

**BLOCK MULTISTEP METHODS FOR SOLVING ORDINARY  
DIFFERENTIAL EQUATIONS**

**ZARINA BIBI BT IBRAHIM**

**DOCTOR OF PHILOSOPHY  
UNIVERSITI PUTRA MALAYSIA**

**2006**

**Abstract of thesis presented to the Senate of Universiti Putra Malaysia in  
fulfilment of the requirement for the degree of Doctor of Philosophy**

**BLOCK MULTISTEP METHODS FOR SOLVING ORDINARY  
DIFFERENTIAL EQUATIONS**

**By**

**ZARINA BIBI BT IBRAHIM**

**September 2006**

**Chairman: Associates Professor Fudziah Ismail, PhD**

**Faculty: Science**

**Multistep methods for the solution of systems of Ordinary Differential Equations (ODEs) were described. The first part of the thesis is about the construction and derivation of new Block Backward Differentiation Formula (BBDF) method of constant step size and variable step size for solving first order stiff Initial Value Problems (IVPs). Their regions of stability were presented and numerical results of the methods were compared with existing methods.**

**The second part of the thesis describes the derivation of the Adams type block method to solve second order nonstiff systems directly whilst a mixture of the Adams type formulae and the new implicit BBDF method were used to solve second order stiff problems directly. Partitioning strategies for the block method were discussed in detail and numerical results of the block partitioning**

are compared with the nonblock Variable Step Variable Order (VSVO) Direct Integration method for solving second order ODEs directly.

Finally, this thesis deals with parallel numerical algorithms for the solution of systems of ODEs. The constructed BBDF methods are then tested and parallelism is obtained by using a Message Passing Interface (MPI) library run on High Performance Computer (HPC). The parallel implementation of the new codes produced superlinear speedup as the dimension of the ODEs systems increased. Comparisons and illustrations with sequential codes are provided.

In conclusion, the numerical results clearly demonstrates the efficiency of using the new block multistep methods for solving ODEs. Application of these multistep block method to a widely used test problems reveals the reduction in the total number of steps and execution time when compared with sequential methods.

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

**KAEDAH BLOK MULTILANGKAH BAGI MENYELESAIKAN  
PERSAMAAN PEMBEZAAN BIASA**

**Oleh**

**ZARINA BIBI BT IBRAHIM**

**September 2006**

**Pengerusi: Profesor Madya Fudziah Bt Ismail, PhD**

**Fakulti: Sains**

**Kaedah multilangkah bagi menyelesaikan sistem Persamaan Pembezaan Biasa (PPB) dihuraikan. Bahagian pertama tesis ini berkenaan pembinaan dan pemerolehan kaedah baru Blok Formulasi Beza Ke Belakang (BFBB) menggunakan panjang langkah tetap dan panjang langkah berubah bagi menyelesaikan Masalah Nilai Awal (MNA) kaku peringkat pertama. Rantau kemantapan kaedah blok didedahkan dan keputusan berangka dibandingkan dengan kaedah sedia ada.**

**Bahagian kedua tesis ini menghuraikan pemerolehan kaedah blok Adams bagi menyelesaikan sistem tak kaku peringkat kedua secara terus manakala campuran daripada kaedah Adams dan kaedah tersirat BFBB yang baru digunakan bagi menyelesaikan masalah kaku peringkat kedua secara terus. Strategi pemetakan bagi kaedah blok dibincangkan secara terperinci dan keputusan berangka bagi pemetakan dalam blok dibandingkan dengan kaedah**

bukan blok Saiz Langkah Berubah Peringkat Berubah (SBPB) bagi menyelesaikan PPB peringkat kedua secara terus.

Akhirnya, tesis ini membincangkan algoritma berangka selari bagi menyelesaikan PPB. Kaedah BFBB yang dibentuk diuji dan keselarian diperolehi dengan menggunakan perpustakaan Penghantaran Mesej Antaramuka (MPI) yang dilarikan atas komputer berkeupayaan tinggi (HPC). Pelaksanaan selari kod baru tersebut menunjukkan kecekapan superlinear apabila dimensi sistem PBB meningkat. Perbandingan dan ilustrasi dengan kod sesiri diberi.

Kesimpulannya, keputusan berangka dengan jelas menunjukkan kecekapan menggunakan kaedah blok bagi menyelesaikan PPB. Pemakaian kaedah blok multilangkah kepada masalah secara meluas mendedahkan pengurangan dalam jumlah langkah dan masa pelaksanaan apabila dibandingkan dengan kod kaedah sesiri.

## ACKNOWLEDGEMENTS

*In the Name of Allah the Most Compassionate, the Most Merciful*

First and foremost, I wish to express my sincere and deepest gratitude to the chairman of the supervisory committee, YBhg. Professor Dato' Dr. Mohamed bin Suleiman for his invaluable advice, guidance, assistance and most of all, for his constructive criticisms. This work would not have been completed without his help that I received in various aspects of the research. I am also grateful to the member of the supervisory committee, Associate Professor Dr. Fudziah bt Ismail and Dr. Rozita bt Johari.

A special thank you to Dr. Zanariah bt Abdul Majid for her advice and encouragement which has contributed in one way or another in completing this thesis. Special acknowledgement is extended to Khairil Iskandar bin Othman who have spent exceptional amounts of time in discussing and developing the algorithms during the course of my research.

I am also indebted to the Universiti Putra Malaysia for the scholarship and study leave which enables me to pursue this research.

Finally, I cannot put into words how much I appreciate the continuous support, understanding and patience of my husband, Azman, and my children, Sarah, Nabilah, Nina, Syasya and Luqman; and special thanks to my parents for their continuous encouragement. Thank you.

**This thesis submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy. The members of the Supervisory Committee are as follows:**

**Fudziah Ismail, PhD**  
**Associate Professor**  
**Faculty of Science**  
**Universiti Putra Malaysia**  
**(Chairman)**

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

**Rozita Johari, PhD**  
**Lecturer**  
**Faculty of Computer Science and Information Technology**  
**Universiti Putra Malaysia**  
**(Member)**

---

**AINI IDERIS, PhD**  
**Professor / Dean**  
**School of Graduate Studies**  
**Universiti Putra Malaysia**

**Date:**

## **DECLARATION**

**I hereby declare that the thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at UPM or other institutions.**

**ZARINA BIBI BT IBRAHIM**

**Date:**



## TABLE OF CONTENTS

	<b>Page</b>
<b>DEDICATION</b>	<b>ii</b>
<b>ABSTRACT</b>	<b>iii</b>
<b>ABSTRAK</b>	<b>v</b>
<b>ACKNOWLEDGEMENTS</b>	<b>vii</b>
<b>APPROVAL</b>	<b>viii</b>
<b>DECLARATION</b>	<b>x</b>
<b>LIST OF TABLES</b>	<b>xiv</b>
<b>LIST OF FIGURES</b>	<b>xvii</b>
<b>LIST OF ABBREVIATIONS</b>	<b>xxi</b>
<b>CHAPTER</b>	
<b>I INTRODUCTION</b>	<b>22</b>
Literature Review	<b>23</b>
Codes for solving stiff ODEs	<b>23</b>
Sequential Block Method for solving ODEs	<b>23</b>
Partitioning ODEs	<b>24</b>
Parallel block methods for solving ODEs	<b>25</b>
Objectives of the Thesis	<b>26</b>
Outline of the Thesis	<b>27</b>
Problem to be solved	<b>29</b>
Stiff Systems of Ordinary Differential Equations	<b>30</b>
Determining Convergence and Stability of Multistep methods	<b>32</b>
Errors in the solution of ODEs	<b>36</b>
<b>II IMPLICIT 2-POINT AND 3-POINT BLOCK BACKWARD DIFFERENTIATION FORMULAE OF CONSTANT STEP SIZE FOR SOLVING FIRST ORDER STIFF ODEs</b>	<b>38</b>
Introduction	<b>38</b>
Derivation of Implicit 2-point block BDF method	<b>38</b>
Derivation of Implicit 3-point block BDF method	<b>42</b>
Stability of the methods	<b>45</b>
Stability of the implicit 2-point block BDF method	<b>46</b>
Stability of the implicit 3-point block BDF method	<b>48</b>
Implementation of the 2-point and 3-point block BDF method	<b>51</b>
Newton Iteration of the implicit 2-point block BDF method	<b>53</b>
Newton Iteration of the implicit 3-point block BDF method	<b>53</b>
Problems tested	<b>54</b>

