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Direct Modeling for Computational Fluid Dynamics

Construction and Application of Unified Gas-Kinetic Schemes

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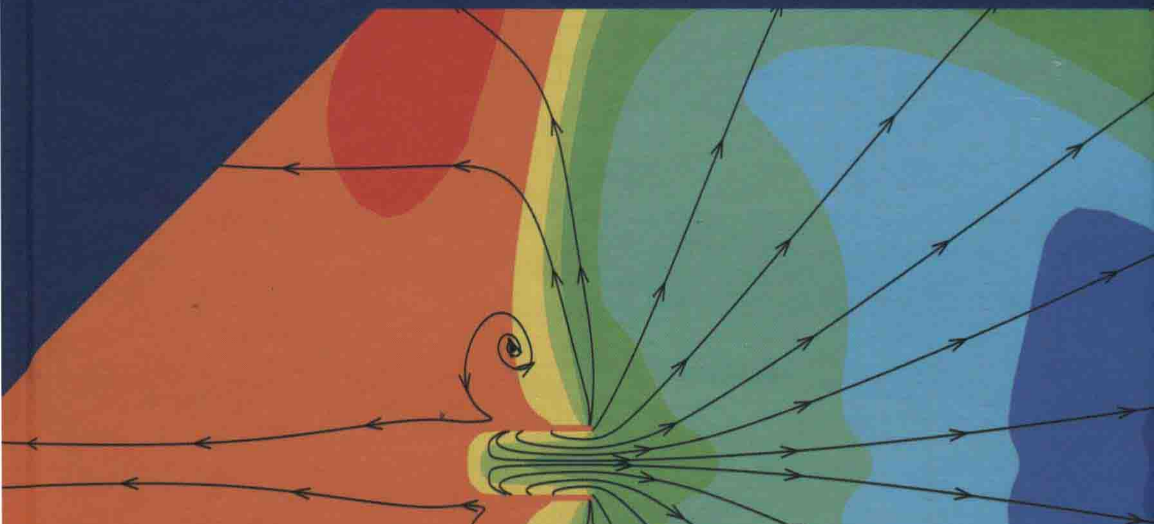

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Direct Modeling for Computational Fluid Dynamics

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Advances in Computational Fluid Dynamics

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The author would like to devote this book to Prof. T.D. Lee of Columbia University who initiated CUSPEA program for many Chinese students to continue their study aboard in 1980s.

Preface

The current Computational Fluid Dynamics (CFD) focuses mainly on the numerical solution of partial differential equations (PDEs). The aim of the CFD is to get the exact solution of the governing equations. Besides introducing the so-called numerical errors, it seems that the numerical mesh size has no any positive dynamic contribution on the solution. As the mesh size and time step go to zero, the CFD algorithm is supposed to converge to the exact solution of the equations, and the limited mesh size is associated with truncation errors only. This CFD principle is based on the belief of the fluid dynamic equations, and makes the equivalence between the fluid dynamics and the equations. Instead of numerical PDE, we propose that the CFD algorithm may be a direct flow modeling in a discretized space, which identifies the flow physics on the scales of mesh size and time step. In other words, the CFD algorithm is to construct discrete numerical governing equations in a space with limited resolution. This monograph will present such a direct modeling principle for CFD algorithm development, and the construction of unified gas-kinetic scheme under such a principle for the flow simulation in all flow regimes.

All fluid dynamic equations have their intrinsic valid modeling scales, such as the mean free path scale of the Boltzmann equation and the hydrodynamic scale of the Navier-Stokes equations. The lost information in the hydrodynamic scale is partially supplied with the modeling of constitutive relationship, which is related to the kinetic scale physics. The current CFD methodology targets on the equations and has no account on the physical modeling scales of these equations anymore. Even with limited mesh size, the CFD is to recover the solution of the PDEs as the mesh size and time step approaching to zero. Under such a CFD practice, the best result is to luckily get the exact solution of the governing equations. But, the flow physics described by the CFD solution is still limited by the modeling scale of the original governing equations. In reality, due to the limited cell resolution, we could never get the exact solution of the original governing equations due to the truncation error. Theoretically, we never know what is the exact underlying governing equation of the CFD algorithm, especially in the cases with unresolved "discontinuities". Therefore, there is NO unique solution when using the approach of numerical PDEs. That is probably the reason why there are so many CFD algorithms for the same PDEs, such as the gigantic amount of approximate Riemann solvers for the Euler equations. The above CFD practice also prevents us from developing multiple scale method if there is no such a governing equation, which is valid in all scales. For example, for the flow around a re-entry air vehicle in near space, the mesh size can vary significantly with respect to the local particle mean free path. There is no such a well-defined governing equation with a continuum variation of modeling scale. Many literatures may claim that the Boltzmann equation is valid in all flow regimes from free molecular to the continuum Navier-Stokes solution. This statement is based on the assumption of fully resolving the mean free path scale physics of the Boltzmann equation everywhere even in the continuum flow regime. It is more or less a statement of brutal force, which cannot be affordable in a real computation. If it were necessary to resolve up to the smallest scale everywhere, there should have no any other scientific discipline except particle physics. In the continuum flow regime, it is unrealistic to set the mesh size to the order of particle mean free path. Instead, we need to construct the governing equations directly in the mesh size scale, and these equations cannot be the Boltzmann equation or the Navier-Stokes equations if the mesh size scale is between the kinetic and hydrodynamic scales. What we are interested in at hydrodynamic scale is the wave propagation and interaction, and at kinetic scale the individual particle transport and collision. Even in the hydrodynamic scale, such as in the unresolved shock region, the macroscopic description seems inadequate to provide necessary mechanism to construct a stable non-equilibrium shock transition. When the shock capturing schemes encounter "carbuncle phenomena", the continuous attempt on different kind of discretization of the PDEs, with the hope of introducing appropriate flow physics which has been ignored in the original Euler equations, can only lead the CFD into a maze. In a discretized space, the CFD should be a multiple scale and multiple physics modeling method.

