UNIVERSITI PUTRA MALAYSIA

APPLICATION OF HIGHER ORDER COMPACT FINITE DIFFERENCE METHODS TO PROBLEMS IN FLUID DYNAMICS

YAP WEN JIUN

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

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To beloved Chen Wai,

my dad, my mum,

Wen Lih and Wen Shan

whose love and support is overwhelming

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfillment of the requirements for the degree of Master of Science

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Chairman : Associate Professor Waqar Asrar, Ph.D.

Faculty : Engineering

Finite difference schemes used in the field of computational fluid dynamics is generally only of second-order accurate in representing the spatial derivatives. Numerical algorithms based on higher order finite difference schemes that can achieve fourth-order accuracy in space have been developed. Higher order schemes will enable a larger grid size with fewer grid points to sufficiently give fine results. A compact scheme, which preserves the smaller stencil size, is preferred due to its simplicity and computational efficiency, as opposed to the normal approach to expand the stencil to achieve higher accuracy. Two approaches are used to obtain the fourth-order accurate compact scheme. In Lax-Wendroff approach, the governing differential equations are used to approximate the leading truncation error in the second-order central difference of the governing equations. In Hermitian scheme, the fourth-order approximations to the derivatives are treated as unknowns. These unknowns are solved explicitly with Hermitian relations that relate the variables and its spatial derivatives. The numerical algorithms are first developed for viscous Burgers' equation on uniform and clustered grids. The fourth-order accuracy and

convergence rate is demonstrated. The performance of the two different approaches are compared and found on par with each other. Second, the numerical algorithms are used to solve the quasi-one-dimensional subsonic-supersonic nozzle flow. The Hermitian scheme shows excellent agreement with the analytical result but the Lax-Wendroff approach failed to do so due to instability problem. Third, only the numerical algorithm based on Hermitian scheme is used to solve the flow past a backward-facing step. The reattachment lengths of the first separation bubble compare favourably with previously published results in the literature. The success of the fourth-order compact finite difference schemes in solving the viscous Burgers' equation is not repeated in the isentropic nozzle flow and the flow past a backward-facing step. Further efforts have to be made to improve the convergence rate of the numerical solution of the isentropic nozzle flow using the Hermitian scheme and to overcome the instability in the numerical solution of the same problem using the Lax-Wendroff approach.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Master Sains

APPLIKASI KAEDAH-KAEDAH BEZA TERHINGGA PADAT TERTIB LEBIH TINGGI KEPADA MASALAH-MASALAH DINAMIK BENDALIR

Oleh

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Skim-skim beza terhingga yang digunakan di dalam bidang dinamik bendalir pengiraan biasanya hanya mempunyai kejituan tertib kedua untuk mewakili terbitan-terbitan ruangan. Algoritma-algoritma berangka berdasarkan skim-skim beza terhingga tertib lebih tinggi yang dapat mencapai kejituan tertib keempat dalam ruangan telah dibina. Skim-skim tertib lebih tinggi membolehkan grid yang lebih besar dengan bilangan grid yang kurang cukup untuk memberikan keputusan yang baik. Skim padat yang mengekalkan saiz stensil yang kecil lebih disukai kerana keringkasannya dan kecekapannya dalam pengiraan, ini berlawan dengan pendekatan biasa yang mengembangkan stensil untuk mencapai kejituan yang lebih tinggi. Dua pendekatan digunakan untuk memperolehi skim padat kejituan tertib keempat. Dalam pendekatan Lax-Wendroff, persamaan-persamaan pembezaan penentu digunakan untuk menghampiri ralat pemangkasan terdepan dalam perbezaan terhingga pusat tertib kedua persamaan-persamaan tersebut. Dalam skim Hermitian, penghampiran-penghampiran tertib keempat kepada terbitan-terbitan dianggap sebagai anu-anu. Anu-anu ini diselesaikan secara tak-tersirat dengan hubungan-hubungan Hermitian yang mengaitkan pembolehubah-pembolehubah dengan

