CONTINENTAL J. APPLIED SCIENCES
Mustafa and Hamza (2017) 12 (2): 33 – 46 DOI: 10.5281/zenodo.801635

Research Article

Convergence Analysis of A- Stable Implicit Runge- Kutta Methods of Reformulated Block Hybrid Multistep Methods

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Abstract

A number of techniques and solvers have been suggested, developed, and described, but a clear definition of stiffness has not been provided. In this paper, an analysis of the A-stable implicit Runge-Kutta methods is undertaken using stability function and the region of absolute stability, which shows region of each of the methods. Also to compare various stiff solvers based on their region of absolute stability. It helps a stiff ordinary differential equation solver, to identify appropriate numerical methods with unbounded region of absolute, appropriate for stiff problems solving.

Keywords: Block Method, Chebyshev Polynomials, Region of Absolute Stability

Received: 19 December 2016 Accepted: 28 May 2017

Introduction

Ordinary differential equations (ODEs) are widely used for modeling real processes. Practice shows that an initial value problem for ODEs can be attributing to the following types: soft, stiff, ill-conditioned and rapid oscillating. Each type is connected with specific demands to Numerical methods. Stiff problem can be exemplified by problems of chemical kinetics in complex electrical circuits, (Kahaner, 1989) non stationary processes in complex electric circuit (Hairer H. , 1980);(Kalitkin, 1993) system emerging while solving equations of heat conductions and diffusion (Butcher, 2003), movement of celestial bodies and satellites (Gear, 1993). The method of construction are A-stable numerical based on multistep continuous collocation method developed for purpose of obtaining numerical values at each mesh point or grid point (Babatola, 2011). In this paper we are interested in a special family of Runge-Kutta methods the so called Lobatto IIIA formulae, whose coefficient satisfy (Elakhe, 2011). Through the reformulation of block hybrid linear Multistep method, were the off grid points are obtained from zeros of second kind shifted Chebyshev polynomials. These methods are A-stable, but they are neither L-stable nor algebraically- stable. In view of this, one may wonder why to study these type of methods for numerical solution of stiff differential equations. As we will see, there are other theoretical and practical features that make it worthwhile to analyze its potential properties. Lobatto IIIA methods are stiffly accurate as state in (Semenov, 2011).

The paper is organized as follows: the review of definitions of stiff ordinary differential equations is presented in section 2. The approaches to finding a numerical solution of the stiff are discussed in section 3. In section 4, the stability function and region of absolute stability for the derived methods were drawn.

Stiff Differential Equations

Stiff differential equations are characterized as those whose exact solution has a term of the form e-ct where c is a large positive constant (Cohen, 1995). This is usually only a part of the solution called the transient solution. The more important portion of stiff equations will rapidly decay to zero as time (t) increases; therefore step size needed for accuracy must be quite small to resolve the initial rapid change in solution.

Definition: Initial Value Problems (Lambert, 1991)

$$y' = f(x, y) \quad y(t_o) = y0 \qquad (1)$$

is called an Initial Value Problem (IVP) of ordinary differential equation.

Definition: Stiffness ratio

$$y_{n+1} = y_n + h \textstyle\sum_{j=1}^{s} b_j k_j$$
$$k_j = f\left(x_n + c_j h, y_n + h \sum_{t=1}^{s} a_j k_i\right), \qquad j = 1,2 \ldots \ldots s \qquad (2)$$

$$\frac{\max_{i=1..m}|Re(\lambda_i)|}{\max_{i=1..m}|Re(\lambda_i)|} \gg 0 \qquad (3)$$

Definition: A-stable

A Numerical method applied to equation (1) as well as its stability function R (z) is called A-stable if the left half-plan i.e, $\{z: Re(z) \leq 0\}$ is contained in the region.

Definition: Chebyshev polynomials

The Chebyshev polynomial

$$x = \cos\theta \qquad (5)$$

of the second kind is a polynomial of degree n in x defined by

$$U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta} \qquad (6)$$

When then we have

$$U_0(x) = 1, U_1(x) = 2x, U_2(x) = 4x^2 - 1 \qquad (7)$$

then the recurrence relation is given as

$$U_n(x) = 2xU_{n-1}(x) - U_{n-2}(x), n = 2,3 \qquad (8)$$

Where $\epsilon[-1 \ \ 1]$ which together with the initial conditions

$$U_n(x) = 2xU_{n-1}(x) - U_{n-2}(x), n = 2,3 \qquad (9)$$

$$U_0(x) = 1, U_1(x), = 2x \qquad (10)$$

Definition: Shifted Chebyshev polynomials (Butcher, 2003)

The transformation of a Chebyshev polynomials appropriate to any given finite range [a,b] of x, by making this range correspond to the range [-1 , 1] of a new variable s under linear transformation provides an efficient procedure for generating the second kind polynomials,

$$\mu = \frac{2x-(a+b)}{b-a} \quad (10a)$$

Stiffness

Several attempts at a rigorous definition of stiffness have been made in the numerical analysis literature. In this paper, we follow the definition of Lambert (1991).