The aim of CFD is to identify and simulate flow physics in the mesh size scale. This principle of direct modeling is not to solve any specific equation, but to construct flow evolution model. With the variation of the ratio between the mesh size and the local particle mean free path, a direct modeling should be able to capture the flow physics from the kinetic scale particle collision and transport to the hydrodynamic scale wave propagation. The unified gas-kinetic scheme (UGKS) presented in this monograph is mainly about such a direct modeling method, where a continuum spectrum of "governing equations" will be directly obtained through the modeling. The success of the UGKS is due to the adaptation of a time-dependent crossing scale gas evolution solution in the algorithm development, and this local modeling solution recovers the physics from free molecular transport to the macroscopic wave propagation. The specific solution adopted locally in the numerical algorithm depends on the ratio between the numerical time step and the local particle collision time. As a result, with a variation of cell resolution, the UGKS provides a smooth transition of the flow physics of different scales. This methodology is different from other multiscale methods, which target to connect distinctive governing equations.

The author started to work on the gas-kinetic scheme (GKS) more than twenty years ago from the postgraduate period at astronomy department of Columbia university. During the early years, the scheme is mainly to solve the compressible Euler and Navier-Stokes equations through the kinetic formulation. So, in the CFD community, the GKS is mostly regarded as a kind of approximate Riemann solvers, such as the modified flux vector splitting scheme. In the following years, with the further development of kinetic schemes to the non-equilibrium flows and its fully comparison with other CFD algorithms, such as the Godunov method, it is realized that the dynamics in the GKS is rich, which is beyond the Euler and NS equations, especially in the physical modeling of a discontinuous shock layer of a shock capturing gas kinetic scheme. The dissipation in the GKS is provided from the non-equilibrium kinetic particle transport. The dissipative mechanism of the GKS and the Godunov method will be analyzed in Chapter 4. In order to extend the GKS to the rarefied flow computation, much effort has been paid to add more physical ingredients into the GKS construction, such as the generalization of constitutive relationship through the introduction of direction-dependent viscosity coefficient, and the extension of the translational temperature from a scalar to a tensor. But, all these attempts have gotten only partially success in the non-equilibrium flow study. At end, instead of trying different kinds of modification on the macroscopic level, such as the inclusion of Burnett or Super-Burnett terms, a discretized particle velocity is used to capture the peculiarity of the gas distribution function in the nonequilibrium flow regime. The newly developed unified gas-kinetic scheme (UGKS) is an extension of the GKS with the update of both macroscopic flow variables and the microscopic distribution function, and the scheme works very well in all flow regimes. In terms of the algorithm construction, the idea of the UGKS becomes even simpler than GKS, because there is no much kinetic theory needed. With further study, it becomes clear that the gas-kinetic scheme is more or less a direct modeling method. This monograph is basically to present such an understanding. The direct modeling concept may benefit to the CFD community. The current CFD research is mainly about the numerical discretization of well-defined PDEs. The difficulties encountered in the Godunov type shock capturing schemes, such as the shock instability in high Mach number flow computations, may come from the inadequate flow physics in the governing equations in the description of a "discontinuity" in a space with limited resolution. This may be the reason for the non-uniqueness of the CFD solutions as well. Also, the methodology underlying the UGKS is useful for developing multiple scale schemes for other transport process, such as radiative transport and plasma evolution.

