In the interval $[t_n, t_n + \Delta t]$ in (2.1.1) to deduce the general ETD2RK2 scheme as follows

$$u_{n+1} = u_n e^{c\Delta t} + \left\{\left((c\Delta t - 2)e^{c\Delta t} + c\Delta t + 2\right)F_n + 2(e^{c\Delta t} - c\Delta t - 1)F\left(a_n, t_n + \frac{\Delta t}{2}\right)/(c2\Delta t)\right\} \quad (2.2.0)$$

In fact, there is a one-parameter family of such $ETD2RK_J$ schemes. For $j \in R^+$, one can start with any fraction $1/j$ of Δt for the first step (2.1.8) which gives

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

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

$$F = F_n + \frac{(t - t_n)}{\Delta t/j}\left(F\left(a_n, t_n + \frac{\Delta t}{j}\right) - F_n\right) + 0(\Delta t^2),$$

In the interval $[t_n, t_n + \Delta t]$ in (2.1.1) to deduce the general $ETD2RK_J$ schemes as follows

$$u_{n+1} = u_n e^{c\Delta t} + \left\{\left((c\Delta t - j)e^{c\Delta t} + (j - 1)c\Delta t + j\right)F_n + j(e^{c\Delta t} - c\Delta t - 1)F\left(a_n, t_n + \frac{\Delta t}{j}\right)/(c2\Delta t)\right\}$$

Stability Analysis

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

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

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

Stability of ETD2RK1 Scheme

Equation (2.1.9) 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 $F_n = \lambda u_n$ into the above equation gives

$$\frac{u_{n+1}}{u_n} = e^{c\Delta t} + \frac{(e^{c\Delta t} - 1)\lambda u_n}{cu_n} + (e^{c\Delta t} - c\Delta t - 1)(F(a_n, t_n + \Delta t)/c^2\Delta t u_n \quad (2.2.1)$$

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

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

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

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

(2.2.1a) If

$$r = e^y + \left(\frac{e^y - 1}{y}\right) + \left(\frac{(e^y - y - 1)(e^y - 1)}{y^2}\right)x^2 < 1 \quad (2.2.1b)$$

Then ETD2RK1 is asymptotically stable.

Stability of ETD2RK2 Scheme

Equation (2.2.0) can be written as

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

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

$$r = e^y + \left(\frac{2(e^y-y-1)e^{\frac{y}{2}}+(y-2)e^y+y+2}{y^2}\right)x + \left(\frac{2(e^y-y-1)\left(e^{\frac{y}{2}}-1\right)}{y^3}\right)x^2 \qquad (2.2.2a)$$

if

$$r = e^y + \left(\frac{2(e^y-y-1)e^{y/2}+(y-2)e^y+y+2}{y^2}\right) + \left(\frac{2(e^y-y-1)\left(e^{y/2}-1\right)}{y^3}\right)x^2 < 1 \quad (2.2.2b)$$

Then ETD2RK2 is asymptotically stable.

ANALYSIS OF RESULTS

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 (2.0.8), where λ is real and c is fixed, 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 3.1: **x and y values given that c is fixed and negative and λ is Real 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 3.1 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.

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Table 3.2: x and y Values Given 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 λ is complex and both c and λ are real, both the values of $x \, and \, y$ decrease as Δt increases.

Computations Of The r Values Of ETD2RK1 and ETD2RK2 Schemes

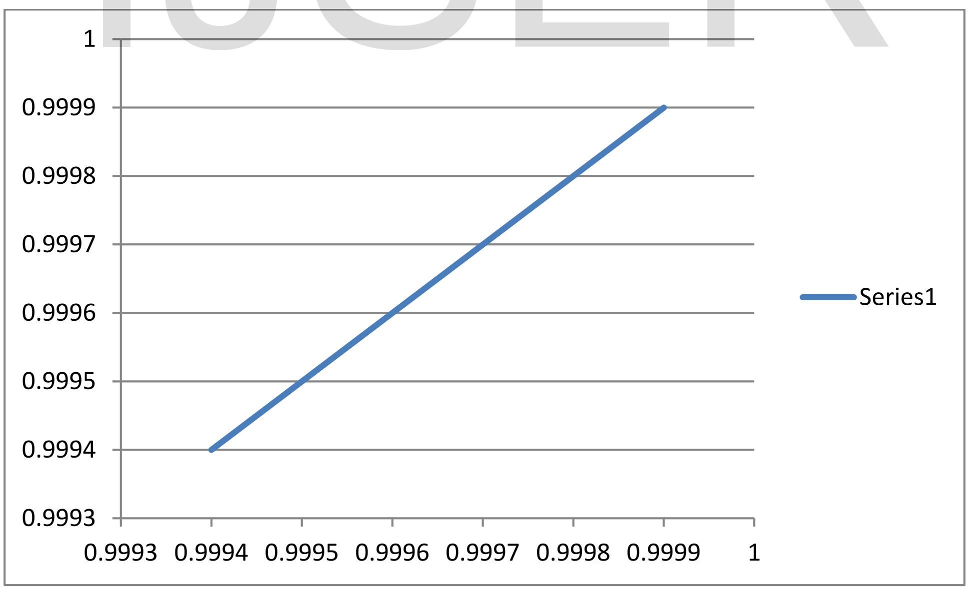
From tables (3.1), the computed values of $x \, and \, y$ were used to carry out the computations for the r values of ETD2RK1 and ETD2RK2.

