

On the reliability and stability of direct explicit Runge-Kutta integrators

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Abstract

Recently, efficient direct numerical integrators of Runge-Kutta type (called RKD and RKT methods) for solving third-order ordinary differential equations (ODEs) of the form $y''' = f(x, y)$ have been proposed. In this paper, we investigate the reliability of these RKD and RKT approaches, with focus on their stability and accuracy. We compare the stability regions of RKD and RKT methods. It is found that RKD stability region is adaptable, in the sense that its area can be controlled using a free parameter to get a more stable solution. To test the accuracy of RKD, we present some examples of this approach towards solving third-order ordinary differential equations. Simulation results show that the RKD approach, in addition to outperforming the existing RKT methods in terms of accuracy and time consumption, gives better control over stability region.

AMS subject classification:

Keywords: Reliability, stability, RKD method, ordinary differential equation (ODE), third-order.

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1. Introduction

Stability of numerical methods for solving ordinary differential equations (ODEs) means that the solution keeps bounded while moving further away from a starting point. An important characterization of a numerical method for solving ODEs is the region of absolute stability [4, 1]. For example, if we consider first-order ODE $y' = f(x, y)$, a numerical method is called stable if the eigenvalues of the test equation, taken as the first-order ODE $y' = f(x, y)$, are all inside the unit circle of the complex plane. If the second-order ODE $y'' = f(x, y, y')$ is solved by reducing it to a system of first-order ODEs, the same condition above applies to the resulting eigenvalues of the generalized eigenvalue problem. No such stability regions could be found for general numerical methods of solving first and second-order ODEs, but for some methods a region of absolute stability can be defined for single first or second-order ODEs. The absence of a region of absolute stability may be due to solving different members of a system of first-order ODEs using different methods. In the theory of differential equations and dynamical systems, a particular stationary or quasistationary solution to a nonlinear system is called linearly unstable if the linearization spectrum contains eigenvalues with positive real part. If there are no such eigenvalues, the solution is called linearly stable. Other names for linear stability include spectral, or exponential, stability. This paper is concerned with the study of the behavior of the solution obtained when integrating by using a Runge-Kutta-Type RKD method of solving third-order ODEs. A general approach for studying the linear stability of Runge-Kutta-Type (RKD & RKT) methods is presented. In the case that different orders for RKD methods are integrated, we present a condition that RKD methods must satisfy so that a uniform bound for stability can be achieved. To the best of our knowledge, this condition has not been studied in the literature. Numerical examples are presented in Section 4.

2. Overview of numerical methods

2.1. The third-order ODE problems

Special third-order ODEs, especially those which do not include any explicit dependence on the first-order derivative $y'(x)$ and the second-order derivative $y''(x)$, are found in many problems of physics and engineering, such as thin film flow, electromagnetics, and gravity [2, 8]. These equations can be written as per the following form

$$y'''(x) = f(x, y(x)); \quad x \geq x_0, \quad (1)$$

having the initial conditions,

$$y(x_0) = \alpha^0, \quad y'(x_0) = \alpha^1$$

and

$$y''(x_0) = \alpha^2.$$

where,

$$f : \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}^N,$$

and

$$\begin{aligned} y(x) &= [y_1(x), y_2(x), \dots, y_N(x)], \\ f(x, y) &= [f_1(x, y), f_2(x, y), \dots, f_N(x, y)], \\ \alpha^0 &= [\alpha_1^0, \alpha_2^0, \dots, \alpha_N^0], \\ \alpha^1 &= [\alpha_1^1, \alpha_2^1, \dots, \alpha_N^1], \\ \alpha^2 &= [\alpha_1^2, \alpha_2^2, \dots, \alpha_N^2]. \end{aligned}$$

If the ODE (1) is in an N - dimensional space, it could be simplified as follows

$$z'''(x) = g(z(x)), \quad (2)$$

with the assumptions,

$$z(x) = \begin{pmatrix} y_1(x) \\ y_2(x) \\ y_3(x) \\ \vdots \\ y_N(x) \\ x \end{pmatrix}, \quad g(z) = \begin{pmatrix} f_1(z_1, z_2, \dots, z_N, z_{N+1}) \\ f_2(z_1, z_2, \dots, z_N, z_{N+1}) \\ f_3(z_1, z_2, \dots, z_N, z_{N+1}) \\ \vdots \\ f_N(z_1, z_2, \dots, z_N, z_{N+1}) \\ 0 \end{pmatrix}.$$

with the initial conditions

$$z(x_0) = \bar{\alpha}^0, \quad z'(x_0) = \bar{\alpha}^1, \quad z''(x_0) = \bar{\alpha}^2$$

where

$$\begin{aligned} \bar{\alpha}^0 &= [\alpha_1^0, \alpha_2^0, \dots, \alpha_N^0, x_0], \\ \bar{\alpha}^1 &= [\alpha_1^1, \alpha_2^1, \dots, \alpha_N^1, 1], \\ \bar{\alpha}^2 &= [\alpha_1^2, \alpha_2^2, \dots, \alpha_N^2, 0]. \end{aligned}$$

Many scientists and engineers solve equations (1) or (2) by first converting the third-order ODE above to a system of first-order ODEs [3]. Also, many researchers handled these equations using multi-step methods. However, the approach based on using direct numerical methods with constant step-size could be shown as more efficient. Recently, two efficient direct numerical methods (called RKD and RKT) for solving third-order ODEs with the form $y''' = f(x, y)$ have been proposed [7, 6, 10], while an RKD numerical method with variable step-size has been proposed in [9]. In [5], direct numerical RKD methods have been used for solving class III of PDEs.

In this paper, we investigate stability conditions and properties for the constant step - size RKD methods.

The following sub-section presents an overview of direct RKD methods.

2.2. Direct RKD numerical methods: simplified order conditions and free parameters

It is possible to write a generalized form for RKD methods with s -stage to solve the equations (1) or (2) as per the following equations

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{2}y''_n + h^3 \sum_{i=1}^s b_i k_i, \quad (3)$$

$$y'_{n+1} = y'_n + hy''_n + h^2 \sum_{i=1}^s b'_i k_i, \quad (4)$$

$$y''_{n+1} = y''_n + h \sum_{i=1}^s b''_i k_i, \quad (5)$$

where,

$$k_1 = f(x_n, y_n), \quad (6)$$

$$k_i = f\left(x_n + c_i h, y_n + hc_i y'_n + \frac{h^2}{2}c_i^2 y''_n + h^3 \sum_{j=1}^{i-1} a_{ij} k_j\right), \quad (7)$$

for $i = 2, 3, \dots, s$.

Please note that it is assumed that the parameters of RKD methods, $c_i, a_{ij}, b_i, b'_i, b''_i$ (for $i = 1, 2, \dots, s$ and $j = 1, 2, \dots, s$), are all real.

The RKD methods can be expressed compactly using Butcher notation as a table of coefficients.

Note that [7] and [10] have derived direct integrators of RK type to solve special ODEs of different orders: three, four, five and six. This paper, the RKD Methods derived in [7] and [10] are applied to solve equations (1) or (2).

To obtain the order conditions or the error equations of direct RK type for special third-order ODEs for y, y' and y'' , there are two approaches. [7] has derived the order conditions using Taylor series expansion up to order seven, while [10] derived it using the approach of rooted trees. Here, we will study the order conditions of RKD method of order four (RKD4). A similar approach can be utilized to find the order conditions of other RKD methods like RKD3, RKD5 and RKD6.

The order conditions of RKD4 method have been presented in [7]. Here, these conditions would be reduced as follows:

$$\begin{aligned} b''_1 + b''_2 + b''_3 &= 1; \quad b''_2 c_2 + b''_3 c_3 = \frac{1}{2}; \\ b''_2 c_2^2 + b''_3 c_3^2 &= \frac{1}{3}; \quad b''_2 c_2^3 + b''_3 c_3^3 = \frac{1}{4}; \\ b''_2 a_{21} + b''_3 (a_{31} + a_{32}) &= \frac{1}{24}. \end{aligned}$$

using the following relations

$$b_i' = b_i''(1 - c_i), \quad b_i = b_i'' \frac{(1 - c_i)^2}{2}, \quad (8)$$

for $i = 1, \dots, s$. These simplifying assumptions can be reached using simple manipulations with the order conditions.

The free parameters (arbitrary parameters) of the RKD4 method can be chosen to control the regions of stability. The above conditions would result in a system of five non-linear equations with eight unknowns. The system is under-determined, and a solution exists for the system as follows with three free parameters

$$a_{32} = \frac{12a_{21} - c_2(16a_{21} + a_{31}(432c_2^3 - 864c_2^2 + 576c_2 - 128) - 24c_2^3 + 50c_2^2 - 36c_2 + 9)}{16c_2(27c_2^3 - 54c_2^2 + 36c_2 - 8)};$$

$$b_1'' = \frac{6c_2^2 - 6c_2 + 1}{6c_2(4c_2 - 3)};$$

$$b_2'' = \frac{1}{6c_2(6c_2^2 - 8c_2 + 3)};$$

$$b_3'' = \frac{2(27c_2^3 - 54c_2^2 + 36c_2 - 8)}{3(4c_2 - 3)(6c_2^2 - 8c_2 + 3)};$$

$$c_3 = \frac{4c_2 - 3}{2(3c_2 - 2)}$$

Obviously three parameters c_2 , a_{21} and a_{31} can be freely chosen. If we define two of them as follows

$$a_{21} = \frac{1}{48}, \quad \text{and} \quad a_{31} = \frac{1}{12}.$$

then we end up with one free parameter which can control the stability region of the RKD method. The Butcher tableaux representing the RKD methods with different orders are shown in Tables 1, 2, 3 and 4, respectively, while the Butcher tableau representing the RKT method with order four is shown in Table 5.

3. Absolute stability of RKD methods

Stability plays a significant role in evaluating numerical approaches. Here, we study the stability of the proposed RKD, and will show that it has sufficiently-wide stability region. An additional asset is that the stability of Runge-Kutta type (RKD) methods can be controlled by free parameters. The main interest is the stability of initial-value problems with third-order ODEs as per (1). Following an approach similar to that of [4], the analysis presented below is based on examining what happens when a method is applied to a simple scalar linear third-order ODE of the form

$$y''' = -\lambda^3 y.$$

The reason for choosing a third-order test equation as above should be evident, as the paper is dealing with third-order differential equations. The RKD method yields the following equations

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{2}y''_n + h^3 \sum_{i=1}^s b_i(-\lambda^3 Y_i), \quad (9)$$

$$y'_{n+1} = y'_n + hy''_n + h^2 \sum_{i=1}^s b'_i(-\lambda^3 Y_i), \quad (10)$$

$$y''_{n+1} = y''_n + h \sum_{i=1}^s b''_i(-\lambda^3 Y_i), \quad (11)$$

where,

$$Y_i = y_n + c_i hy'_n + \frac{c_i^2}{2} h^2 y''_n + h^3 \sum_{j=1}^{i-1} a_{ij}(-\lambda^3 Y_j), \quad (12)$$

for $i = 1, 2, 3, \dots, s$. Now re-arranging terms will give

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{2}y''_n + h^3 \sum_{i=1}^s (-\lambda^3 b_i Y_i), \quad (13)$$

$$hy'_{n+1} = hy'_n + h^2 y''_n + h^3 \sum_{i=1}^s (-\lambda^3 b'_i Y_i), \quad (14)$$

$$h^2 y''_{n+1} = h^2 y''_n + h^3 \sum_{i=1}^s (-\lambda^3 b''_i Y_i), \quad (15)$$

If z_n is defined as follows

$$z_n = \begin{pmatrix} y_n \\ hy'_n \\ h^2 y''_n \end{pmatrix},$$

then the above equations give

$$z_{n+1} = \begin{pmatrix} 1 & 1 & \frac{1}{2} \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix} z_n + (\lambda h)^3 \begin{pmatrix} b_1 & b_2 & \dots & b_s \\ b'_1 & b'_2 & \dots & b'_s \\ b''_1 & b''_2 & \dots & b''_s \end{pmatrix} \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{pmatrix},$$

and equation (12) gives

$$\begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ \vdots \\ Y_s \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & c_2 & \frac{c_2^2}{2} \\ 1 & c_3 & \frac{c_3^2}{2} \\ \ddots & & \\ 1 & c_s & \frac{c_s^2}{2} \end{pmatrix} z_n + H \begin{pmatrix} 0 & 0 & 0 & \dots & 0 \\ a_{21} & 0 & 0 & \dots & 0 \\ & & \ddots & & \\ a_{s1} & a_{s2} & a_{s3} & \dots & a_{ss} \end{pmatrix} \begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ \vdots \\ Y_s \end{pmatrix},$$

or, in compact form

$$\Gamma_n = (I - HA)^{-1} C z_n,$$

where

$$\Gamma_n = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{pmatrix},$$

$$H = \lambda^3 h^3 = (\lambda h)^3,$$

$$A = \begin{pmatrix} 0 & 0 & & \dots & 0 \\ a_{21} & 0 & & \dots & 0 \\ a_{31} & a_{32} & 0 & \dots & 0 \\ & & & \ddots & \\ a_{s1} & a_{s2} & a_{s3} & \dots & a_{ss} \end{pmatrix},$$

$$C = \begin{pmatrix} 1 & 0 & 0 \\ 1 & c_2 & \frac{c_2^2}{2} \\ & \ddots & \\ 1 & c_s & \frac{c_s^2}{2} \end{pmatrix}.$$

Now a recursive relation on z_n can be written as follows

$$z_{n+1} = D_H z_n,$$

where,

$$D_H = \begin{pmatrix} 1 + Hb^T N^{-1}e & 1 + Hb^T N^{-1}c & \frac{1}{2} + Hb^T N^{-1}d \\ Hb'^T N^{-1}e & 1 + Hb'^T N^{-1}c & 1 + Hb'^T N^{-1}d \\ Hb''^T N^{-1}e & Hb''^T N^{-1}c & 1 + Hb''^T N^{-1}d \end{pmatrix}, \quad (16)$$

$$\begin{pmatrix} b \\ b' \\ b'' \end{pmatrix} = \begin{pmatrix} b_1 & b_2 & \dots & b_s \\ b'_1 & b'_2 & \dots & b'_s \\ b''_1 & b''_2 & \dots & b''_s \end{pmatrix},$$

$$e = (1, 1, \dots, 1)^T, \quad c = (0, c_2, c_3, \dots, c_s)^T,$$

and

$$d = \left(0, \frac{c_2^2}{2}, \frac{c_3^2}{2}, \dots, \frac{c_s^2}{2}\right)^T, \quad N^{-1} = I - HA,$$

The stability function for the s -stage formula associated with this method is an eigenvalue problem given by

$$\varphi(\xi, H) = |\xi I - D_H|,$$

where D_H , as defined by (16), represents the stability matrix whose characteristic equation is given as follows

$$\phi(\xi, H) = P_0(H)\xi^3 + P_1(H)\xi^2 + P_2(H)\xi + P_3(H). \quad (17)$$

The complex roots of (17) with $|\xi| = 1$ define the border of the stability region, in which the magnitude of the eigenvalues should be less than one. Running for all possible values of complex $|\xi|$ such that $|\xi| = 1$, we can find the border \mathcal{B}_S of stability region \mathcal{S} by finding the corresponding roots of reduced (17) as follows

$$\mathcal{B}_S = \{H \mid \phi(\gamma, H) = 0 \ \& \ |\gamma| = 1.\} \quad (18)$$

Since the values of H defines the accuracy step h of the method, then a wider stability region gives more flexibility for the corresponding method; also makes it more time efficient as it can reach stable solution with bigger step-size. Observe that the stability function for the s -stage formula associated with RKD method depends on the number of stages, s . Taking RKD4 as an example and looking at its Butcher's Table (Appendix A), we see that the order conditions for this approach leaves c_2 as a free parameter, giving more flexibility for the stability region as compared to RKT4 proposed by [10] (Appendix B). Figure (1) shows a comparison using a few values of the free parameter.

4. Implementation

The purpose of this section is to apply the recently proposed theory of the direct methods to solve ordinary differential equations (ODEs) of third-order, using the RKD and RKT methods, which have been proposed to solve special ODEs of the form $y''' = f(x, y)$ [7, 10].

Numerical implementation and testing are based on selected examples as shown in Problems 1-6 below. Note that these problems are carefully chosen as they have exact solutions, making it possible to examine the accuracy of the methods under test. In these examples, the RKD methods are implemented and compared with the existing RK methods; where the results show that the RKD methods are more reliable as they present more accurate solutions.

Results for implementing Problems 1-3 below using various RKD methods are shown in Figure (2), while results of implementing Problems 4-6 are shown in Figure (3).

4.1. Test problems and numerical results

Problem 4.1. (Non-linear ODE)

$$y'''(x) = \frac{3}{8}y^5(x), \quad 0 < t \leq b.$$

Initial conditions,

$$y(0) = 1, y'(0) = \frac{1}{2}, y''(0) = -\frac{1}{4}.$$

Exact solution: $y(x) = \sqrt{1+x}$, $b = 1$.

Problem 4.2. (ODE with non-constant coefficients)

$$y'''(x) = 4(3 - 2t^2)y(x), \quad 0 < t \leq b.$$

Initial conditions,

$$y(0) = 1, y'(0) = 0, y''(0) = -2.$$

Exact solution: $y(x) = e^{-x^2}$, $b = 1$.

Problem 4.3. (Non-homogenous, nonlinear ODE)

$$y'''(x) = y^2(x) + \cos(x)(\cos(x) - 1) - 1, \quad 0 < t \leq b.$$

Initial conditions,

$$y(0) = 0, y'(0) = 1, y''(0) = -1.$$

Exact solution: $y(x) = \sin(x)$, $b = \pi$.

Problem 4.4. (Non-homogeneous ODE)

$$y'''(x) = 2(e^x \cos(x) - y(x)), \quad 0 < t \leq b.$$

Initial conditions,

$$y(0) = 0, y'(0) = 1, y''(0) = 2.$$

Exact solution: $y(x) = e^x \sin(x)$, $b = 1$.

Problem 4.5. (Non-homogeneous ODE)

$$y'''(x) = y(x) + \cos(x), \quad 0 < t \leq b.$$

Initial conditions,

$$y(0) = 0, y'(0) = 1, y''(0) = 2.$$

Exact solution: $y(x) = \cos(x) - \sin(x)$, $b = 1$.

Problem 4.6. (Linear System of ODEs)

$$\begin{aligned} y_1'''(x) &= -20y_1(x) - 12y_2(x) - 19y_3(x), \\ y_2'''(x) &= 19y_1(x) + 11y_2(x) + 19y_3(x), \\ y_3'''(x) &= -26y_1(x) - 26y_2(x) - 27y_3(x). \end{aligned}$$

Initial conditions:

$$\begin{aligned} y_1(0) &= 1, & y_1'(0) &= -2, & y_1''(0) &= 6; \\ y_2(0) &= 0, & y_2'(0) &= 1, & y_2''(0) &= -5; \\ y_3(0) &= 0, & y_3'(0) &= -2, & y_3''(0) &= 8. \end{aligned}$$

The system is integrated over the interval $[0, 2]$.

The exact solution is given by:

$$\begin{aligned} y_1(x) &= e^{-x} - e^{-2x} + e^{-3x}; \\ y_2(x) &= e^{-2x} - e^{-3x}; \\ y_3(x) &= e^{-3x} - e^{-x} \end{aligned}$$

5. Conclusion

This paper presents a study on the reliability of a recently proposed direct numerical approach (called RKD and RKT methods) to solve ordinary differential equations. The study is focused on stability analysis and accuracy of the above approach. It has been shown that the stability region of RKD can be controlled using free parameters, giving more reliability (through wider stability region) than existing methods (including direct methods). Regarding accuracy, numerical results based on RKD3, RKD4, RKD5 and RKD6 methods are compared with those obtained from the existing methods RK3, RK4, RK5 and RK6. Comparisons show that RKD methods outperform the existing RK methods in terms of accuracy and time consumption.

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A.

Table 1: Butcher tableau representing RKD3 method of third-order.

0		
$\frac{2}{3}$	$\frac{11}{200}$	
$\frac{3}{3}$		
	$\frac{1}{8}$	$\frac{1}{24}$
	$\frac{1}{4}$	$\frac{1}{4}$
	$\frac{1}{4}$	$\frac{3}{4}$

Table 2: Butcher tableau representing RKD4 method of fourth-order.

0			
$\frac{1}{2}$	$\frac{1}{48}$		
1	$\frac{1}{12}$	$\frac{1}{12}$	
	$\frac{1}{12}$	$\frac{1}{12}$	0
	$\frac{1}{6}$	$\frac{1}{3}$	0
	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$

Table 3: Butcher tableau representing RKD5 method of fifth-order.

0	0		
$\frac{3}{5} - \frac{\sqrt{6}}{10}$	$\frac{27}{500} - \frac{19\sqrt{6}}{1000}$	0	
$\frac{3}{5} + \frac{\sqrt{6}}{10}$	$\frac{33}{2500} + \frac{51\sqrt{6}}{5000}$	$\frac{51}{1250} + \frac{11\sqrt{6}}{1250}$	0
	$\frac{1}{18}$	$\frac{1}{18} + \frac{\sqrt{6}}{48}$	$\frac{1}{18} - \frac{\sqrt{6}}{48}$
	$\frac{1}{9}$	$\frac{7}{36} + \frac{\sqrt{6}}{18}$	$\frac{7}{36} - \frac{\sqrt{6}}{18}$
	$\frac{1}{9}$	$\frac{4}{9} + \frac{\sqrt{6}}{36}$	$\frac{4}{9} - \frac{\sqrt{6}}{36}$

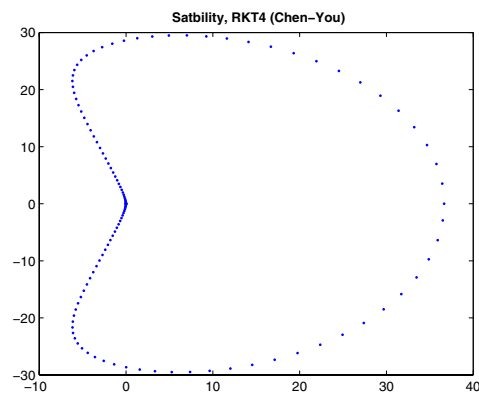
Table 4: Butcher tableau representing RKD6 method of sixth-order.

0	0			
$\frac{1}{2} - \frac{\sqrt{15}}{10}$	$\frac{7}{120} - 3\frac{\sqrt{15}}{200}$			
$\frac{1}{2}$	$\frac{-1}{96} + \frac{\sqrt{15}}{480}$	$\frac{1}{32} - \frac{\sqrt{15}}{480}$		
$\frac{1}{2} + \frac{\sqrt{15}}{10}$	$-\frac{1}{600} + \frac{\sqrt{15}}{600}$	$\frac{\sqrt{15}}{50}$	$\frac{3}{50} - \frac{\sqrt{15}}{150}$	0
	0	$\frac{1}{18} + \frac{\sqrt{15}}{72}$	$\frac{1}{18}$	$\frac{1}{18} - \frac{\sqrt{15}}{72}$
	0	$\frac{5}{36} + \frac{\sqrt{15}}{36}$	$\frac{2}{9}$	$\frac{5}{36} - \frac{\sqrt{15}}{36}$
	0	$\frac{5}{18}$	$\frac{4}{9}$	$\frac{5}{18}$

B.

Table 5: Butcher tableau representing RKT4 method of fourth-order.

$\frac{3 - \sqrt{3}}{6}$	0	0
$\frac{3 + \sqrt{3}}{6}$	$\frac{1}{12}$	0
	$\frac{2 + \sqrt{3}}{24}$	$\frac{2 - \sqrt{3}}{24}$
	$\frac{3 + \sqrt{3}}{12}$	$\frac{3 - \sqrt{3}}{12}$
	$\frac{1}{2}$	$\frac{1}{2}$



(a) Stability Region, RKT

Figure 1: Stability regions for RKD4 and existing methods. The RKD4 approach offers a free parameter to control the stability region.

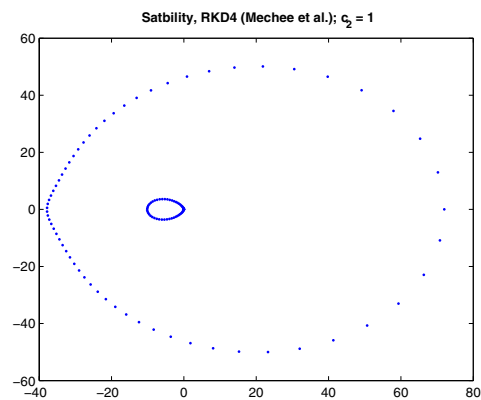
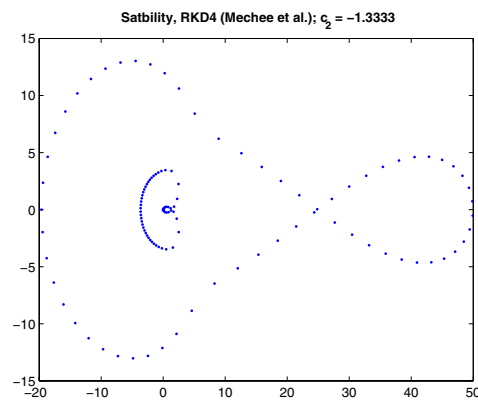
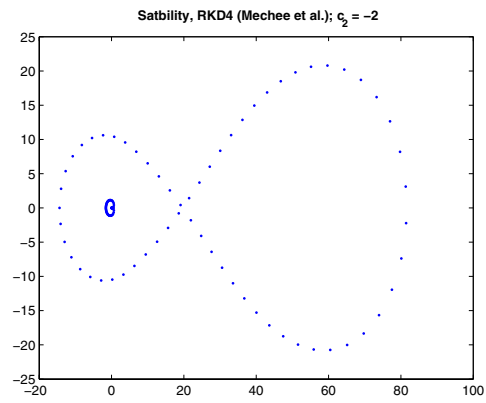


Figure 1: Continued.