terbitan-terbitan ruangan mereka. Algoritma-algoritma berangka dibina dahulu untuk persamaan Burgers likat di atas grid seragam dan berkelompok. Kejituan dan kadar penumpuan tertib keempat telah dipertunjukkan. Kebolehan kedua-dua pendekatan telah dibandingkan dan mereka didapati setanding dengan satu sama yang lain. Kedua, algoritma-algoritma berangka digunakan untuk menyelesaikan aliran muncung subsonik-supersonik mirip satu-matra. Skim Hermitian mempamerkan persetujuan baik dengan keputusan beranalisis tetapi pendekatan Lax-Wendroff gagal untuk berbuat demikian disebabkan masalah ketakstabilan. Ketiga, hanya algoritma berangka yang berdasarkan skim Hermitian digunakan untuk menyelesaikan aliran melalui tangga berhadapan belakang. Jarak pencantuman semula buih perpisahan pertama bersetuju dengan baiknya dengan keputusan di dalam rujukan sebelum ini. Kejayaan skim beza terhingga padat tertib keempat di dalam penyelesaian berangka persamaan Burgers likat tidak dapat diulangi di dalam aliran muncung subsonic-supersonik isentropik dan aliran melalui tangga berhadapan belakang. Usaha lanjutan perlu dilakukan untuk meningkatkan kadar penumpuan bagi penyelesaian berangka aliran muncung isentropik menggunakan skim Hermitian dan mengatasi masalah ketakstabilan dalam penyelesaian berangka bagi masalah yang sama menggunakan pendekatan Lax-Wendroff.

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I certify that an Examination Committee met on 21 February 2003 to conduct the final examination of Yap Wen Jiun on his Master of Science thesis entitled "Application of Higher Order Compact Finite Difference Methods to Problems in Fluid Dynamics" 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:

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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.

YAP WEN JIUN

Date: 1/4/2003

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LIST OF ABBREVIATIONS

ADI	Alternating-Direction-Implicit
CDS	Central Difference Scheme
CFL	Courant-Friedrichs-Lewy
ENO	Essentially Non-Oscillatory
Eq	Equation
FE	Forward Euler
Fig	Figure
KFVS	Kinetic Flux Vector Splitting
MUSCL	Monotone Upstream-centered Schemes for Conservation Laws
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
Re	Reynolds number
SSP	Strong Stability Preserving
SSPRK	Strong Stability Preserving Runge-Kutta
TV	Total Variation
TVD	Total Variation Diminishing
WENO	Weighted Essentially Non-Oscillatory

CHAPTER 1

INTRODUCTION

The advent of the high-speed computers combined with the development of accurate numerical algorithms for solving physical fluid flow problems on these computers have revolutionized the way fluid dynamics is studied and practiced today. The governing equations for the engineering design of fluid flow and thermal systems, namely the Navier-Stokes equations, are too complex to be solved analytically except in some trivial cases. Finite difference methods have long been used to approximate the solution of these partial differential equations (PDEs), in which the domain of interest is discretized into a structured mesh of nodes and derivatives are approximated by difference quotients.

The common finite difference schemes generally are only up to second-order accurate in discretizing spatial derivatives. In many problems the accuracy of a second-order method is not sufficient and it is best to use a higher order method. A higher order method also allows fewer grids with a larger grid size to sufficiently give reasonably good results. In classical finite difference approximations, the higher the approximation, the higher the number of discretization grid points involved. Classical fourth-order finite difference method leads to an algebraic system with a pentadiagonal matrix, as opposed to a tridiagonal matrix used in a second-order method. Problems with pentadiagonal matrix are more expensive to solve and difficulties usually appear in implementing boundary conditions.

Higher order compact schemes have attracted much attention in recent years due to their narrow grid stencil and a possible enhanced accuracy over the non-compact schemes. Compact schemes only utilize a patch of grid points immediately surrounding a given grid point to form the fourth-order finite difference schemes and therefore have a better computational efficiency. Different approaches for higher order compact finite difference schemes have been proposed. Two of these approaches are considered in present study, the Lax-Wendroff approach and the Hermitian scheme. These higher order compact finite difference schemes will be implemented in some model problems in fluid dynamics. The numerical solutions will be examined to evaluate the potential of such higher order compact methods in computational fluid dynamics.

The objectives of the current research are:

1. To develop numerical algorithms to solve problems in fluid dynamics utilizing higher order finite difference schemes with superior accuracy and reasonable computational efficiency.
2. To compare the numerical solutions using the higher order finite difference schemes with the standard second order central difference schemes in terms of accuracy and convergence rate.