Considering the condition that λ is complex and c is fixed and negative and both $\lambda$and c are purely real, equations (2.1.6), (2.2.1) and (2.2.1a) computes the r values for ETD2RK1 while, equations (2.1.6), (2.2.2) and (2.2.2a) computes the r values for ETD2RK2. Below is a summary of the computed values for r for the schemes.

Table 3.3: The r Values of the Schemes when Parameter c fixed and Negative and λ is complex

$|r|$ ***VALUES OF THE SCHEMES***

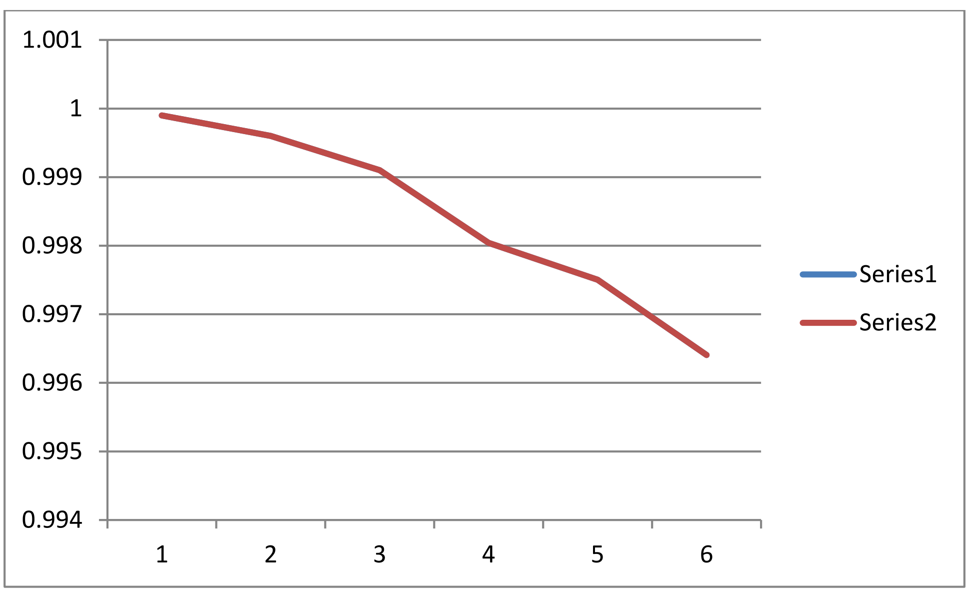
$ETD2RK1$	$ETD2RK2$
0.9999	0.9999
0.9998	0.9998
0.9997	0.9997
0.9996	0.9996
0.9995	0.9995
0.9994	0.9994



From Table 3.3, all values corresponding to the 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. Again descending down the table, the values of r corresponding to the schemes decreases, hence making the schemes more asymptotically stable.

Table 3.4: The r Values of the Schemes when Parameters c is changing and Negative and λ is Complex

$ETD2RK1$	$ETD2RK2$
0.9999	0.9999
0.9996	0.9996
0.9991	0.9991
0.9980401	0.9980401
0.997503	0.997503
0.996406	0.996406



Summary

From Table 3.1, 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

From Table 3.2, all values corresponding to ETD2RK1 and ETD2RK2 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 order. Again descending down the table, the values of r corresponding to the schemes decrease, hence making the schemes more stable.

CONCLUSION

This research suggests that the comparison of the asymptotic stability of ETD2RK1 and ETD2RK2 schemes in solving the stiff semi-linear differential equation (2.1.6) was properly executed. This was made possible when some parameter c, λ and Δt were adopted and used for computations.

To ensure that the first objective was met, ETD2RK1 and ETD2RK2 schemes were used to solve the stiff semi-linear differential equation (2.1.6) to obtain the asymptotic stability expressions (2.2.1b) and (2.2.2b).

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.
- At each Δt, the $|r|$ values of all the schemes are the same, that is; at Δt= 0.001, $|r|$ value of 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 ETD2RK1 and ETD2RK2 are efficient schemes for solving stiff semi-linear differential equations.

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