Definition: Stiffness

A linear constant coefficient system is stiff if all its eigenvalues have negate real part and the stiffness ratio is large.

Definition: Stiffness

Stiffness occurs when stability requirement rather than of accuracy, constrain the step length.

Definition: Stiffness

If a numerical method with a finite region of absolute stability, applied to a system with any initial conditions is forced to use in a certain interval of integration a step length which is excessively small in relation to the smoothness of the exact solution in that interval, then the system is said to be stiff in that interval.

Definition: Stiffness

Paper system is called stiff if real components of all the eigenvalues of Jacobian are negative, $Re(\lambda_i) < 0$, i **=…**N, the system is asymptotically stable and the ratio is

$$s = \frac{max\{|Re(\lambda_i)|, i = 1,2, \dots N\}}{max\{|Re(\lambda_i)|, i = 1,2, \dots N\}} \quad (11)$$

Large the parameter s is called the stiffness ratio. Since, in stiff system, some components of the solution decay much more rapidly than others, for a numerical method with a finite region of stability, we force to use excessively small step sizes in relation to the smoothness solution, which inevitably decreases computational efficiency and accumulators more machine round off error (Lambert, 1991). As a result, stiffness leads to some practical difficulties for explicit methods. There are number of interpretation of stiffness, each of which reflects certain aspects of the numerical solution (e.g.

impossibility of using explicit methods of integration, presence of rapidly damped disturbance.

Approaches to Finding a Numerical Solution of Stiff ODEs

Consider a stiff initial value problem of the form (1) ,since the discovery of stiffness in development of numerical methods for integrating stiff systems, the following trends have appeared: The most completed overview of the current numerical methods for solving stiff (ODEs) systems with as extensive bibliography is presented in the papers (Aiken, 1985),(Petzold, 1998).

Taylor Series

One of the ways to construct the solution to the system (1) at a point, is a method based on the expansion of solutions in a Taylor series in the neighbourhood of that point. Consider,

$$y(x_n+1) = y(x_n) + hf(x_n, y_n, h) \qquad (13)$$

where

$$f(x_n, y_{n,} h) = y'(x_n) + \frac{hy''(x_n)}{2!} + \frac{hy'''(x_n)}{3!} + \cdots \qquad (14)$$

If this series is truncated at q-th term and replace with the approximate value of (1), we obtain, the explicit Euler method obtained as,

$$y_{n+1} = y_n + hf(x_{n,} y_n) \qquad (16)$$

Linear Multistep Methods

Another important way to construct the solution to the system (1) is the use of linear multistep methods. In 1883, Bashforth and Adams proposed the idea of extending the Euler method using previous solution and derivative values in computing the solution. The general form of a linear k-step method for (1) is given as.

$$\sum_{J=0}^{k} \propto_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \qquad (17)$$

Where y_n is numerical approximation to the exact solution at the point x_n and $\propto_1, \propto_2, \ldots\ldots \propto_k, \beta_1, \beta_2 \ldots \beta_k$ are fixed numbers. The values of $\propto_1, \propto_2, \ldots\ldots \propto_k, \beta_1, \beta_2 \ldots \beta_k$ are chosen to obtain the highest possible order and characterize a method. If $\propto_1 = 1$ *and* $\propto_i = 0$ *and* $\beta_0 = 0$ the methods are known as Adams Bashforth methods. If $\beta_0 = 0$ *is not* 0, the methods are known as Adams Moulton methods.

Runge-Kutta Methods

Runga and Kutta proposed the idea of solving (1), which is characterized by allowing for a multiplicity of evaluations of function f within one step, then using the information obtained to match a Taylor-series expansion up to some higher order.

