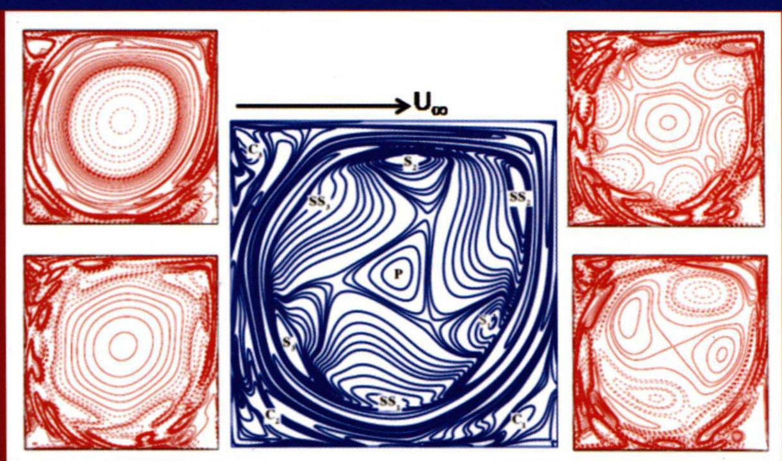
High Accuracy Computing Methods

Fluid Flows and Wave Phenomena

Tapan K. Sengupta



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To my teachers, students
and my family members

Foreword

This book aims at covering the foundations of high accuracy computing methods within the framework of Computational Fluid Dynamics (CFD) in an era of rapidly developing and evolving hardware and software.

From the hardware point of view, huge parallel machines with tens of thousands cores are installed at national facilities and research laboratories giving the practioners of scientific computing tools that they could not have dreamt of a decade ago. The advent of Graphical Processing Units (GPUs) also modifies the course of CFD as everyone tries to strain the computational tools to their last bits and extracts the highest speed-up. This is not surprising as one of the unsolved problems in classical physics is the understanding and control of turbulence in nature and technological applications.

From the software viewpoint, the advent of commercial packages including mesh generators, solvers and graphics tools, provide the numericists with appealing users interfaces and deliver numerical results for extremely different and various problems involving complicated geometries, peculiar boundary conditions and complex physics to be captured. This has had a major impact on the CFD community.

A question that is often raised consists in asking "Why should we not use the simplest schemes and run them on millions (billions) of processors?" The problem as we will discover rapidly is that simple schemes are very often too naive and lead to numerical disaster. We cannot assume that our intellectual indolence will be compensated by the computer's power. At the end of the day, a bad method will produce inconsistent and poor results.

The book is clearly oriented to the application of finite differences (FD), although Chapter 12 presents a long introduction to finite volume and finite element methods. FD methods are simple, easy to implement and test, and allow deep analysis, as we will observe. It is by all means an unavoidable step among the numerical methods as FD is prone to simple but profound analysis of numerical phenomena like numerical dissipation and dispersion. Scientific computing is a serious and most elaborate subject where the unexperienced numericist must fear the many dangers that lurk in the jungle of numerical methods. This book will definitely help to circumvent the traps and pitfalls where our candid behaviour might bring our fall in the computer's oubliette hidden in some remote memory. Let us recall that Jean Bernoulli, Newton, Leibniz and L'Hospital already used FDs in the calculation of the brachistochrone. Therefore they deserve a new presentation as this monograph intends to propose.

Chapter one sets the scene of the numerical landscape at the beginning of this century. High performance computing (HPC) with all the armada of simulation softwares and packages is giving the scientist and engineer an efficient way to understand complicated physical phenomena and the ability of taking them into account in the design process.

Chapter two gives the basic equations in fluid mechanics, both for incompressible and compressible fluids. However, the numerical methods will essentially address incompressible fluid flow applications through the set of Navier-Stokes equations. Compressible flows require by themselves a full monograph as, for example, the presence of discontinuities like shocks bring extra difficulties. The various formulations are presented like the primitive variables, velocity and pressure, the vorticity-vector potential, or the possibility of solving a Poisson pressure equation. Boundary and initial conditions are treated and explained.

Chapter three is of mathematical flavour as it studies the classification of quasi-linear partial differential equations. This analysis is a necessary condition in the sequel to distinguish the very nature of each problem with the associated intrinsic properties that derive consequently. The choice of the discretization methods is linked to the mathematical nature of the problem at hand.

