OVERVIEW ON SOLVING STIFF PROBLEMS USING ONE-STEP METHODS

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A Dissertation submitted as a partial fulfilment of the requirements for the award of the degree of Master of Science (Mathematics)

Faculty of Science
Universiti Teknologi Malaysia

OCTOBER, 2001

UNIVERSITI TEKNOLOGI MALAYSIA

BORANG PENGESAHAN STATUS TESIS◆

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I humbly dedicate to...

my beloved family members (especially Chee Wooi)

who has shaped my life

and

who has influenced my life in a wonderful way.

ACKNOWLEDGEMENT

Firstly, the author would like to take this opportunity to express her heartfelt appreciation and thanks to her respectful supervisor, PM DR. Nazeeruddin Yaacob who has relentlessly given a microscopic supervision, guidance, constructive ideas and invaluable advice, enabling the author to achieve the objective of this dissertation.

The author is very grateful to the author's family members especially my husband, Chee Wooi. No amount of gratitude could repay their kindness of being there as well as the patience to put up with the author's whim. The author also would like thanks to her friends especially Lee Lean Eng for many helpful comments and suggestions.

ABSTRACT

Stiff problems in ordinary differential equations can now be solved more routinely. In the past four decades, many researchers were interested in finding effective stiff solution methods. This dissertation is intended for the readers who are interested in solving stiff problems with one-step methods. The focus is on one-step methods, more particularly to implicit Runge-Kutta methods and a recent explicit one-step method. This review explains what stiff differential equations are and what are the requirements for the stiff solution methods. The development of one-step methods in solving stiff problems is outlined. The advantages and disadvantages of each method are also presented. Further, practical implementation of implicit Runge-Kutta methods and the development of one-step methods are discussed briefly. Finally, the dissertation is concluded by presenting a summary of historical reviews of one-step methods in solving stiff problems and some suggestions for future research in this area.

ABSTRAK

Masalah kekakuan dalam persamaan pembezaan biasa dapat diselesaikan dengan lebih sistematik pada masa kini. Sejak empat dekad lepas, ramai penyelidik berminat dalam mencari kaedah penyelesaian masalah kekakuan yang berkesan. Disertasi ini adalah untuk pembaca yang berminat dalam menyelesaikan masalah kekakuan dengan kaedah satu langkah. Penumpuan adalah kepada kaedah satu langkah, khususnya kepada kaedah Runge-Kutta tersirat dan suatu kaedah satu langkah tak tersirat yang dicadangkan baru-baru ini. Ulasan ini menjelaskan makna persamaan pembeza kaku dan syarat-syarat bagi kaedah penyelesaian masalah kekakuan. Perkembangan kaedah satu langkah dalam menyelesaikan masalah kekakuan telah dibentangkan. Kebaikan dan keburukan setiap kaedah juga diberi. Selanjutnya, pelaksanaan kaedah Runge-Kutta tersirat yang praktikal dan perkembangan kaedah satu langkah hanya dibincang secara ringkas. Disertasi ini diakhiri dengan memberikan satu ringkasan catatan sejarah kaedah satu langkah dalam menyelesaikan masalah kekakuan dan memberikan beberapa cadangan untuk penyelidikan yang selanjutnya dalam bidang ini.

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LIST OF ABBREVIATIONS

SDE	-	Stiff Differential Equation
DE	-	Differential Equation
ODE	-	Ordinary Differential Equation
IRK	-	Implicit Runge-Kutta
DIRK	-	Diagonally Implicit Runge-Kutta
SDIRK	-	Singly Diagonally Implicit Runge-Kutta
SIRK	-	Singly Implicit Runge-Kutta
MIRK	-	Mono Implicit Runge-Kutta
ROW	-	Rosenbrock Wanner Methods
VSVO	-	Variable Step-Variable Order
DC	-	Deferred Correction
DESI	-	Diagonally Extended Singly Implicit
BDF	-	Backward Differentiation Formulae
PDIRK	-	Parallel Diagonally Implicit Iteration Runge-Kutta
IVP	-	Initial Value Problem

$\langle\ ,\ \rangle$	-	inner product on ∇^m
λ	-	eigenvalue
$\otimes$	-	direct product
L	-	Lipschitz constant
$\rho(\ )$	-	spectral radius
W	-	***W***-transformation
$\\| \\|$	-	norm corresponding to $\langle\ ,\ \rangle$
e	-	vector of length q with all entries equal one
$L_s(\ )$	-	Laguerre polynomial of degree s
J	-	Jacobian matrix
S	-	non-singular matrix
$\mathfrak{R}$	-	negative half plane
h	-	step size
M	-	symmetric matrix
s	-	number of stages

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CHAPTER I

INTRODUCTION

1.1 Introduction

Stiffness is a property of the differential equation that makes it slow and expensive when solving by numerical methods. It is due to the numerical coefficients in the differential equation (so that there is too wide a spread between the fastest and slowest elements) rather than of the form. Unfortunately, the numerical values occurring in nature are frequently such as to cause stiffness, so a realistic representation of a natural system using differential equation is likely to encounter this phenomenon (Garfinkel *et.al*, 1978). Stiff differential equations arise in almost all chemical kinetics studies. It also arises in biochemistry and physics.

Much has been written about what "stiffness" really means but the property is generally understood in terms of what goes wrong when numerical methods not designed for such problems are being used to solve them (Butcher, 2000a). Stiff problems had been recognized from approximately half way through the 20th century and these have received considerable attention, especially in the last 30 years. The methods for dealing effectively with stiffness involve considerable sophistication, and much of the information regarding them is scattered through departmental or laboratory reports and conference proceedings. Accordingly, this dissertation is to give an overview of the development of one-step methods in solving stiff problems that has the state of the art or offers promise for the future.

1.2 Dissertation Background

Recently, there are so many methods in solving stiff problems. A clear overview and information of solving stiff problems need to be summarized in order to give a good reference for research purposes. An overview of one-step methods in coping with stiffness in differential equations will be discussed in details in this dissertation. In future, choosing the right and the most applicable method not only increases the efficiency of research work, but also gives the most accurate result in shorter time.

1.3 Objective of the Dissertation

i) To give an overview on the one-step methods from the past to the most recent in solving stiff ODE problems.

ii) To compile the advantages and disadvantages of the implicit Runge-Kutta methods in solving stiff ODEs.

iii) To discuss the development of one-step methods related to stiff ODEs.

1.4 Scope of Dissertation

The scope of this dissertation includes:

i) Review the one-step methods, which includes implicit Runge-Kutta methods and a recent explicit one-step method.

ii) Overview of development of one-step methods, without involving the parallel methods.

iii) Review the stiff differential equations from the aspect of stability and without consider the aspect of converge and consistency.

1.5 Contribution of the Dissertation

The contribution of this dissertation can be stated as below:

i) To gather all the information regarding the development of one-step methods in solving stiff ODE problems.

ii) To provide the overview of the implicit Runge-Kutta methods and their differences.

iii) To provide a platform for the future researchers as a reference and yardstick in this research field.

1.6 Summary of the Dissertation

This dissertation contains six chapters: Introduction, Literature survey, Stiff differential equations, One-step methods, Discussion and Conclusion. Figure 1.1 is a framework pertaining to the structure of this dissertation. The first chapter comprises introduction of the dissertation, problem background and dissertation's objectives and scopes. Chapter II discusses the overview done by some researchers, which review the stiff situation from several aspects.

Chapter III gives the historical review of stiff differential equations, various definitions of stiffness and stability criteria of stiffness. The details of stiff differential equations will be presented by using examples and graphs in order to give a better understanding to readers. Chapter IV reviews development of one-step methods in solving stiff problems. The scope here is primarily on implicit Runge-Kutta methods and a recently established explicit one-step method. Table 4.5 provides an executive summary of the historical development of the one-step methods. The last part of this chapter highlights the development process of various special classes under the implicit Runge-Kutta methods.

Chapter V focuses on the advantages and disadvantages of the implicit Runge-Kutta methods. The algorithm towards the implementation of implicit Runge-Kutta is shared through some numerical experiments to enhance a better understanding.

The procedure of solving the stiff problems will be presented in Figure 6.1. Table 6.1 summarized the suitability of these one-step methods in different categorizes of stiff problems. The last part of Chapter VI gives a snap shot, which outlined probable numerical methods relevant to the stiff problem.

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