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Computational Fluid Dynamics Based on the Unified Coordinates

Wai-How Hui Kun Xu

(统一坐标系下的计算流体力学方法)

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Preface to the Series in Information and Computational Science

Since the 1970s, Science Press has published more than thirty volumes in its series Monographs in Computational Methods. This series was established and led by the late academician, Feng Kang, the founding director of the Computing Center of the Chinese Academy of Sciences. The monograph series has provided timely information of the frontier directions and latest research results in computational mathematics. It has had great impact on young scientists and the entire research community, and has played a very important role in the development of computational mathematics in China.

To cope with these new scientific developments, the Ministry of Education of the People's Republic of China in 1998 combined several subjects, such as computational mathematics, numerical algorithms, information science, and operations research and optimal control, into a new discipline called Information and Computational Science. As a result, Science Press also reorganized the editorial board of the monograph series and changed its name to Series in Information and Computational Science. The first editorial board meeting was held in Beijing in September 2004, and it discussed the new objectives, and the directions and contents of the new monograph series.

The aim of the new series is to present the state of the art in Information and Computational Science to senior undergraduate and graduate students, as well as to scientists working in these fields. Hence, the series will provide concrete and systematic expositions of the advances in information and computational science, encompassing also related interdisciplinary developments.

I would like to thank the previous editorial board members and assistants, and all the mathematicians who have contributed significantly to the monograph series on Computational Methods. As a result of their contributions the monograph series achieved an outstanding reputation in the community. I sincerely wish that we will extend this support to the new Series in Information and Computational Science, so that the new series can equally enhance the scientific development in information and computational science in this century.

Shi Zhongci

2005.7

Preface

Computational fluid dynamics (CFD) uses large scale numerical computation to solve problems of fluid flow. It has been known since its onset that the numerical solution to a given flow depends on the relation between the flow and the coordinates (mesh) used to compute it. Each of the two well-known coordinate systems for describing fluid flow—Eulerian and Lagrangian—has advantages as well as drawbacks. Eulerian method is relatively simple, but its drawbacks are: ① it smears contact discontinuities badly; ② it needs generating a body-fitted mesh prior to computing flow past a body. Lagrangian method, by contrast, resolves contact discontinuities (including material interfaces and free surfaces) sharply, but it also has drawbacks: ① the gas dynamics equations could not be written in conservation partial differential equations (PDE) form, rendering numerical computation complicated; ② it breaks down due to cell deformation.

A fundamental issue in CFD is, therefore, the role of coordinates and, in particular, the search for "optimal" coordinates. It is in the long search for an optimal coordinate system that a unified coordinate (UC) system was developed by the first author and his collaborators over the last decade. While the search for an optimal coordinate system in CFD would undoubtedly continue, the unified coordinate system developed so far is found to combine the advantages of both Eulerian and Lagrangian system, while avoiding their drawbacks. Indeed, it goes beyond these. For instance, the UC system provides a foundation for automatic mesh generation by the flow being computed.

This monograph first reviews the relative advantages and drawbacks of Eulerian and Lagrangian coordinates as well as the Arbitrary-Lagrangian-Eulerian (ALE) and various moving mesh methods in CFD for one- and multi-dimensional flow. It then systematically introduces the unified coordinate approach to CFD, illustrated with numerous examples and comparisons to clarify its relation with existing approaches.

The content of this monograph is based on a graduate course taught by the first

author from 2000 to 2007 at the Hong Kong University of Science and Technology, Academia Sinica in Taiwan, Hong Kong Polytechnic University and Hong Kong Baptist University, and by the second author since 2009. We thank Prof. T. Tang for his comments on the first draft of the book. We also acknowledge the permission of Communication in Computational Physics (CiCP) for allowing us to use the material presented in a review paper①.

Many scientists have made substantial contributions in the course of development of the UC approach to CFD. Here is a partial list: Chien-Cheng Chang, De-Lin Chu, Bo Gao, Yuan-Ping He, Jeu-Jiun Hu, Changqiu Jin, Sergei Kudriakov, Chih-Yu Kuo, Claude Lepage, Zuo-Wu Li, Ping-Yiu Li, Meng-Sing Liou, Ching Yuen Loh, Yang-Yao Niu, Keh-Ming Shyue, Ronald Ming Cho So, Yih-Chin Tai, Henry Van Roessel, Zi-Niu Wu, Jaw-Yen Yang, Gui-Ping Zhao, Yanchun Zhao. Without their valuable contributions, the UC approach to CFD could not have reached its current state of maturity. We also thank our secretary Odissa Wong for her help for many years in editing and preparing the figures. We give special thanks to our wives, Kwok Lan Hui and Jie Shen, for their strong support to us in writing this monograph.

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December 1, 2011

① The unified coordinate system in computational fluid dynamics. *Communications in Computational Physics*, 2: 577-610, 2007.