Chapter 2 provides the literature review on higher order schemes. Chapter 3 discusses the basics of the Lax-Wendroff and Hermitian fourth-order compact finite difference scheme. The time integration used in this study, the optimal Strong Stability Preserving Runge-Kutta (SSPRK) scheme is also discussed in this chapter. In Chapter 4 the numerical algorithms are developed to solve a popular one-

dimensional model problem, the viscous Burger's equation. There are a number of numerical studies done on this problem. Chapter 5 deals with quasi-one-dimensional isentropic nozzle flow and Chapter 6 deals with the two-dimensional flow over a backward-facing step enclosed in a channel. Chapter 7 provides the conclusion on the fourth-order compact schemes and some recommendations for further study.

The following list of contributions is a description of the original works presented in this thesis. First, a non-uniform grid is utilized in the numerical solution of the viscous Burgers' equation using the fourth-order compact schemes. Second, the numerical solution of the viscous Burgers' equation in a large domain is obtained. Third, a conclusion that low-order boundary conditions in fourth-order compact schemes lead to a poor numerical solution is drawn based on the numerical solution of the flow in a convergent-divergent nozzle. Finally, the fluid dynamics problem of flow past a backward-facing step is solved using the Hermitian scheme via the incompressible Navier-Stokes equations in the primitive variables with the artificial compressibility approach. These research works is hoped to contribute to the further development of higher order compact finite difference schemes.

CHAPTER 2

LITERATURE REVIEWS

Numerical experiments with a class of fourth-order accurate compact schemes were conducted by Hirsh [1]. The idea behind his scheme was proposed by Kriess, as documented in [2]. The original method was used in a hyperbolic problem and Ciment and Leventhal [3] applied this method to such problem. Hirsh [1] applied this fourth-order compact scheme to parabolic problems and discussed several of the test problems with different boundary conditions. The fundamental idea behind this scheme is that the approximations to the derivatives are treated as unknown variables at each point of the computational grid. Thus, for a second-order differential equation, a system of two high-order relations, known as Hermitian relations [4] are used to evaluate the derivatives. The advantage of the scheme is that it produces a tridiagonal matrix for all the unknowns. The stability properties of the scheme are studied by Hirsh [1] using a linearized model problem.

Adam [4] has proposed two different techniques to eliminate the second-order derivatives in parabolic equations using the same approach as Hirsh to produce a fourth-order compact scheme. This is done either implicitly by using the governing equation or explicitly by using another compact relation between the first and the second derivatives. Adam [4] has derived additional boundary relations to solve the tri-diagonal system of equations. These relations yield third-order accuracy near the boundary of the computational grid, which is compatible with the fourth-order accuracy at the inner points. This scheme requires less computational effort than that of Hirsh [1] for the same accuracy.

Lele [5] has presented a more generalized form of the Hermitian scheme and introduced the idea of resolution efficiency as a measure of accuracy. Lele [5] provided compact schemes for the first and the second order derivatives on a cell-centered mesh, and has shown that such scheme has better resolution efficiency. Lele [5] discussed the aliasing errors, boundary condition approximations, assessment of boundary condition errors and the stability restrictions of his compact schemes. Wilson *et al.* [6] has used the higher order compact schemes presented by Lele [5] to solve one and two-dimensional convection equation as well as Euler equations for temporally-developing plane mixing layer and two-dimensional viscous wave decay. The continuity equation is enforced through the solution of the Poisson equation for pressure in Wilson *et al.* [6].

Rubin and Khosla [7] have presented a sixth-order compact Hermitian technique. They also developed higher order compact procedures on non-uniform grids derived from polynomial spline interpolation combined with Hermitian-type finite difference discretization. Another hybrid scheme using two polynomial approximations for the first and second derivatives was discussed. This scheme leads to a non-uniform-grid extension of the Pade's difference technique. Appropriate boundary conditions for all the procedures were derived. They showed that the spline procedure has the smallest truncation error among the fourth-order techniques they studied. A remarkable feature of the spline technique is that it requires one-quarter of the number of grid points as that of a central difference scheme of equal accuracy. The procedures derived were applied to boundary layer equations and the driven cavity problem.