Chapter four introduces waves and space-time dependence in CFD. This chapter is very important as Prof. Sengupta mentions: "If you are unable to solve accurately a one- dimensional (1D) convection (or convection dominated) problem, it is hopeless that you will be able to solve with precision the full Navier-Stokes equations". This is a chapter that departs from classical CFD books. The concept of wave equation is developed with special cases like plane waves or surface gravity waves. Then the notion of group velocity is described and applied to several problems. The Rayleigh-Taylor problem is afterwards investigated and the shallow water equations are proposed. The chapter ends with very useful considerations about spatial resolution of turbulent flows. Is direct numerical simulation (DNS) efficient and sufficient to resolve those problems? The question of temporal scales is tackled for turbulent flows. Time-averages and fully transient flows are also questioned. Reynolds-averaged Navier-Stokes (RANS) equations are evoked as well as unsteady RANS (URANS). Finally, large eddy simulations (LES) constitute the state-of-the-art of turbulent flow simulations as they separate the dynamics of the gross structures with respect to the subgrid scales that are modelled.

Chapter five is devoted to spatial and temporal discretizations. The methodology relies on classical developments like Taylor series and the FD operators. The time integrators cover single and multiple step methods. Special attention is paid to Runge-Kutta methods.

Chapter six treats the parabolic equations with the heat equation as the model. Explicit and implicit schemes are described and studied for stability and consistency. Stability conditions of explicit methods are given. A truncation error analysis yields the order of the method. Stability, consistency and convergence are all linked through the Lax equivalence theorem.

Chapter seven summarizes the basic knowledge of numerical linear algebra. Starting with the Jacobi and Gauss-Seidel method, the following sections offer successive over-relaxation, alternating direction implicit (ADI) methods, fractional step methods. Convergence of the iterative procedures is carried out by the careful inspection of the iteration matrix and the associated spectral radius. The chapter ends with the multigrid technique, which is the optimal algorithm in terms of convergence and computational complexity.

Chapter eight is central to the book and addresses the solution of hyperbolic equations. The book relies heavily on Prof. Sengupta's expertise of this problem and on the many contributions he made to this important topic. The model is the 1D convection equation with a constant advection speed. Explicit and implicit time schemes are applied to the problem. The Courant number shows up. For an explicit treatment the stability condition imposes the Courant number to be equal or less than one. As a first non-linear problem, the inviscid Burgers equation is integrated by a predictor-corrector method due to MacCormack. The dispersion error analysis involves resorting to Fourier transforms in space. Time discretization is performed by standard schemes like Euler first order or Runge-Kutta methods. This leads to the numerical amplification factor that in principle should be one. A dynamic equation is eventually obtained for the numerical error with all the possible sources. The chapter closes with the description of two new phenomena that destroy the accuracy through dispersion error: focussing and caustics. As a final conclusion, the reader is warned that despite the classical assumption that error and signal follow the same dynamics, the new analysis shows that the speed of propagation of the computed signal is the numerical group velocity and the numerical phase speed is different from the physical phase speed.

Curvilinear coordinates and grid generation are the central themes of Chapter nine. The goal is to obtain a mesh that is body-conforming in order to deal with the complex geometries without any loss of the geometrical details. Body-fitted coordinates are used for that purpose. This task is more than ancillary work. The accuracy of the numerical results depends strongly on the grid quality. Extremely helpful examples with various airfoils are described in detail. Overset grid techniques and chimera approach are also illustrated. The problem of the flow behind a circular cylinder is solved with a single grid and an overset grid. The comparison of the numerical result for a Reynolds number equal to 100 is carried out using proper orthogonal decomposition (POD) applied to the vortex shedding. The advantages and drawbacks of each type of mesh are discussed at length.

Chapter ten entitled "Spectral analysis of numerical schemes and aliasing error" is again full of novelties brought forward by Professor Sengupta and his research group. The Laplace-Fourier transform is the tool of investigation. Spectral analysis is performed for various spatial discretizations including central and upwind schemes. The essence of compact schemes is introduced and this procedure leads to high accurate approximations. The time discretization is then taken into account through one- and multi-step schemes. The end of the chapter treats the aliasing error that is always present when using high accurate methods. Filtering is one way to solve the problem.

More theory is given for compact schemes in Chapter 11. Optimized discretizations are built up and applied to the previous 1D convection equation. Symmetrized and combined compact schemes are investigated. Channel flow problems and lid-driven cavity are used as test benches. In particular in the cavity problem results show vorticity patterns with a triangular core shape. This is a consequence of the accuracy reached by compact schemes.

The finite volume and finite element methods form the topics presented in chapter 12. They are both using a "weak" formulation where Green's theorems have been used. Standard methods like QUICK and MUSCL are obtained and tested. The finite element approach relies on the Galerkin method. The Petrov-Galerkin (PG) formulation allows for upwinding the test functions. The streamline upwind PG (SUPG) scheme is designed to solve multi-dimensional schemes by following locally the direction of the streamlines.

In chapter 13, the Navier-Stokes equations are solved in the vorticity- streamfunction formulation. Then the MAC method is described with the use of the staggered mesh for velocity components and pressure. A velocity-vorticity approach is also considered. The lid-driven cavity flow serves as a benchmark problem.

The fourteenth and final chapter presents recent material based on filters and applied to LES or detached eddy simulations. Dispersion relation preserving (DRP) schemes are used throughout the chapter and applied to various problems: airfoils, cavities, cylinders, etc.

The book is very complete and may be used in an introductory course with the first chapters as the textbook. It may also be used at the undergraduate level and at the very beginning of the doctoral school with the last seven chapters as the CFD cornerstone. The book is timely as we enter a new paradigm in HPC, where the demand is obviously high quality numerical results and high-fidelity simulations. Richard Hamming in the introduction of his 1962 book *Numerical Methods for Scientists and Engineers* gives the motto 'The purpose of computing is insight, not numbers'. We could rephrase it in 2013, as 'The purpose of computing is insight and prediction through accurate numbers'. Behind numbers is hidden the question of the design and choice of the models, but this is another issue.

The reader will discover many exciting topics in this beautifully written account on numerical approximations of partial differential equations coming from fluid flow problems. I highly recommend Professor Sengupta's book as an inspiring source of high quality, high accuracy numerics that will give us the tools of achieving perfection and satisfaction in our never ending quest for excellence...and as Aristotle said 'Excellence is an art that needs constant effort'.

M. Deville
Emeritus EPFL Professor
Lausanne, Switzerland
January 23, 2013

Preface

Scientific theories by design, are always vulnerable to destruction just like a species, subjected to environmental pressure and is subjected to extinction ... Even when scientific theories fail to survive ... their evolutionary progeny carry the best "genes"— the ideas that still work — of the previous theory intact. — **Hans Pagel**

There are many new developments in scientific computing, in its application to fluid flows and wave phenomena, which warrant their consolidation in a single source, covering some of the key developments. I have been convinced by many students and peers that there is a definitive need for a single source book which deals with topics covered here. I would like to acknowledge their inspiration. My main motivation in writing this manuscript is to communicate something new and powerful as opposed to conventional derivatives of products churned out by existing schools of thought.

However, this book also provides general introduction to computational fluid dynamics (CFD), using well tested classical methods of solving partial differential equations (PDEs) for the sake of completeness. These are to be found in Chaps. 1 to 9 and 13, but re-interpreted using the spectral analysis method introduced in Chaps. 4, 8 and 10. This provides an unity of approach in understanding numerical methods for parabolic, elliptic and hyperbolic PDEs. The spectral analysis tool has been refined in recent years by the author's group, with which disparate methods can be easily compared.

This spectral analysis enables one, as shown in Chap. 8, that celebrated von Neumann analysis is actually flawed, in which it is assumed that for a linear dynamical system the error and signal follow the same dynamics. While this appeals to anyone as logical in an intuitive framework, the correct error analysis shows that this is indeed a false assumption when viewed for the numerical solution of the one-dimensional convection equation, which is an ideal model equation for non-dissipative, non-dispersive system. A correct error analysis for this equation shows that numerical schemes must be neutrally stable and dispersion error-free to provide high accuracy solution. The error dynamics is noted to be distinctly different from the signal for this simple model equation. One of the singular achievement of this analysis is identification of the correct numerical dispersion relation, which in turn has enabled the creation of a general spectral theory of analysis of numerical methods over the full domain for any discrete computations. Such analysis can also be done for linear shallow water equation, as an example for dispersive dynamic system and that also shows different error dynamics from signal behaviour.

In proposing the new error analysis through a simple one-dimensional convection equation, we follow the Scottish philosopher, David Hume's logic about fallibility of method of induction in knowledge creation by the theory of black swan (*No amount of observation of white swans can allow the inference that all swans are white, but the observation of a single black swan is sufficient to refute the conclusion*). While the *white swan* of von Neumann analysis was a mere assumption related to behaviour of linear systems, the one-dimensional convection equation is the *black swan* which negates the assumption of identical dynamics of signal and error for linear systems.

To understand numerical wave properties and related physical concepts, one can use Chaps. 4, 8, 10, 11, 12 and 14 after familiarizing oneself with discretization methods in Chap. 5. Chapter 9 introduces readers to governing equations in curvilinear co-ordinate systems and grid generation with emphasis on orthogonal grid generation, which can be used with chimera grid technique in solving complex geometry problems which involve multiply connected computing domain. Our emphasis in this regard is simply from the point of view of obtaining higher accuracy. Although, we admit that chimera method itself is a work in progress. Spectral analysis also allows one to compare finite volume and finite element methods with any other methods, as described in Chap. 12. Practitioners in these areas emphasize that they are capable of solving practical and complex problems and their tools should be immune to scrutiny, other than truncation error analysis. We have other ideas and results about it in Chap. 12. In Chap. 13, various formulations of Navier-Stokes equation using different methods have been studied, which have been described in previous chapters.

The other aspect of the present book is to develop computational methods in their ability for direct numerical simulation (DNS) and large eddy simulation (LES). Nearly two thirds of the book addresses in detail, issues of high precision computing in Chaps. 4, 8 to 14. Studying dispersion properties from physical and numerical perspective requires understanding wave properties — an absolute necessity to compute physically unstable, transitional and turbulent flows. A common misperception exists among many users of DNS who not only modify the governing differential equations, but they do not check for the essential numerical properties of the basic methods used in their code. It is quite common to note that the basic method remains numerically unstable, which is *controlled* by adding *hyperviscosity*! The present book strongly discourages this practise.

Accuracy and precision of numerical methods are more important than the order of the method, which is emphasized time and again in the book, with the associated concepts originating from spectral analysis, in terms of wave propagation properties and its application to DNS and LES. Development of DNS and ever growing activities of LES for practical applications have convinced us that wave mechanics is central to such activities. Spectral analysis of model 1D convection equation for correct error propagation equation in Chap. 8 forms the foundation of DNS for convection dominated flows and wave propagation phenomena.

This error and dispersion analysis require considering spatial and temporal discretization together, which is the foundation of dispersion relation preserving (DRP) schemes. The basic analysis in Chap. 8 is method independent and leads to identifying the correct numerical dispersion relation vis-a-vis physical dispersion relation. This must be supplemented by explaining aliasing error (Chap. 10) to develop high accuracy compact schemes described in Chaps. 11 and 12, for finite difference and finite volume methods, respectively. Absolute control of flow simulation for DNS also requires understanding implicit Padè filters applied in adaptive manner (Chap. 14) and how these exclude spurious numerical waves (*q*-waves) without compromising accuracy. These are the core elements of the second part of the book, which can be used in an advanced course on scientific computing related to fluid flows and wave phenomena, by using materials in Chaps. 2, 4, 8 to 14.

No special attempts have been made to deal with compressible flows in the book, for two reasons. First, there are excellent books and monographs dealing specifically with this topic. Secondly, if computing is performed with high accuracy avoiding problems of capturing discontinuities, then there is no need to develop special methods for compressible flows specifically. This is also related to developing DRP scheme, as capturing discontinuity implies faithful reproduction of all scales which propagate at the correct speed without numerical dispersion.

It is my solemn duty to declare my debts of gratitude to pioneers in the field, whose ideas have been expanded to obtain new developments in a single book. In research there are two classes of noteworthy initiatives. In one class, researchers try to provide the 'first word' by initiating new ideas and in the other class, attempts are made to provide the 'last word' on a topic. The present book uses both these tracks to present concisely, classical and recent developments. I have benefited immensely from many colleagues and students who have read early drafts of various chapters and provided insightful comments. I would specially like to acknowledge Prof. Michel Deville, who read a portion of the book and provided many valuable suggestions. This book has benefited tremendously from three students: Yogesh Bhumkar, Swagata Bhaumik and Manoj Rajput who created many new figures for the manuscript. Without their support, this effort would be much poorer and my heartfelt gratitude is expressed here. I am also deeply indebted to V. V. S. N. Vijay and A. Dipankar for reading many chapters, correcting errors and providing suggestions. I also would like to sincerely acknowledge help provided by my other students (past and present) in providing figures and materials used in the book. I specifically thank M. T. Nair, Gaurav Ganeriwal, A. