UNIVERSITI PUTRA MALAYSIA

TWO STEP RUNGE-KUTTA-NYSTRÖM METHOD FOR SOLVING SECOND ORDER ORDINARY DIFFERENTIAL EQUATIONS

LATIFAH BINTI MD ARIFFIN

FS 2016 81

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By

LATIFAH BINTI MD ARIFFIN

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfillment of the Requirement for the Degree of Doctor of Philosophy

December 2016

DEDICATIONS

To

My beloved parents, Mr. Md Ariffin Md Nor and Madam Mahfuzah Abd Ghaffar,

my faithful husband, Major Mohd Safiee Idris Mat Ali (Amdias),

my loyal and beautiful princesses,

Ms. Syasya Syahmina Amdias,

Ms. 'Adlina Safiyy Amdias,

Ms. 'Aaliah Syakirah Amdias and

future Amdias's clan.

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfillment of the requirement for the Degree of Doctor of Philosophy

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Chairman: Professor Dato' Mohamed Bin Suleiman, PhD
Faculty: Science

In this research, methods that will be able to solve the second order initial value problem (IVP) directly are developed. These methods are in the scheme of a multi-step method which is known as the two-step method. The two-step method has an advantage as it can estimate the solution with less function evaluations compared to the one-step method. The selection of step size is also important in obtaining more accurate and efficient results. Smaller step sizes will produce a more accurate result, but it lengthens the execution time.

Two-Step Runge-Kutta (TSRK) method were derived to solve first-order Ordinary Differential Equations (ODE). The order conditions of TSRK method were obtained by using Taylor series expansion. The explicit TSRK method was derived and its stability were investigated. It was then analyzed experimentally. The numerical results obtained were analyzed by making comparisons with the existing methods in terms of maximum global error, number of steps taken and function evaluations.

The explicit Two-Step Runge-Kutta-Nyström (TSRKN) method was derived with reference to the technique of deriving the TSRK method. The order conditions of TSRKN method were also obtained by using Taylor series expansion. The strategies in choosing the free parameters were also discussed. The stability of the methods derived were also investigated. The explicit TSRKN method was then analyzed experimentally and comparisons of the numerical results obtained were made with the existing methods in terms of maximum global error, number of steps taken and function evaluations.

Next, we discussed the derivation of an embedded pair of the TSRKN (ETSRKN) methods for solving second order ODE. Variable step size codes were developed and numerical results were compared with the existing methods in terms of maximum

global error, number of steps taken and function evaluations. The ETSRKN were then used to solve second-order Fuzzy Differential Equation (FDE). We observe that ETSRKN gives better accuracy at the end point of fuzzy interval compared to other existing methods.

In conclusion, the methods developed in this thesis are able to solve the system of second-order differential equation (DE) which consists of ODE and FDE directly.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk Ijazah Doktor Falsafah

KAEDAH RUNGE-KUTTA-NYSTRÖM DUA LANGKAH BAGI MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA PERINGKAT DUA

Oleh

LATIFAH BINTI MD ARIFFIN

Disember 2016

Pengerusi: Profesor Dato' Mohamed Bin Suleiman, PhD
Fakulti: Sains

Di dalam kajian ini, kaedah yang boleh menyelesaikan masalah nilai awal secara terus dibangunkan. Kaedah ini adalah di dalam skim multi-langkah di mana ia dikenali sebagai kaedah dua-langkah. Kaedah dua-langkah mempunyai kelebihan di mana ia boleh menganggar penyelesaian dengan kurang penilaian fungsi berbanding dengan kaedah satu-langkah. Pemilihan saiz langkah juga penting bagi memperolehi keputusan yang lebih jitu dan efisyen. Saiz langkah yang kecil akan menghasilkan keputusan yang lebih jitu, tetapi ia akan memanjangkan tempoh masa pelaksanaan.

Kaedah Runge-Kutta Dua Langkah (RKDL) diterbitkan bagi menyelesaikan Persamaan Pembezaan Biasa (PPB) peringkat satu. Syarat peringkat bagi kaedah RKDL tak tersirat diperolehi dengan menggunakan kembangan siri Taylor. Kaedah RKDL tak tersirat diterbitkan dan kestabilannya dikaji. Ia kemudiannya dianalisa secara eksperimen. Keputusan berangka yang diperolehi dianalisa dengan membuat perbandingan bersama kaedah-kaedah sedia ada berdasarkan kepada ralat global maksimum, bilangan langkah dan penilaian fungsi.

Kaedah Runge-Kutta-Nyström Dua Langkah (RKNDL) tak tersirat diterbitkan mengikut teknik seperti penerbitan kaedah RKDL. Syarat peringkat bagi kaedah RKNDL juga diperolehi dengan menggunakan kembangan siri Taylor. Strategi pemilihan parameter bebas juga dibincangkan. Kestabilan kaedah-kaedah ini juga dikaji. Kaedah RKNDL tak tersirat ini kemudiannya dianalisa secara eksperimen dan perbandingan dilakukan bersama kaedah-kaedah sedia ada berdasarkan kepada ralat global maksimum, bilangan langkah dan penilaian fungsi.

Seterusnya kami membincangkan penerbitan kaedah Benaman RKNDL (BRKNDL) bagi menyelesaikan PPB peringkat dua. Kod langkah berubah dibangunkan dan keputusan berangka dibandingkan dengan kaedah-kaedah sedia ada berdasarkan kepada ralat global maksimum, bilangan langkah dan penilaian fungsi. Kaedah BRKNDL ini

kemudiannya digunakan untuk menyelesaikan Persamaan Pembezaan Kabur (PPK). Kami mendapati bahawa kaedah BRKNDL memberi kejituan yang lebih baik pada titik hujung selang kabur berbanding dengan kaedah-kaedah sedia ada.

Kesimpulannya, kaedah-kaedah yang diterbitkan di dalam tesis ini dapat menyelesaikan sistem persamaan pembezaan (PP) yang merangkumi PPB dan PPK peringkat dua secara terus.

ACKNOWLEDGEMENT

I am grateful to the Almighty Allah for with His blessings, I am able to complete this thesis. May blessing and peace be upon Prophet Muhammad *Sallalahu ‘Alaihi Wasallam.*.

I would like to express my utmost appreciation to my supervisor, Professor Dato’ Dr. Mohamed bin Suleiman for his patient, guidance throughout my PhD studies and until the completion of this thesis. I am also very grateful to my co-supervisor, Associate Professor Dr. Norazak bin Senu who had guided me throughout this project. His guidance, continuous help and encouragement had been the key to the success of this project. I would also like to thank Professor Dr. Zanariah binti Abdul Majid for being such an inspiring icon for me and Dr. Mansor bin Monsi for being supportive morally.

Many thanks to Dr. Ali Ahmadian and Dr. Nor Shamsidah binti Amir Hamzah for guiding me to complete the final findings in this thesis. Not to forget, all of my friends who have continuously helped me through the hard times throughout my studies. Thank you to UTHM’s Study Leave Committee for the financial support. Finally, I am forever grateful to my husband, my children, my parents, my best friend, Dr. Balkis binti Hj. A. Talip and other family members for their moral support, patience, ideas and understanding that made the completion of this thesis possible.

This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfillment of the requirement for the Degree of Doctor of Philosophy. The members of the Supervisory Committee were as follows:

Dato' Mohamed Suleiman, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Chairman)

Norazak Senu, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

Zanariah Abdul Majid, PhD
Professor
Faculty of Science
University Putra Malaysia
(Member)

Mansor Monsi, PhD
Lecturer
Faculty of Science
University Putra Malaysia
(Member)

ROBIAH BINTI YUNUS, PhD
Professor and Dean
School of Graduate Studies
Universiti Putra Malaysia

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Name and Matric No.: Latifah Binti Md Ariffin (GS23633)

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Name of Chairman of Supervisory Committee: Professor Dato' Dr. Mohamed Bin Suleiman

Signature: ______________________________
Name of Member of Supervisory Committee: Associate Professor Dr. Norazak Bin Senu

Signature: ______________________________
Name of Member of Supervisory Committee: Professor Dr. Zanariah Binti Abdul Majid

Signature: ______________________________
Name of Member of Supervisory Committee: Dr. Mansor Bin Monsi

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LIST OF ABBREVIATIONS

BVP	Boundary Value Problem
DE	Differential Equation
ERK3(2)D	A second-order three-stage explicit RK method embedded into third-order three-stage RK method derived by Dormand (1996).
ERK4(3)B	A third-order four-stage explicit RK method embedded into fourth-order four-stage RK method derived by Butcher (1987).
ERK4(3)F	A third-order four-stage explicit RK method embedded into fourth-order four-stage RK method derived by Fehlberg (1970).
ETSRKN	Embedded Two-Step Runge-Kutta-Nyström
ETSRKN3(2)	The two-stage second-order embedded in two-stage third-order TSRKN method
ETSRKN4(3)	The three-stage third-order embedded in three-stage fourth-order TSRKN method
FCN	Number of Function Evaluations
FDE	Fuzzy Differential Equation
FETSRKN	Fuzzy Embedded Two-Step Runge-Kutta-Nyström
FIVP	Fuzzy Initial Value Problem
H-derivative	Hukuhara-Differentiability
HPC	High Performance Computing Machine
IVP	Initial Value Problem
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
PLTE	Principal Local Truncation Error
RK	Runge-Kutta
RK3(3)B	The three-stage third-order explicit RK method derived by Butcher (1987)
RK3(3)D	The three-stage third-order explicit RK method derived by Dormand (1996)

RK4(3)B	The four-stage third-order embedded in four-stage fourth-order RK method derived by Butcher (1987)
RK4(3)F	The four-stage third-order embedded in four-stage fourth-order RK method derived by Fehlberg (1970)
RKN	Runge-Kutta-Nyström method
RKN3(3,12,3)	A three-stage third-order RKN method with dispersive order twelve and dissipative order three derived by van der Houwen and Sommeijer (1987).
RKN4(4,10,5)	A four-stage fourth-order RKN method with dispersive order ten and dissipative order five derived by van der Houwen and Sommeijer (1987)
TSRK	Two-Step Runge-Kutta method
TSRK2(3)	The two-stage third-order explicit TSRK method
TSRKN	Two-Step Runge-Kutta-Nyström method
TSRKN2(3)	The two-stage third-order explicit TSRKN method
TSRKN3(4)	The three-stage fourth-order explicit TSRKN method
$C_2(p)$	Simplifying conditions for m −stage TSRKN method
$B_2(p)$	Simplifying conditions for m −stage TSRKN method
$B'_2(p)$	Simplifying conditions for m −stage TSRKN method

CHAPTER 1

INTRODUCTION

1.1 Introduction

Many problems in engineering and science can be formulated in terms of differential equations. These problems arise in mechanical and electrical systems, celestial and orbital mechanics, molecular dynamics, seismology and many other engineering problems. A differential equation is defined as an equation that involves a relation between an unknown function with one or more of its derivatives. Basically, a differential equation involving only ordinary derivatives with respect to single independent variable is called Ordinary Differential Equation (ODE). Meanwhile, a differential equation involving partial derivatives with respect to more than one independent variable is called Partial Differential Equation (PDE). Furthermore, ODE may be classified as either initial-value problem (IVP) or boundary-value problem (BVP).

The most discussed IVP are in class of the first and second order. These problems can be solved analytically when they are linear. However, very few nonlinear problems can be solved analytically. Thus, one must rely on numerical scheme to solve these problems. Methods for solving IVP numerically are classified into two schemes, which are the one-step method and the multi-step method. Many numerical one-step methods have been developed such as Euler method, Runge-Kutta (RK) method and Taylor series method where these methods are used to solve the first order IVP directly. These methods are also being used to solve the second order IVP indirectly by reducing it to the first order equations system. Even though this approach is easy to implement but it will enlarge the equation system and will increase the cost for the process.

1.2 Objectives of the Thesis

The main objective of this thesis is to develop a two-step Runge-Kutta-Nyström (TSRKN) method with a constant step-size and a variable step-size for solving special second-order IVP directly. The objectives can be accomplished by:

1. Develop the order conditions for two-step Runge-Kutta (TSRK) by using Taylor series expansion, derive the TSRK method and implement the method to solve first order IVP using constant step-size code;
2. Develop the order conditions for TSRKN by using Taylor series expansion, derive the TSRKN method and implement the method to solve special second order IVP using constant step-size code;
3. Investigate the stability and convergence of the derived TSRK and TSRKN methods;

4. Derive the embedded two-step Runge-Kutta-Nyström (ETSRKN) method and implement the method to solve special second order IVP using variable step-size code;
5. Solve second order fuzzy differential equations (FDE) by using ETSRKN method that had been derived previously to show the ability of the method to solve other type of DEs.

1.3 Outline of the Thesis

In Chapter 1, a brief introduction on differential equations and the application of numerical methods for solving different types of differential equations are given.

In Chapter 2, a brief introduction to IVP and Taylor series expansion were given. Then earlier researches related to TSRK and TSRKN methods for solving first order ODE and, second order ODE and FDE were provided. The stability properties for these methods were also presented. Some basic definitions and theorems related to the subject were also given. FDE and FIVP were discussed at the end of this chapter.

In Chapter 3, we start with the development of the order conditions from order one up to order four for TSRK method by using Taylor series expansion. Based on the order conditions obtained, we derived the two-stage third-order TSRK explicit method. The strategies of choosing the free parameters of the method for developing a more accurate computed solution are also discussed. The convergence of the method is proven and the stability regions of the method are presented. To illustrate the efficiency of the method, a number of tested problem are validated and the numerical results are compared with existing RK method of the same order derived by Dormand (1996) and Butcher (1987). Stability interval for all methods will also be presented.

Chapter 4 will discuss the development of order conditions from order one up to order four for TSRKN method by using Taylor series expansion. A two-stage third-order and three-stage fourth-order explicit TSRKN method were derived using the same strategy as found in Chapter 3. Several problems are solved and their numerical results are compared with the existing RK method of the same order. For existing RK method of order three, comparisons are made with methods derived by Butcher (1987) and van der Houwen and Sommeijer (1987). Likewise, comparisons are made with RK method of order four derived by Lambert (1991) and RKN method of order four derived by van der Houwen and Sommeijer (1987). Stability interval for all methods will also be presented.

For variable step-size, the development of an embedded pair for explicit TSRKN (ETSRKN) methods based on formulas derived in Chapter 4 are discussed in Chapter 5. The choices of free parameters in obtaining the optimized pair are also discussed. Special second-order IVP are solved including oscillating problems. Numerical results and their performances are presented. For the new ETSRKN 3(2) pair, comparisons are made with an existing embedded RK 3(2) pair derived by Dormand (1996).

Meanwhile, for the new ETSRKN 4(3) pair, comparisons are made with an existing embedded RK 4(3) pair derived by Butcher (1987) and Fehlberg (1970). The ETSRKN 4(3) pair method then is adapted for solving second-order fuzzy differential equations. Two fuzzy problems are solved and their numerical results are compared with the existing embedded RK method.

Finally, the summary of the whole thesis, conclusions and future research are given in Chapter 6.

1.4 Motivation and Contribution of the Thesis

Many differential equations which appear in practice are systems of second order IVP. This system can be reduced into first order differential equations of doubled dimension. In this study we are focusing on solving the second order IVP directly. Our proposed method able to solve the second order problems directly that is TSRKN method. We focus only on the explicit type of method. In addition to the implementation of the method, accuracy and stability are two other factors used for judging the efficacy of the methods.

1.5 Scope of the Thesis

This study concentrate on the development of new coefficient and efficient codes that are based on explicit TSRKN methods for numerical solution of IVP. These methods will then be used for solving system of second order ODEs directly for both constant and variable step size mode. The properties of this method will be analyzed in terms of order, consistence and convergence. Our main motivation is to reduce the number of steps taken in solving second order IVP directly by using this method as well as to reduce the number of function evaluations where it will ensure cost efficiency.

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BIODATA OF STUDENT

Latifah Binti Md Ariffin was born on the 9th of January, 1979 in Kajang, Selangor. She received her primary level education at Air Panas Primary School in Setapak, Kuala Lumpur. The author then continued her secondary level education at Convent Bukit Nanas Secondary School in Kuala Lumpur.

In May 1997, the author furthered her studies at the Matriculation of Biological Science at Kurniawan College, Cheras, Kuala Lumpur in collaboration with Universiti Putra Malaysia (UPM) and continued her Bachelor of Science degree with honours, majoring in Mathematics at the Faculty of Science(formerly known as the Faculty of Science and Environmental Studies), at UPM. She then graduated with second class upper in February 2002.

After completing her degree, the author worked as a lecturer at Kurniawan College, Cheras, Kuala Lumpur. In September 2002, she became a tutor at Kolej Universiti Teknologi Tun Hussein Onn (KUiTTHO) which is situated in Batu Pahat, Johor. She obtained her Masters of Science in Theoretical Structure and Modelling in October 2006. In November 2007, she was appointed as a permanent lecturer at Universiti Tun Hussein Onn Malaysia (previously known as KUiTTHO). Currently, she is attending a Ph. D. programme at the Department of Mathematics, UPM and working on a TSRKN Method for Solving Second Order Ordinary Differential Equation.