Goedheer and Potters [8] have presented a Hermitian approach of fourth-order compact finite difference scheme for second order differential equations with a non-uniform grid. Schemes underlying the Hermitian approach have also been utilized by Cockburn and Shu [9] who have developed compact schemes for computations of flows with shocks. Following the ideas from Total Variation Diminishing (TVD) method, they introduced a local mean that serves as a reference for using a local nonlinear limiter to control spurious numerical oscillations. They used a TVD-type Runge-Kutta time discretization which is proven to be stable under certain restrictions on the time step. Numerical results are presented for hyperbolic equations.

Mackinnon and Johnson [10] use a different approach to obtain a fourth-order accurate formulation. Convection-diffusion equations with variable coefficient are considered in their study. Choo and Schultz [11] independently use the same approach as Mackinnon and Johnson [10] to solve the heated cavity problem. They all use a formulation procedure similar to Dukowicz and Ramshaw [12]. This higher order compact finite difference scheme is based on the ideas first used by Lax and Wendroff [13] to increase the accuracy of time dependent schemes for hyperbolic problem. Lax and Wendroff [13] used the original governing equation, which is a partial differential equation, to approximate the second-order time derivative in the Taylor series expansion, thus raising the method from first-order to second-order. This idea has been extended and developed for spatial problems by Mackinnon and Carey [14], Abarbanel and Kumar [15] and later by Spotz and Carey [16], Spotz [17], Asrar *et al.* [18] and Asrar *et al.* [19]. In this approach the governing equation is utilized to approximate the leading truncation error terms of the standard second-

order central difference scheme. The governing equation is differentiated compactly and the resultant relations are included in the finite difference formulation. Wong and Raithby [20] and Gupta *et al.* [21] have also derived schemes similar to this although in a different manner. Gupta *et al.* [21] have used the scheme to solve two-dimensional constant and variable coefficient convection-diffusion equation, and showed numerically that the scheme is both highly accurate and computationally efficient.

Rai and Moin [22] showed that upwind-bias schemes are very robust even when they are made high-order accurate. They used a spatially fifth-order upwind finite-difference scheme using an upwind-bias stencil for the Navier-Stokes equations. Tolstykh [23] proposed a fifth-order compact upwind scheme for moisture transport equation in atmosphere. Christie [24] proposed a fourth-order compact upwind scheme because the standard central compact schemes break down in convection dominated problems. Zingg *et al.* [25] tested the accuracy of a fifth-order explicit upwind finite-difference scheme with built-in filtering terms in a central grid stencil for linear wave propagation problems. Adams and Shariff [26] proposed fifth-order upwind compact schemes with spectral-like resolution using central grid stencils for the direct numerical simulation of shock-turbulence interaction. Zhong [27] has presented a family of upwind compact and explicit finite-difference schemes of third, fifth, and seventh-order and their stable high-order boundary schemes for the direct numerical simulation of hypersonic boundary-layer transition. These upwind schemes are similar to the upwind schemes of Zingg *et al.* [25] and those of Adams and Shariff [26].

Ravichandran [27] has used high-order compact upwind difference schemes together with the split fluxes of the Kinetic Flux Vector Splitting (KFVS) scheme to obtain high-order semi-discretizations of the two-dimensional Euler equations. A TVD multistage Runge-Kutta time stepping scheme is then used to compute steady states for transonic and supersonic flow problems. Fu and Ma [28] have presented a high-order difference scheme for compressible flows with shocks. This scheme used a fifth-order upwind compact difference relation for the convective terms, a sixth-order symmetric compact difference scheme for the viscous terms and a three-stage Runge-Kutta method for advance in time. They analyzed the reason for numerical oscillations and observed that it is due to non-uniform group velocity of wave packets. They proposed a method for controlling the group velocity and hence better shock resolution and elimination of spurious oscillations.

Yanwen *et al.* [29] developed a numerical scheme for the solution of incompressible Navier-Stokes equations utilizing a fifth-order accurate compact upwind scheme for the convection terms and a sixth-order accurate symmetrical compact difference scheme for the viscous terms on a staggered mesh. The continuity and the pressure gradient in the momentum equations are discretized using a fourth-order cell-centered difference approximation. Time integration is performed using a three-stage Runge-Kutta method. Wilkes [30] has also developed a high-order scheme based on upwind differencing and has used this scheme to solve elliptic flow problems.

Deng and Maekawa [31] have developed cell-centered compact high-order nonlinear schemes for shock-capturing. They have used compact adaptive interpolations of variables at cell edges to eliminate spurious numerical oscillations. This technique,