Contents

Chapter 1

Introduction

1.1 CFD as Numerical Solution to Nonlinear Hyperbolic PDEs

The great majority of research work in CFD, especially those in the first several decades, treats it as numerical solution to nonlinear hyperbolic partial differential equations (PDEs). For a good summary, see Hirsch[1]. Most part of this monograph also treats CFD as numerical solution to nonlinear hyperbolic PDEs. But it is concerned mainly about the role of coordinates in CFD and, in particular, will base all CFD study on the newly discovered unified coordinates. To put it in perspective we shall first give an overview of the major developments of CFD as numerical solution to the initial value problem of nonlinear hyperbolic PDEs as follows.

The theoretical foundation for nonlinear hyperbolic PDEs was laid by Riemann in his pioneering work[2] where he introduced the concept of Riemann invariants and posed the special initial value problem—since has been known as the Riemann problem. It turns out that the Riemann problem plays a central role in most numerical methods in CFD.

Nothing very significant happened during the following six decades until Richardson proposed weather prediction by numerical process (Lewis Fry Richardson, Cambridge University Press, 1922). Even without an electronic computer, wanting to find numerical solutions to nonlinear hyperbolic PDEs immediately raises many interesting theoretical and practical questions, and progresses are made in answering them.

(1) The first of these is the discovery of the CFL condition[3]. It simply says that in a time-marching process to find a numerical solution, marching too fast causes numerical instability and destroys the solution.

(2) Practical methods for computing solutions with shock discontinuities are developed: the artificial viscosity method of von Neumann and Richtmyer which smears shock discontinuities[4]; the Godunov method which reduces the general initial value problem to a sequence of Riemann problems with cell-averaging data[5]; the Glimm random choice method which also reduces the general initial value problem to a sequence of Riemann problems but with data of randomly chosen representative states[6, 7]; and the shock-fitting (front tracking) method[8]. The last two methods are not easily extended to the three-dimensional flow.

(3) A very important discovery was made by Lax and Wendroff[9] that in order to numerically capture shock discontinuities correctly, the governing PDE should be written in conservation form to begin with. This is easily done in Eulerian coordinates (in any dimensions) and also for one-dimensional flow in Lagrangian coordinates. But for a long time, it was not known how to use Lagrangian coordinates to write the governing PDEs for multidimensional flows in conservation form. This problem was solved by Hui et al.[10].

(4) To extend Godunov's method to higher order accuracy, the important concepts of limiters and TVD were introduced which avoid non-physical oscillations in high resolution schemes[11, 12].

(5) From the onset of CFD, it was known that the numerical solution to a given flow depends on the coordinates (mesh) used to compute it; hence great efforts have been devoted to search for the optimum coordinate system: the Particle-in-Cell method[13]; the Arbitrary-Lagrangian-Eulerian method[14]; various moving mesh methods[15]; and the unified coordinate method[10].

(6) Finally, to compute a flow past a body, which is the central problem in fluid dynamics, it is necessary to construct a body-fitted mesh prior to computing the flow. Even after decades of research, mesh-generation remains tedious and time-consuming. The unified coordinate approach to CFD has opened up a way of automatic mesh-generation[16].

1.2 Role of Coordinates in CFD

1.2.1 Theoretical Issues

For more than 200 years, two famous coordinate systems have existed for describing fluid flow: Eulerian system is fixed in space, whereas Lagrangian system follows the fluid. An immediate question arises:

"*Are these two coordinate systems equivalent to each other theoretically?*"

This question must have been asked by numerous researchers in fluid dynamics (FD), and the answer presumably was positive. Surprisingly, the first mathematical proof of equivalency, meaning the existence of a one-to-one map between the two sets of weak solutions obtained by using the two systems, was given as late as 1987 by Wagner[17] and holds only for one-dimensional flow①. For 2-D and 3-D flows, Hui et al.[10, 18] showed that they are *not equivalent* to each other theoretically (see Section 8.3).

Although Lagrangian and Eulerian approaches to FD are each self-contained and general, prior to the advent of computer most text books [19−22] are written in Eulerian coordinates, with the exception of [23], which is devoted solely to Lagrangian approach. There are at least two reasons for this historical bias.

Firstly, steady flow is the most important class of flow in application of FD, and Eulerian coordinate system has a clear advantage in describing it: the time variable drops out, reducing the number of independent variables from 4 to 3. This greatly simplifies the mathematics of the governing equations. By contrast, the time variable in Lagrangian coordinates is essential and cannot disappear, so apparently we still need 4 independent variables for three-dimensional flow even when the flow is steady. Of course, one might argue that among the 4 apparent independent variables, there must be a relation expressing the steadiness of the flow. Indeed, such a relation does exist, see Eq.(20) in [24], but it is solution-dependent; hence without knowing the flow solution it is difficult to use the relation to reduce the number of independent variables from 4 to 3. On the other hand, when the flow solution is known there is no need to use that relation. This is the dilemma of Lagrangian approach for steady flow: the governing equations of FD in Lagrangian coordinates do not simplify as Eulerian coordinates do, and steady flow has to be obtained by solving the unsteady flow equations. This dilemma was resolved in [25−27] when the Lagrangian time variable was introduced which played the dual role as time and as a Lagrangian label (see also the variable λ in (9.4) when $h = 1$).