	Numerical results	56
	Discussion and Conclusion	60
<b>III</b>	<b>VARIABLE STEP SIZE OF IMPLICIT 2-POINT BLOCK BACKWARD DIFFERENTIATION FORMULAE FOR SOLVING FIRST ORDER STIFF SYSTEMS OF ODEs</b>	<b>62</b>
	Introduction	62
	Derivation of Variable Step Size Block BDF by Doubling and Halving	62
	Derivation of the predictors	67
	Stability of the Methods	69
	Implementation of the method	75
	Estimating the Error and Step Size Selection	79
	Estimating the Local Truncation Error, LTE	79
	Estimating the Maximum error, MAXE	79
	Step size selection	80
	Problems tested	81
	Numerical results	85
	Discussion and Conclusion	94
<b>IV</b>	<b>DERIVATION OF IMPLICIT BLOCK ADAMS AND BDF METHOD FOR SOLVING SECOND ORDER ODEs DIRECTLY</b>	<b>96</b>
	Introduction	96
	Derivation for BGBDF for $j = 1$ , variable step size	97
	Derivation for BGBDF for $j = 2$ , variable step size	103
	Derivation of BGBDF predictors for $j = 1$	108
	Estimating the error	111
	Some Aspect of Stability	115
	Stability region for the Block Adams, $j = 0$	115
	Stability region for the BGBDF for $j = 1$	117
	Stability region for the BGBDF for $j = 2$	120
<b>V</b>	<b>IMPLEMENTATION OF BLOCK PARTITIONING USING BLOCK ADAMS AND BDF METHODS FOR SOLVING SECOND ORDER ODEs DIRECTLY</b>	<b>125</b>
	Introduction	125
	Implementation of implicit block Adams method, $j = 0$	125
	Derivation of Newton iteration matrix for BGBDF	129
	Newton iteration for BGBDF method for $j = 1$	129
	Newton iteration for BGBDF method for $j = 2$	134
	Strategy for Block Multistep Formulas Intervalwise Partitioning	139
	Detailed test for Detecting Stiffness	139

	<b>Strategy for choosing <math>j</math></b>	<b>141</b>
	<b>Convergence of the corrector iteration</b>	<b>146</b>
	<b>Problems tested</b>	<b>147</b>
	<b>Numerical result</b>	<b>151</b>
	<b>Discussion and Conclusion</b>	<b>157</b>
<b>VI</b>	<b>PARALLELISATION OF IMPLICIT BLOCK MULTISTEP METHOD FOR SOLVING LARGE ODES</b>	<b>158</b>
	<b>Introduction</b>	<b>158</b>
	<b>Computers Architectures: An Overview</b>	<b>160</b>
	<b>SISD Model</b>	<b>161</b>
	<b>SIMD Model</b>	<b>161</b>
	<b>MISD Model</b>	<b>162</b>
	<b>MIMD Model</b>	<b>163</b>
	<b>Memory Architectures</b>	<b>163</b>
	<b>Shared memory</b>	<b>164</b>
	<b>Distributed memory</b>	<b>164</b>
	<b>Message Passing Interface</b>	<b>165</b>
	<b>Performance of parallel processing</b>	<b>166</b>
	<b>Speedup</b>	<b>166</b>
	<b>Efficiency</b>	<b>168</b>
	<b>Parallel implementation</b>	<b>168</b>
	<b>Matrix multiplication for Jacobian matrix</b>	<b>170</b>
	<b>High Performance Computer SunFire 1280 Architecture</b>	<b>171</b>
	<b>Problems tested</b>	<b>172</b>
	<b>Numerical results</b>	<b>174</b>
	<b>Discussion and Conclusion</b>	<b>192</b>
<b>VII</b>	<b>CONCLUSION</b>	<b>194</b>
	<b>Summary</b>	<b>194</b>
	<b>Future Work</b>	<b>195</b>
	<b>BIBLIOGRAPHY</b>	<b>197</b>
	<b>APPENDICES</b>	<b>204</b>
	<b>BIODATA OF THE AUTHOR</b>	<b>224</b>