The content of this monograph is based on a graduate course taught by the author in the past several years at Hong Kong University of Science and Technology, and short courses at Peking University and National Laboratory of Aerodynamics. This monograph is written for different levels of readers. For students and beginners, the ideas presented here will be useful to give them a wide exposure in CFD study. The mathematics involved in this book is not sophisticated. It can be understood by anyone with basic training on calculus and linear algebra. Some basic knowledge on differential equation and statistical mechanics will be helpful, but not necessary. The book will also benefit to the CFD researchers working on the Euler and Navier-Stokes equations. At least, it presents algorithms which could be a supplement to the existing CFD methods. To understand the similarity and differences between the gas-kinetic scheme and their own in-house CFD method will be a joyful experience. The method presented in this book may be useful in practical engineering applications, especially for vacuum pumps and high speed non-equilibrium flow simulation of near space flight.

Many people have helped and made substantial contributions to the development of the gas-kinetic scheme. I give my sincerely thanks to my collaborators and colleagues: K.H. Prendergast, L. Martinelli, A. Jameson, W.H. Hui, M.D. Su, M. Ghidaoui, T. Ohwada, M. Torrilhon, E. Josyula,

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K. Xu

Contents

Chapter 1

Direct Modeling for Computational Fluid Dynamics

Computational fluid dynamics (CFD) is a scientific discipline, which aims to capture fluid motion in a discretized space. The description of the flow behavior depends closely on the scales which are used to identify or "see" it. All theoretical equations, such as the Boltzmann equation or the Navier-Stokes equations, are constructed and valid only on their modeling scales, even though these scales cannot be explicitly observed in these equations. The mechanism of these governing equations depends on the physical modeling, such as the constitutive relationship in the stress and strain of the hydrodynamic equations, and the separation of transport and collision of the kinetic equation. The existence of a few distinct governing equations, such as the Boltzmann equation, the Navier-Stokes equations, and the Euler equations, only presents a partial picture about flow physics in their specific modeling scales. The governing equations between these scales have not been fully explored yet due to the tremendous difficulties in the modeling, even the flow variables to be used for the description of a non-equilibrium flow in the scale between the Navier-Stokes and the Boltzmann equation are not clear. However, the CFD provides us an opportunity to present the flow physics in the mesh size scale. With the variation of the mesh size to resolve the flow physics, the direct modeling of CFD may open a new way for the description and simulation of flow motion. This book is mainly about the construction of numerical algorithms through the principle of direct modeling. The ultimate goal of CFD is to construct the discrete flow dynamic equations, the so-called algorithm, in a discretized space. These equations should be able to cover a continuum spectrum of flow dynamics with the variation of the ratio between the mesh size and the particle mean free path.

Instead of direct discretization of existing fluid dynamic equations, the direct modeling of CFD is to study the corresponding flow behavior in the cell size scale. The direct discretization of a well-defined governing equation may not be an appropriate way for CFD research, because the modeling scale of partial differential equations (PDEs) and mesh size scale may not be matched. Here, besides introducing numerical error the mesh size doesn't actively play any dynamic role in the flow description. For example, the Fourier's law of heat conduction is valid in a scale where the heat flux is proportional to temperature gradient. How could we imagine that such a law is still applicable on a mesh size scale, which can be freely chosen, such as $1cm$, $1m$, or even $1km$? To avoid this difficulty, one may think to resolve everything through the finest scale, such as the molecular dynamics. But, the use of such a resolution numerically in the simulation is not practical due to the overwhelming computational cost, and it is not necessary at all in real engineering applications, since in most times only macroscopic flow distributions are needed, such as the pressure, stress, and heat flux on the surface of a flying air vehicle. Instead of direct discretization of PDEs or resolving the smallest scale of molecular dynamics, a possible way is to model and capture the flow dynamics in the corresponding mesh size scale, and the choice of the mesh size depends on how much information is sufficient to capture the flow evolution in any specific application. Depending on the flow regimes, there is a wide variation between the cell size and the local particle mean free path. Therefore, a multiple scale modeling is needed in the CFD algorithm development, i.e, the construction of the so-called discrete governing equations.

1.1 Physical Modeling and Numerical Solution of Fluid Dynamic Equations

There are different levels in flow modelings. The theoretical fluid mechanics is to apply physical laws in a certain scale with the modeling of the flux and constitutive relationship. Then, based on the construction of discrete physical law, as the control volume shrinking to zero, and with the assumption of smoothness of flow variables in the scale of control volume, the corresponding PDEs are obtained. For the PDEs, even with a continuous variations of space and time, the applicable regime of these equations is on its modeling scale, such as the scale for the validity of constitutive relationship and the fluxes. For the Boltzmann equation, the modeling scale is the particle mean free path and the particle collision time, where the particle collision and transport in such a scale are separated and modeled in an operator splitting way. For the Navier-Stokes (NS) equations, the scale is the dissipative layer