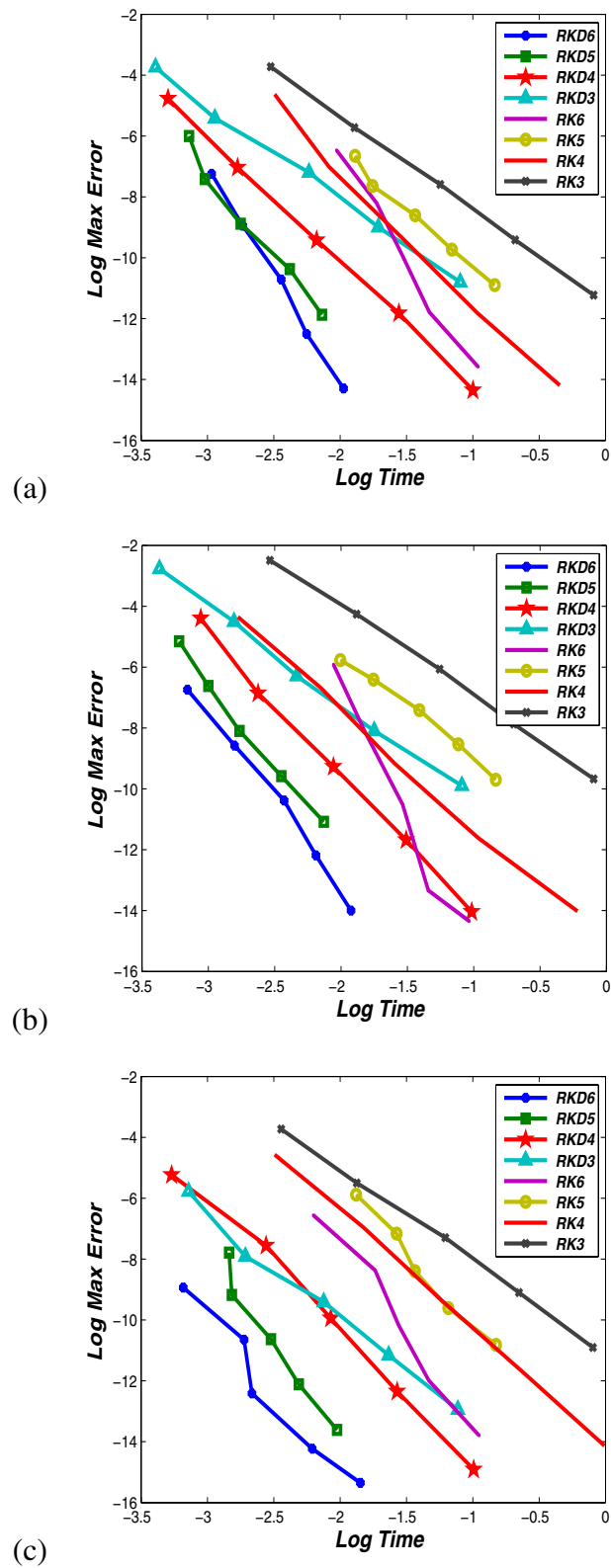


Figure 2: Error versus Computational Time for RKD6, RKD5, RKD4 and RKD3 Methods for Problems (a) 1 (b) 2 and (c) 3.

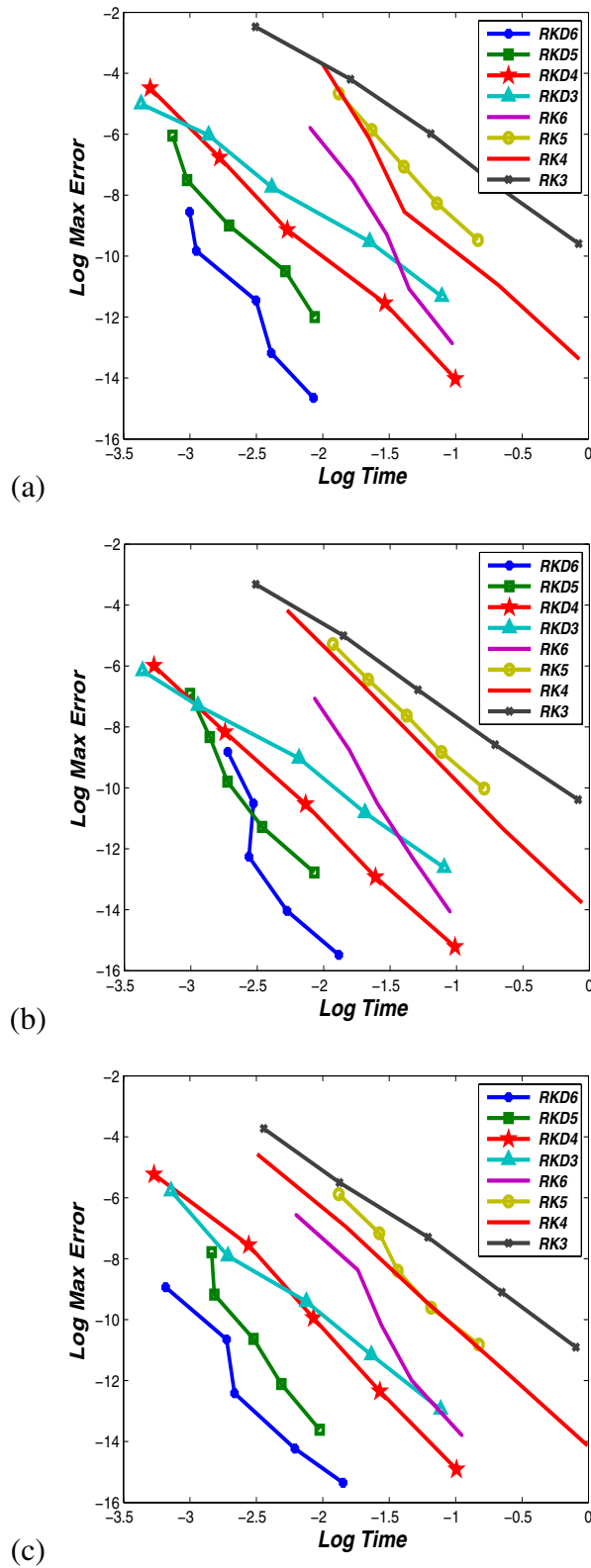


Figure 3: Error versus Computational Time for RKD6, RKD5, RKD4 and RKD3 Methods for Problems (a) 4 (b) 5 and (c) 6.

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