The general s- stage Runge-Kutta method for problem (1) is defined by Jesus *et al*. (2007) as,

$$y_{n+1} = y_n + h\sum_{j=1}^{s} b_j k_j$$

where

$$k_j = f\left(x_n + c_n h, y_n + h\sum_{j=1}^{s} b_j k_j\right), \qquad j = 1,2,\ldots\ldots\ldots.s \qquad (19)$$

The formula of this methods are ideally applicable for practical calculations, they allow changing the integration step h easily. Perhaps the most famous is the formula of the 4-th order Runge-Kutta method [21]. Where $k_1, k_{2\ldots}\ldots k_s$ are called the stage values, which are approximations to solution values, $y(x_{n-1} + c_i h)$ at point $x_{n-2} + c_i h$, The integer is the number of stages of the method. The c_i represents the position of the internal stages within one step. The Runge-kutta formula can be conveniently represented by Butcher tableau below.

$$\frac{c|A}{\;\;|b^T} \qquad (20)$$

Where A = $\{a_{ji}\}, b^T = \{b_j\}$ *and* $c = \{c_j\}$ .The set of numbers a_j are the coefficients used in finding the internal stages using linear combination of the stage derivatives. The component of the vector b is coefficient which represents how the numerical solution at this step depends on the derivative of internal stages. The vector $c = [c_1, c_2 \ldots . c_s]^{T}$ is called the abscissas. If the matrix A strictly lowered triangular, i.e., the internal stage can be calculated without depending on later stages, the method is explicit. An example of widely used ERK method was proposed by (Dorman, 1980), which is used as build in MATLAB solver for initial value problem as (ode45). One of the major problems with use of Runge-Kutta method, especially the explicit form of it, lies in choosing the size of the integration step, which provides extra computational expensive. And also stability restriction on the methods.

A-stability and Implicit methods

A well- known result in the numerical ODE literature, for example, (Butcher, 2008) is that an ERK method with order p has stability function given as

$$R(z) = 1 + z + \frac{z^2}{2!} \dots\dots\dots\dots\dots\dots \frac{z^p}{p!} + O(z^{p+1}) \qquad (21)$$

Which determine the stability region of the underlying method

$$S = \{z\epsilon\, C : |R(z) \leq 1|\} \qquad (22)$$

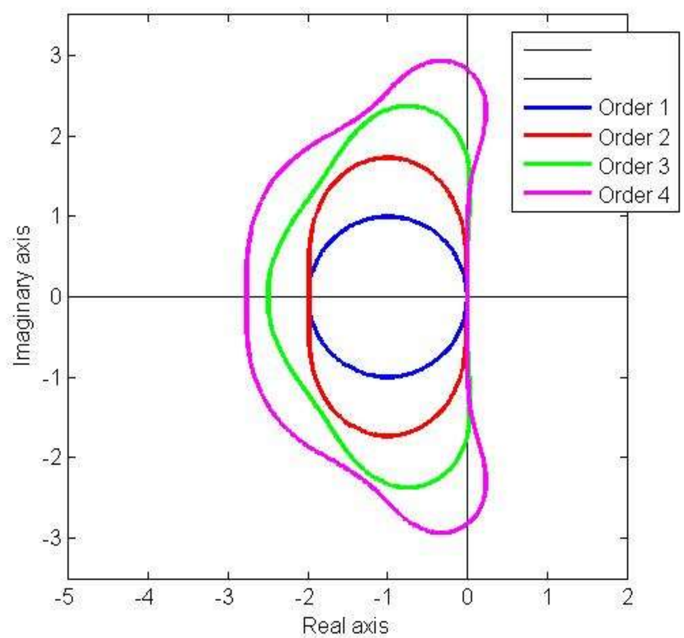

Fig.1 Region of absolute stability for Explicit RK-Methods

As result, all explicit Runge-Kutta methods have bounded stability regions. The stability region order one, two, three, and four, ERK methods with P=1, 2, 3, 4 and given in figure 3. It can be seen that although the stability region of a higher order ERK method is slightly wider than that of the explicit Euler method, it is still highly restrictive. This will create, as shown above, numerical inefficiency for stiff system. To deal with stiffness, a method with a much wider stability region is called for. A typical approach in the numerical ODE literature is to use a method with an unbounded stability region. This is the motivation behind the concept of A –stability (Dahlquist, 2003). Due to ineffectiveness of explicit method either from linear multistep method or Runge-Kutta to handle stiff problem, an explicit methods are no longer consider for solving stiff problem. One source of methods for stiff methods is implicit linear multistep methods. For example the so-called implicit Euler method (the first order) and the trapezoidal method (the second order) are special cases of linear-multistep (Butcher, 2003), given as

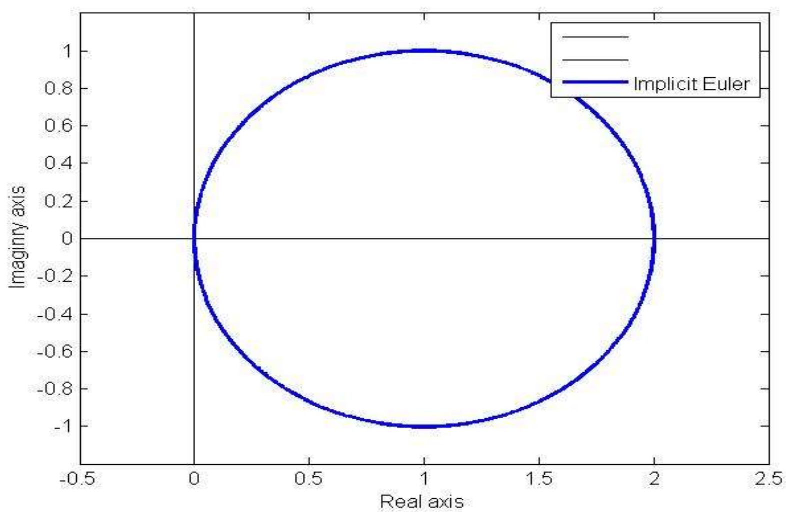

Fig.2 Region of absolute stability for Implicit Euler Method

$$y_{n+1} = y_n + hf_{n+1} \tag{23}$$

This has the desirable property of being A-stable. This means that, for all z in the left half complex plane, and then the stability function, using a test equation $y' = My(x)$ then we've

$$R(z) = \frac{1}{z-1} \tag{24}$$

Then the region of absolute stability is shown below unfortunately, it is not possible to find A-stable linear multistep methods with order higher than 2 due to Dahlquist barrier, which states that no linear multistep method for order greater than two will be A-stable (Hairer E. , 1987). Looking for better methods for solving stiff system (Dahlquist, 2003) discovered the Backward Differentiation Formulae (BDF). Still BDF has only A-stability properties with order less than or equal to six, which restricted the method from having a higher order A-stable BDF method. For example the regions from order 1, to order 2 are A-stable while as the order increase the region becomes unstable as shown below.

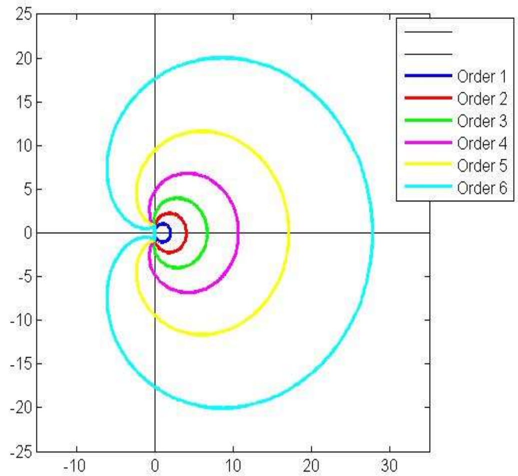

Fig.3 Region of absolute stability for Backward Differentiation Method

Therefore for BDF methods of the seventh order, will be worst in terms of region of absolute stability, it turns out that the BDF methods of order greater than sixth does not meet the requirements of stiff stability (Semenov, 2011).

The new family block linear multi-step methods

Another family of stiff ODE solvers is developed based on the implicit Runge-Kutta approach. Compared to a BDF algorithm, an implicit Runge-kutta (IRK) scheme is a single step method, which not only can have a high order of accuracy but also favorable numerical stability properties. Thus the coefficient of the family can be obtained through reformulation of the block hybrid linear-Multistep as Runge-Kutta method was established in (Jesus, 2007) where the Runge-Kutta coefficient was obtained by combing the Adams-Moulton formula and Adams-Bashforth formula. But in this paper we only employ block Adams-Moulton with off grid points from zeros of orthogonal polynomials to derive the Lobatto Runge-kutta Method, for derivation we adopt the method by (Onumanyi, 1994). After which it was reformulated as Runge-Kutta method. In this paper offgird point were obtained from the zeros of shifted second kind Chebyshev polynomials and inserted into 1-step Adams-Moulton method to derive Lobatto implicit Runge-Kutta method, since Lobatto method include the endpoints of the polynomials. When any of the method applied to the Dahl-Quists test $y' = \lambda y, Re(\lambda) < 0$ it results in an algebraic linear system in the unknown $y(x_n + \mu_j h) for\ j = 0,1,2,3, \dots \dots N$ then we obtain the difference equation.

$$y_{n+1} = R(\lambda h) y_n \qquad (25)$$

Where the stability function $R(z) = C \to C$ given by

$$R_s(z) = 1 + zb^T(1 - zA)^{-1}\mathrm{e} \qquad (26)$$

Where e is the (s+1)-vector e=(1,-1) T,I is the (s+1) –identity matrix, A is the matrix

$$A = (a_{ij})_{i,j=1}^{s+1} and\ b = (b1 .. bs + 1).$$

In this context, the method is called A-stable (Hairer *et al.*, 1996)) if the left-half complex plane is included in the stability domain, that is

$$C^- = \{z; Rez < 0\} \subset S = \{z; |R(z)|1\} \qquad (27)$$

The stability function of the derived methods are the rational function ,which is referred o to as transition function of a dynamical system, then its solution is A-stable if and only if the numerator P(z) is a *Hurwitz polynomial*

$$R(z) = \frac{N(z)}{D(z)} \qquad (28)$$

Definition: Let P(z) be a polynomial of real coefficients. If all zeros lie in the open left half plane Řz<0, then P (z) is called a Hurwitz polynomials.

Theorem:
Given polynomial

$P(z) = a_0 z^n + a_1 z^{n-1} + \ldots + a_n$, $a_0, a_1, \ldots a_n \in R$

of real coefficients. A necessary condition that $P(z)$ is a Hurwitz polynomial is that $a_0, a_1, \ldots a_n$ are all positive, or all are negative. Also if $a_0 < 0$, then

$$\frac{1}{a_0} P(z) = z^n + \frac{a_1}{a_0} z^{n-1} + \ldots + \frac{a_n}{a_0} \; ,$$

has an only positive coefficient, so $a_0, a_1, \ldots a_n$ have all the same sign either all positive or all negative.

Remark:
If n=1 or n=2, then necessary condition of the above theorem is also sufficient. For $n \geq 3$ this is no longer true

Then, for our derive methods, we subject it into the Dahlquist test equations to verify whether the methods are A-stable base on the stability function in 28. For N=1, the stability function is given as

$$R_1(z) = \frac{12+6z+z^2}{12-6z+z^2} \tag{29}$$

For N= 2, the stability function is given as

$$R_2(z) = \frac{384+192z+38z^2+z^3}{384-192z+38z^2+z^3} \tag{30}$$

For N =3, the stability function is given as

$$R_3(z) = \frac{1920 + 960z + 204z^2 + 22z^3 + z^4}{1920 - 960z + 204z^2 - 22z^3 + z^4} \tag{31}$$

For N =4, the stability is given as

$$R_4(z) = \frac{184320+92160z+20352z^2+2496 \quad ^3 +170z^4 +5z^5}{184320-92160z \qquad\qquad ^2-2496z^3 +170z^4 -5z^5} \tag{33}$$

For N = 5, the stability is given as

$$R_5(z) = \frac{2580480+1290240z+291840z^2+38400z^3+3108\ {}^{4}+146z^5+3z^6}{2580480-1290240z+291840z^2-38400z^3+3108\ {}^{4}-146z^5+3z^6} \qquad (34)$$

Region of Absolute Stability of the Methods

To determine a geographical locus of points described in equation (30) to (34) a computer algebra system Mathematica and Maple were used. As result, a geometrical locus of derive methods as shown in Figures 4 - 7.

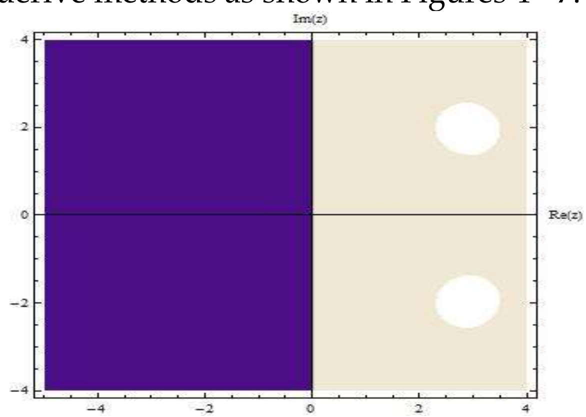

Fig.4: Stability Region for N=2

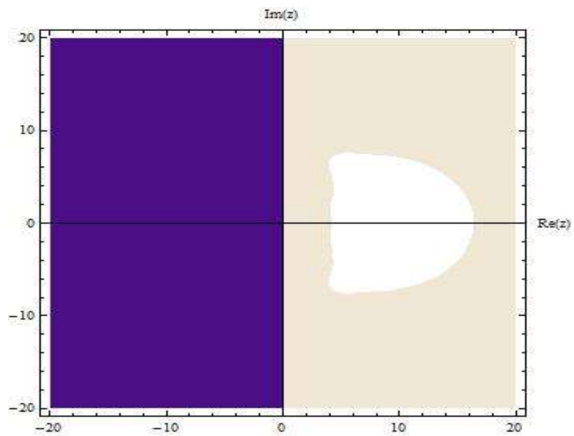

Fig.5: Stability Region for N=3

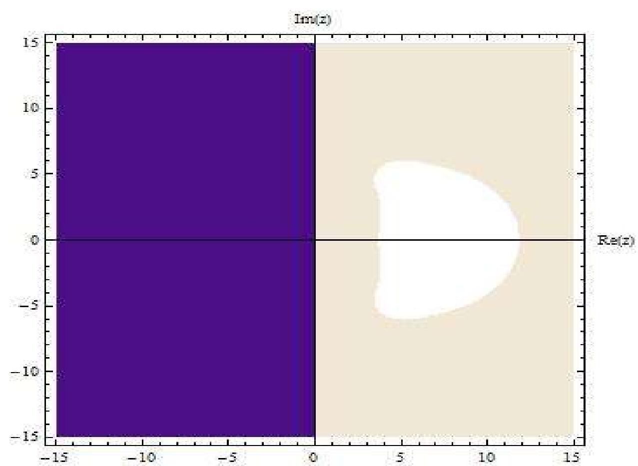

Fig.6: Stability Region for N=4

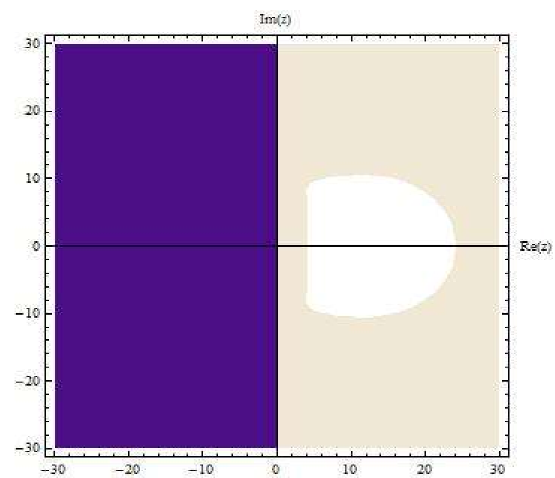

Fig.7: Stability Region for N=5

The study of region of absolute stability of the derive method (simple closed curved) show that the methods from order 4 to 10 inclusive are all A-stable, they also are stiffly accurate. Implicit methods such as our derived methods can be applied for the calculation of a big category of the stiff ordinary differentials equations. In this case, decrease of step size to minimum possible will not alter the convergence to exact solution, compare to other implicit methods as can be seen in figures 4 to 7, as order of the method increases also the stability region of the method increases.

Conclusion

The area of the numerical methods for solving ODEs is one of the well investigated topics in the mathematical literature. A number of techniques and solvers have been suggested, developed, and described, but a clear definition of stiffness has been provided. As a rule in most solvers for ordinary differential equations the explicit first order in most solvers for ordinary differential equations (Euler method) or a second order method (trapezoidal method) is applied. Implicit Gear methods (backward differentiation formula) are stiff by considering the region of absolute stability in fig.3, but as the order of the method increases, the Gears method turns out not to be A-stable rather it become A (alpha)-stable, but orders from 1 to 6 inclusive are all A-stable from the definition of A-stable, so for accurate solution of stiff differential equations an order of method has to be considered.

Now for our derived methods it can be seen from Figs 4 to 7, all the methods are A-stable and as the order of the method increases the stability region of the method increases and becomes more suitable for stiff solution, this shows that, the reformulated Runge-Kutta methods are favourable for solving stiff differential equations compared to some Implicit Method.

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