Secondly, in the problem of flow past a body, which is the central problem

① In the presence of a vacuum, the definition of weak solution for the Lagrangian equations must be strengthened to admit test functions which are discontinuous at the vacuum.

in FD, very often one is interested only in the flow quantities on the body surface, e.g., pressure, temperature, velocity and shear stresses on the airfoil surface. Eulerian approach naturally and easily produces these quantities. By contrast, in Lagrangian approach, we need to calculate the motion histories of all fluid particles and then trace them back to find the flow quantities on the body surface. This is quite cumbersome.

With the advent of computer and the birth of computational fluid dynamics, the advantages and drawbacks of Eulerian and Lagrangian approach need be critically re-examined from the computational point of view.

1.2.2 Computational Issues

Computationally, Eulerian and Lagrangian systems are not equivalent even for 1-D flow. Indeed, it has been known since the onset of CFD that the numerical solution to a given flow depends on the relation between the flow and the coordinates used to compute it. For 1-D flow, we shall show in Chapter 4 that Lagrangian system is superior to the Eulerian and, in turn, the UC (i.e., the generalized Lagrangian plus shock-adaptive Godunov scheme) is superior to both the Lagrangian and the Eulerian, and is completely satisfactory.

The situation for 2-D and 3-D flow is more complicated. Each of the two well-known coordinate systems for describing fluid flow has advantages as well as drawbacks. Eulerian method is relatively simple, but its drawbacks are: ① it smears contact discontinuities badly; ② it needs generating a body-fitted mesh prior to computing flow past a body. Lagrangian method, by contrast, resolves contact discontinuities (including material interfaces and free surfaces) sharply, but it also has drawbacks: ① the gas dynamics equations could not be written in conservation partial differential equations (PDE) form, rendering numerical computation complicated; ② it breaks down due to cell deformation.

A fundamental issue in CFD is, therefore, the role of coordinates and, in particular, the search for "optimal" coordinates. The search for optimal coordinates has led to the development of the unified coordinate (UC) system[28], in a series papers beginning with [25–27]. See also [29–33]. This monograph first reviews the relative advantages and drawbacks of Eulerian and Lagrangian coordinates in CFD for 1-D and multi-dimensional flow, and then systematically discusses the unified coordinate system and its applications.

For 1-D flow, UC uses a material coordinate and also applies the shock-adaptive Godunov scheme [34–36] instead of the classical Godunov scheme[5]. For 2-D flow, it uses one material coordinate, with the other coordinate determined so as to preserve mesh othorgonality (or preserve the Jacobian), whereas for 3-D flow, it uses two material coordinates, with the third one determined so as to preserve mesh skewness (or preserve the Jacobian). The unified coordinate system may be regarded as a generalization of Lagrangian system. It combines the advantages of both Eulerian and Lagrangian system while avoiding their drawbacks. The UC formulation also provides a foundation for automatic mesh-generation by the flow being computed. It may also be regarded as a moving mesh method in that the mesh can move in any manner, while the effects of its movement on the flow are fully accounted for.

1.3 Outline of the Book

This book is arranged as follows: Derivation of the equations of physical conservation laws are given in Chapter 2. Chapter 3 reviews shock-capturing methods for 1-D flow based on Eulerian coordinates, pointing out their defects. Although most of the materials in Chapters 2 and 3 can be found in existing texts, e.g., Ref. [1, 37–39], they are included here to give a smooth introduction to the main theme of this monograph and also to make it self-contained. Chapter 4 introduces UC method for 1-D flow and shows how all defects of Eulerian and Lagrangian computation are cured or avoided by UC. Chapter 5 comments on the difficulties encountered in current computational methods for the general case of multi-dimensional unsteady flow. Chapter 6 gives the unified coordinates formulation of CFD for multi-dimensional unsteady flow, whose mathematical properties are studied in Chapter 7. Chapter 8 is devoted to the very important special case of Lagrangian gas dynamics. Chapter 9 uses UC to study the simpler problem of steady 2-D supersonic flow, showing that it can be solved essentially as 1-D unsteady flow. 3-D steady supersonic flow is also discussed. Chapter 10 discusses the general case of unsteady flow computation using UC, illustrated with typical examples and comparisons with existing methods. Chapter 11 discusses viscous flow computation. Chapter 12 is devoted to the applications of the unified coordinates to kinetic theory. Finally, a summary of the book is given in Chapter 13.

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