MULTISCALE LOCALIZED DIFFERENTIAL QUADRATURE IN 2D PARTIAL DIFFERENTIAL EQUATION FOR MECHANICS OF SHAPE MEMORY ALLOYS

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To my beloved family, for your love and support.

To my friends, for your wit, intelligence and guidance in life.

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ABSTRACT

In this research, the applicability of the Multiscale Localized Differential Quadrature (MLDQ) method in two-dimensional shape memory alloy (SMA) model was explored. The MLDQ method was governed in solving several partial differential equations. Besides, the finite difference (FD) method was used to solve some examples of partial differential equations and the solutions obtained were compared with those obtained by MLDQ method in order to show the accuracy of the numerical method. The MLDQ method was developed by increasing the number of grid points in critical region, and approximating the derivatives at the certain selected grid points. This present method together with the fourth-order Runge-Kutta (RK) method has been applied in differential equations such as wave equation and high gradient problems,. The MLDQ method can achieves accurate numerical solutions compared with FD method which is a low order numerical method by using a few number of grid points. The multiscale method was employed at the critical region which can break down the region of interest from coarser into finer grid points. Furthermore, FORTRAN programs were developed based on MLDQ method in solving some problems as above. The shared memory architecture of parallel computing was done by using OpenMP in order to reduce the time taken in simulating the numerical results. Consequently, the results show that the MLDQ method was a good numerical technique in two-dimensional SMA.

ABSTRAK

Dalam kajian ini, kesesuaian kaedah *Multiscal*e Berbeza Kuadratur Setempat (MLDQ) dalam model dua dimensi Aloi Memori Bentuk (SMA) telah diterokai. Kaedah MLDQ telah dibangunkan dalam menyelesaikan beberapa persamaan pembezaan separa. Selain itu, kaedah Perbezaan Terhingga (FD) telah digunakan untuk menyelesaikan beberapa contoh persamaan pembezaan separa dan keputusan yang diperolehi telah dibandingkan dengan keputusan yang diperolehi dari kaedah MLDQ, untuk menunjukkan kejituan kaedah berangka tersebut. Kaedah MLDQ telah dibangunkan dengan memperbanyakkan bilangan titik grid di kawasan kritikal, dan juga menganggarkan terbitan pada titik grid tertentu yang dipilih. Kaedah ini bersama-sama dengan kaedah Runge-Kutta peringkat keempat (RK-4) telah digunakan dalam persamaan pembezaan seperti persamaan gelombang dan masalah kecerunan tinggi. Kaedah MLDQ boleh mencapai penyelesaian yang lebih jitu berbanding dengan kaedah FD yang mempunyai peringkat kejituan yang rendah dengan menggunakan bilangan titik grid yang kecil. Kaedah *multiscale* digunakan di kawasan kritikal kerana mampu memecahkan rantau yang dikehendaki dari titik grid kasar kepada titik grid lebih perinci. Tambahan lagi, program FORTRAN dengan kaedah MLDQ telah dibangunkan untuk menyelesaikan masalah-masalah tersebut di atas. Bagi pengkomputeran selari, seni bina memori perkongsian telah dilaksanakan dengan menggunakan OpenMP bertujuan untuk mengurangkan masa yang diambil dalam simulasi keputusan berangka. Dengan itu, keputusan menunjukkan bahawa kaedah MLDQ adalah teknik berangka yang baik dalam SMA dua dimensi.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF APPENDICES

CHAPTER 1

INTRODUCTION

1.1 Background of Problem

In most of the science and engineering fields, a set of partial differential equations (PDEs), either linear or nonlinear, the solutions to them must be sorted for. Therefore, the numerical computations have attracted considerable attention for solving PDEs problems. There are many available numerical methods used nowadays for solving PDEs, that is, Finite Difference (FD) method, Finite Element (FE) method, Finite Volume (FV) method, Boundary Element (BE) method and others numerical methods. However, many numerical methods have been discussed and applied in the science and engineering areas, the Differential Quadrature (DQ) method is by far the most effective tool available to researchers with interests in numerical computations. The DQ method will be discussed in this study.

The DQ method is more efficient numerical which requires less computational effort and achieves an acceptable and reasonable accuracy for the PDEs. Besides, DQ method is an extension of FD method for the higher order of finite difference scheme. Although DQ method is a numerical technique of high accuracy, but it is sensitive to the number of grid points. Therefore, many researchers have developed new methods to overcome the limitation of the DQ method. A new class of numerical methods for solving the sciences and engineering problems will be discussed in Chapter Two.

Another numerical discretization technique that will be discussed in this study is Localized Differential Quadrature (LDQ) method. According to Zong and Lam (2002), LDQ method is characterized by approximating the derivatives at a grid point using weighted sum of the points in its neighbourhood. This method is used to solve the limitation of the DQ method. Besides, the Runge-Kutta method has been discussed in order to numerically integrate the LDQ numerical system in the time direction.

In this study, parallel programming of shared memory architecture (OpenMP) is introduced in order to reduce the execution time for sequential algorithm in solving the PDEs using LDQ method. Generally, when the number of grid points increase and the simulation time will become longer, this make the whole simulation will become expensive. Therefore, parallel computation technique will be applied in solving PDEs.

Furthermore, Multiscale method is also been discussed in this study. The Multiscale method is a powerful tool for the numerical solution of differential equation which is based on discrezation and subsequent approximation of derivatives by FD formulas. The main idea of Multiscale is to accelerate the convergence of base iterative method by solving a coarse problem. According to Zhu and Cangellaris (2006), the Multiscale method can be applied in combination with any common discretization techniques. Based on the multiscale concept with using various interpolation techniques, in our study, the certain grid point which is out of uniformly distributed grids can be calculated accurately with less computation time. By take into account of the powerful Multiscale approach with LDQ method, we calculate the numerical solution in any point with minimum calculation.

Moreover, in this study, we present our method applied in Shape Memory Alloy (SMA) problems. SMA are novel and special materials which have the ability to return to predetermined shape when heated above a certain transition temperature. Constitutive modelling of SMA has been an interest research subject from 1980s until now. There are many researchers used the various numerical methods in the numerical simulation of SMA problems. Therefore, we present our method applied in simple SMA model to achieve a good numerical solution.

1.2 Statement of the Problem

There are many available numerical methods used to approximate the solution of diffusion equation and wave equation. A set of initial and boundary conditions are needed to solve these equations. Although the DQ method has been applied successfully to a variety of science and engineering problems, however, this method possesses several undesirable limitations and drawbacks. As an example, the total of grid points used in DQ method is limited due to the ill-conditioned matrix form. Besides, asymmetry of the final solution matrix produced by the DQ method makes the solution procedure to be inefficient. Due to overcome this drawback of the DQ method, many researchers have developed and improved new DQ methods. In this study, the Multiscale Localized Differential Quadrature (MLDQ) method is applied in solving the boundary value problems, and also to overcome the limitation of the DQ method. Finally, parallel programming with shared memory architecture using OpenMP is implemented in order to reduce the execution time of FORTRAN program developed in this study.

1.3 Objectives of the Study

The objectives of this research are summarized as:

i. To govern MLDQ method in solving wave equation, diffusion equation and high gradient problem.
ii. To compare the MLDQ method with FD method in terms of their accuracy and convergence study of numerical solution in solving wave equation, diffusion equation and high gradient problem.
iii. To govern MLDQ method in the numerical simulation of SMA model.
iv. To develop FORTRAN program codes based on MLDQ method in solving wave equation, diffusion equation, high gradient problem and SMA problem.
v. To parallelize FORTRAN program codes using OpenMP language for LDQ method and MLDQ method in solving boundary value problems.

1.4 Scope of the Study

In this research, the basic concept of DQ, LDQ and multiscale methods will be discussed, and also, understanding these numerical discretization techniques' application in solving boundary value problems. Another scope of the study will be focused on solving the two dimensional wave equation and two dimensional high gradient problem. The Runge-Kutta (RK) method will be utilized in MLDQ method to numerically integrate it in time direction. Furthermore, FORTRAN program codes will be developed and parallelized by using share memory architecture, that is, OpenMP for LDQ method in solving boundary value problems. The limitation of parallel programming in this study is four cores will be used. In this research, the multi-core computer Intel® Core™ i5 CPU M460 @2.53GHz is used to do the programming. The data of the programming is reasonable for four processors to run. Besides, the MLDQ method will also be implemented in the numerical simulation of SMA problem.

1.5 Significance of the Study

In this research, MLDQ method will be discussed and applied to boundary value problems. This research is important to overcome the limitations and drawbacks of the DQ method. Besides, this method also is applied in SMA problem. Next, the FORTRAN program codes for the LDQ method will be developed in convenience of checking the performances of the numerical methods. Furthermore, the OpenMP language is used to parallelize the FORTRAN program codes in order to reduce the execution time.

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