



UNIVERSITI PUTRA MALAYSIA

**PARTITIONING TECHNIQUES AND THEIR PARALLELIZATION FOR
STIFF SYSTEM OF ORDINARY DIFFERENTIAL EQUATIONS**

KHAIRIL ISKANDAR OTHMAN

FS 2007 39

**PARTITIONING TECHNIQUES AND THEIR PARALLELIZATION FOR
STIFF SYSTEM OF ORDINARY DIFFERENTIAL EQUATIONS**

By

KHAIRIL ISKANDAR OTHMAN

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

April 2007



TO MY FAMILY



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

PARTITIONING TECHNIQUES AND THEIR PARALLELIZATION FOR STIFF SYSTEM OF ORDINARY DIFFERENTIAL EQUATIONS.

By

KHAIRIL ISKANDAR BIN OTHMAN

April 2007

Chairman: Associate Professor Fudziah bt Ismail, PhD

Faculty: Science

A new code based on variable order and variable stepsize componentwise partitioning is introduced to solve a system of equations dynamically. In previous partitioning technique researches, once an equation is identified as stiff, it will remain in stiff subsystem until the integration is completed. In this current technique, the system is treated as nonstiff and any equation that caused stiffness will be treated as stiff equation. However, should the characteristics showed the elements of nonstiffness, and then it will be treated again with Adam method. This process will continue switching from stiff to nonstiff vice versa whenever it is necessary until the interval of integration is completed.



Next, a block method with R -points generate R new approximate solution values, is a strategy for solving a system and also for parallelizing ODEs. Partitioning this block method to solve stiff differential equations is a new strategy; it is more efficient and takes less computational time compared to the sequential methods. Two partitioning techniques are constructed, Intervalwise Block Partitioning (IBP) and Componentwise Block Partitioning (CBP). Numerical results are compared as validation of its effectiveness.

Intervalwise block partitioning will initially treat the systems of equations as nonstiff and solve them using Adams method, by switching to the Backward Differentiation formula when there is a step failure and indication of stiffness.

Componentwise block partitioning will place the necessary equations that cause instability and stiffness into the stiff subsystem and solve using Backward Differentiation Formula, while all other equations will still be treated as non-stiff and solved using Adams formula.

Parallelizing the partitioning strategies using Message Passing Interface (MPI) is the most appropriate method to solve large system of equations. Parallelizing the right algorithm in the partitioning code will give a better performance with shorter execution times. The graphs of its performance and execution time, visualize the advantages of parallelizing.

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

**KAEDAH PEMETAKAN DAN KESELARIAN BAGI
MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA YANG
KAKU.**

Oleh

KHAIRIL ISKANDAR BIN OTHMAN

April 2007

Pengerusi: Profesor Madya Fudziah bt Ismail, PhD

Fakulti: Sains

Suatu kod baru berdasarkan peringkat berubah dan saiz langkah berubah pemetakan blok komponen diperkenalkan bagi menyelesaikan sistem persamaan dinamik. Dalam kajian teknik pemetakan sebelum ini, apabila persamaan dikenalpasti sebagai persamaan kaku, persamaan itu akan kekal dalam subsistem kaku sehingga tamat pengamiran. Dalam teknik semasa, sistem persamaan PBB dianggap sebagai tak kaku dan sebarang persamaan yang menyebabkan kekakuan akan dilayan sebagai persamaan kaku. Walaubagaimanapun, sekiranya terdapat ciri-ciri menunjukkan ada elemen tak kaku, persamaan itu akan diselesaikan semula dengan kaedah Adams. Proses ini akan berterusan berubah dari kaku ke tak kaku dan sebaliknya apabila perlu sehingga tamat selang pengamiran.

Seterusnya, kaedah Blok R -titik menghasilkan R nilai anggaran penyelesaian, iaitu strategi selari menyelesaikan suatu sistem Persamaan Pembezaan Biasa (PPB). Pemetakan kaedah blok untuk menyelesaikan persamaan pembezaan kaku adalah suatu strategi baru yang lebih cekap dan mengurangkan masa pengiraan apabila dibandingkan dengan kaedah jujukan. Dua kaedah pemetakan dibina iaitu Pemetakan Blok Secara Selang (PBSS) dan Pemetakan Blok Secara Komponen (PBSK). Keputusan berangka dibandingkan untuk pengesahan kecekapannya.

Dalam pemetakan blok secara selang, sistem persamaan di anggap sebagai tak kaku pada awalnya dan diselesaikan menggunakan kaedah Adams dan berubah kepada Formulasi Beza Ke Belakang (FBB) apabila berlaku langkah gagal dan adanya petunjuk bagi kekakuan.

Pemetakan blok secara komponen meletakkan hanya persamaan yang menyebabkan ketakstabilan dan kekakuan ke dalam subsistem kaku dan diselesaikan dengan menggunakan FBB, manakala persamaan yang lain akan dianggap sebagai tak kaku dan diselesaikan dengan formula Adams.

Keselarian strategi pemetakan menggunakan Penghantaran Mesej Antaramuka (MPI) merupakan kaedah yang paling sesuai bagi menyelesaikan sistem persamaan yang besar. Algoritma selari yang sesuai dalam kod pemetakan akan

mengurangkan masa pelaksanaan. Graf pelaksanaan dan masa pelaksanaan menggambarkan faedah keselarian.

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 my supervisor, YBhg. Dato' Prof Dr. Mohamed bin Suleiman for his invaluable advice, guidance, discussion, 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 Associate Professor Dr. Mohamed bin Othman.

A special thank you is extended to Dr. Zarina Bibi bt Ibrahim for her constant motivation and being very helpful during the course of my research

I am also indebted to the Public Services Department and Universiti Teknologi MARA for the sponsorship and study leave which enables me to pursue this research.

Finally, my special thanks and appreciation goes to my wife Rozita for her continuous support, encouragement, and patience which is essential to the completion of this work.



I certify that an Examination Committee has met on 13th April 2007 to conduct the final examination of Khairil Iskandar bin Othman on his Doctor of Philosophy thesis entitled “Partitioning Techniques and their Parallelization for Stiff System of Ordinary Differential Equations” in accordance with Universiti Pertanian Malaysia (Higher Degree) Act 1980 and Universiti Pertanian Malaysia (Higher Degree) Regulations 1981. The Committee recommends that the candidate be awarded the relevant degree. Members of the Examination Committee are as follows:

Azmi Jaafar, PhD

Associate Professor

Faculty of Computer Science and Information Technology

Universiti Putra Malaysia

(Chairman)

Malik Hj. Hassan, PhD

Professor

Faculty of Science

Universiti Putra Malaysia

(Internal Examiner)

Leong Wah June, PhD

Lecturer

Faculty of Science

Universiti Putra Malaysia

(Internal Examiner)


Md. Yazid Mohd. Saman, PhD

Professor

Faculty of Science and Technology

Universiti Malaysia Terengganu

(External Examiner)



HASANA HAMED. GHAZALI, PhD
Professor/Deputy Dean
School of Graduate Studies
Universiti Putra Malaysia

Date: 21 JUNE 2007

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)

Mohamed Othman, 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: 17 July 2007

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.


KHAIRIL ISKANDAR OTHMAN

Date: 12 June 2007

LIST OF TABLES

Table		Page
4.1	Absolute stability of Adam-Bashforth-Moulton	48
4.2	The perturbation of case (1)	51
4.3	The perturbation terms in case (2)	53
4.4	Comparison of stiff and non-stiff system	54
4.5	The perturbations when switching to non-stiff	59
4.6	Numerical results when $\mu = 20$	64
4.7	Numerical results when $\mu = 5$	65
4.8	The effect of the non-stiff terms as the step size changes.	69
5.1	Comparison between the partitioning and non-partitioning block method for Solving Problem 1	95
5.2	Comparison between the partitioning and non-partitioning block method for Solving Problem 2	97
5.3	Comparison between the partitioning and non-partitioning block method for Solving Problem 3	98
5.4	Comparison between the partitioning and non-partitioning block method for Solving Problem 4	99
5.5	Comparison between the partitioning and non-partitioning block method for Solving Problem 5	101
6.1	Execution time for solving Problem 6.1	117
6.1(a)	The Speedup and Efficiency for Problem 6.1 at TOL = 10^{-2}	118
6.1(b)	The Speedup and Efficiency for Problem 6.1 at TOL = 10^{-4}	120
6.1(c)	The Speedup and Efficiency for Problem 6.1 at TOL = 10^{-6}	122



6.2	Execution time for solving Problem 6.2	124
6.2(a)	The Speedup and Efficiency for Problem 6.2 at TOL = 10^{-2}	125
6.2(b)	The Speedup and Efficiency for Problem 6.2 at TOL = 10^{-4}	127
6.2(c)	The Speedup and Efficiency for Problem 6.2 at TOL = 10^{-6}	129



LIST OF FIGURES

Figure		Page
3.1	Stiff ODE at short time scale	20
3.2	Stiff ODE at longer time scale	20
3.3	Stiff ODE unstable solution	21
3.4	Solution changes from nonstiff and stiff on a time scale.	21
3.5	SISD model	23
3.6	SIMD model	24
3.7	MISD model	24
3.8	MIMD model	25
3.9	Memory-processor interconnection	26
3.10	General Model of Shared-Memory Interconnection Topology	27
3.11	General Model of Distributed-Memory Interconnection Topology	28
3.12	Basic Message Passing	30
3.13	Transmitting data to all processors via a command MPI_Bcast()	31
3.14	A Distributed Shared Memory model	32
3.15	A linear speedup graph	33
3.16	Hardware Configuration of Sunfire 1280	38



5.1	Iterations using 2-point Block Multistep method	73
5.2	2-point block method of variable step size	74
6.1	Listing of profile program for 200 equations	108
6.2	Listing of profile program for 20 equations	108
6.3	Expanding from nonblock to 2-point block matrix	112
6.4	Algorithm for master in MPI	114
6.5	Algorithm for slaves in MPI	115
6.6	Graph of speedup against the number of processors at TOL = 10^{-2} for Problem 6.1	119
6.7	Graph of efficiency against the number of processors at TOL = 10^{-2} for Problem 6.1	119
6.8	Graph of speedup against the number of processors at TOL = 10^{-4} for Problem 6.1	121
6.9	Graph of efficiency against the number of processors at TOL = 10^{-4} for Problem 6.1	121
6.10	Graph of speedup against the number of processors at TOL = 10^{-6} for Problem 6.1	123
6.11	Graph of efficiency against the number of processors at TOL = 10^{-6} for Problem 6.1	123
6.12	Graph of speedup against the number of processors at TOL = 10^{-2} for Problem 6.2	126
6.13	Graph of efficiency against the number of processors at TOL = 10^{-2} for Problem 6.2	126
6.14	Graph of speedup against the number of processors at TOL = 10^{-4} for Problem 6.2	128
6.15	Graph of efficiency against the number of processors at TOL = 10^{-4} for Problem 6.2	128



6.16	Graph of speedup against the number of processors at TOL = 10^{-6} for Problem 6.2	130
6.17	Graph of efficiency against the number of processors at TOL = 10^{-6} for Problem 6.2	130



LIST OF ABBREVIATIONS

BDF	Backward Differentiation Formula
DI	Direct Integration Method
IVPs	Initial Value Problems
MIMD	Multiple Instruction Multiple Data
MPI	Message Passing Interface
MISD	Multiple Instruction Single Data
ODEs	Ordinary Differential Equations
SIMD	Single Instruction Multiple Data
SISD	Single Instruction Single Data
PBI	Partitioning Block Intervalwise
PBC	Partitioning Block Componentwise
NPBDF	Non-Partitioning Backward Differentiation Formula
VSVO	Variable Stepsize Variable Order



TABLE OF CONTENTS

	Page
DEDICATION	ii
ABSTRACT	iii
ABSTRAK	v
ACKNOWLEDGEMENTS	viii
APPROVAL	ix
DECLARATION	xi
LIST OF TABLES	xii
LIST OF FIGURES	xiv
LIST OF ABBREVIATIONS	xvii
 CHAPTER	
I INTRODUCTION	
Objectives of the Thesis	2
Outline of the Thesis	3
II LITERATURE REVIEW	6
III ORDINARY DIFFERENTIAL EQUATIONS AND PARALLEL PROCESSING	
Introduction	10
Linear Multistep Method	13
Stiff Systems	18
Parallel Computing	22
Classification of Computer Architectures	22
Single Instruction Stream, Single Data Stream (SISD)	23
Single Instruction Stream, Multiple Data Stream (SIMD)	24
Multiple Instruction Stream, Single Data Stream (MISD)	24
Multiple Instruction Stream, Multiple Data Stream (MIMD)	25
Types of Parallel Computers	25
Shared Memory Architecture	25
Message-Passing Multicomputer	27
Distributed Shared Memory	31
Performance for Parallel Systems	32
Factors That Influence Performance	34
Parallel Solution of Ordinary Differential Equations	35
High Performance Computer SUNFIRE 1280 Architecture	37



IV	DYNAMIC PARTITIONING SEQUENTIALLY FOR THE SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS.	
	Introduction	39
	Formula Derivations	41
	Adams type formulae	41
	Backward Differentiation Formula (BDF)	43
	Partitioning System of ODE using Nonconvergence	45
	Order Selection	46
	Choosing Step Size	47
	Switching from Nonstiff to Stiff	48
	Partitioning and Effect of Eigenvalues	49
	Partitioning Technique Switching from Stiff to Nonstiff	57
	The Van de Pol Equation	62
	Numerical results when $\mu = 20$	64
	Numerical results when $\mu = 5$	65
	Comments on the Results	68
	Conclusion	71
V	PARTITIONING SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS USING MULTI STEP BLOCK METHOD.	
	Introduction	72
	The 2-Point Block Multistep Method	73
	2-Point Block Method for Solving Nonstiff ODEs	75
	2-Point Block Backward Differentiation Formula (BDF)	77
	Partitioning System of ODEs in Block Method	81
	Partitioning Block Intervalwise (PBI)	82
	Partitioning Block Componentwise (PBC)	83
	Iterations formulae for Partitioning Block Componentwise	86
	Problems tested	92
	Numerical result	94
	Comments on the Results	102
VI	PARALLELIZATION OF INTERVALWISE PARTITIONING BLOCK MULTISTEP METHOD FOR SOLVING LARGE ODEs.	
	Introduction	104
	Parallel Implementation	105
	Matrix Multiplication in Newton-iteration BDF	109
	Matrix Multiplication in MPI	112
	Problems tested	115
	Numerical results	116
	Discussion and Conclusion	131



VII	CONCLUSION	
	Summary	132
	Future Work	134
	BIBLIOGRAPHY	135
	APPENDICES	139
	BIODATA OF THE AUTHOR	154



CHAPTER 1

INTRODUCTION

Historically, differential equations have originated in chemistry, physics, and engineering. More recently they have also risen in models in medicine, biology, anthropology, and various other branches. The problem of determining the motion of a projectile, rocket, satellite or planet, the vibrations of a wire or a membrane, the steady-state flow of a viscoelastic fluid parallel to an infinite plane with uniform suction and the problem of determining the charge or current in an electric circuit are examples of problems which all can be formulated into differential equations. The differential equations that result from applications – particularly those in engineering and the natural sciences – generally cannot be solved by analytical techniques. Hence with the advent of high-speed electronic computers have led to differential equations being solved by numerical methods in which a finite set of points are generated. These set of points are an approximation to the actual solution function, $y(x)$ and these sets are referred to as numerical solution to the problems. The emphasis in numerical method is the development of accurate and efficient techniques to solve specific problems.

The basic approach used to solve ODE problems in numerical method is the algorithm. An algorithm is a complete, well-defined procedure for obtaining a numerical answer to a given mathematical problem. Algorithms are expressed as a



finite number of ordered computational steps. Many techniques of classical mathematics are expressed as algorithms.

In the past years, the fast development in computer industry has enabled many areas in science and engineering to apply numerical methods to solve large mathematical problems in order to increase the computational speed. Initial effort are mainly concentrated in achieving high performance on a single processors, but more recent attempt were focused in additional performance by taking multiprocessor route.

The numerical solution of large ODE systems requires a large amount of computing power. These large problems arise in a wide variety of applications and these include fluid dynamic, radioactive reaction and weather prediction. Users of parallel computing tend to solve the mathematical problems with the desire to obtain faster and more accurate results (Zanariah and Suleiman, 2004).

Objectives of the thesis

The main objective in this thesis is to solve the system of ODEs by,

1. developing a switching technique that will partition into stiff and nonstiff subsystem continuously.
2. integrating the existing block method formulas and develop the switching techniques which partitioned the system of ODEs.
3. parallelizing the partitioned block method.

Initially, the system of ODEs is solved sequentially by dynamic partitioning. In other words, the entire system is treated as nonstiff ODEs and should instability occur the relevant equations are brought into the stiff subsystem. However, should the transient reappear then the relevant equations are brought back to nonstiff subsystem again.

Another strategy is by partitioning and parallelizing a 2-point block method for a system of equation. By using the multistep method, partitioning the system as stiff and nonstiff subsystem allows each steps to solve numerically 2-point for the system of differential equations. In the 2-point block, matrix multiplication operation is required in the Newton iteration and it requires a considerable amount of time. By parallelizing, this operation will make solving using 2-point block much faster.

Outline of the Thesis

In Chapter I, a brief introduction on the applications of numerical methods.

Chapter II, gives a review of all related researches on partitioning, block methods and parallelizing block methods.



In Chapter III, a brief introduction of the numerical solution of ODEs is given. Basic theory of numerical method like convergence and stability are discussed. This chapter also focuses on the fundamental concepts in parallel programming. Basic architecture of Shared Memory, Distributed Memory and Distributed Shared Memory are explained briefly and some basic commands in MPI are also given in this chapter. Included at the end of this chapter are factors that influenced the performance of parallelism.

Solving a differential equation by partitioning dynamically is discussed in Chapter IV by using the variable stepsize variable order (VSVO). A brief explanation of the VSVO is at the beginning of this chapter. Next, strategy to improve and develop the algorithm using the VSVO to solve any oscillatory system are discussed. An example of this system is the van der Pol equation.

A brief explanation on deriving block method using Adams formula and Backward Differentiation Formula, for solving nonstiff and stiff equations are in Chapter V. Then using these formulas, the partitioning algorithms to solve a system of ODEs in block are developed in this chapter. Initially, the system of ODEs is treated as nonstiff and once there is an indication that stiffness has occurred, the whole system is treated as stiff. This algorithm is known as Intervalwise Partitioning. Another type of partitioning is called Componentwise Dynamic Partitioning, where the components that caused stiffness are placed in the stiff subsystem. Numerical

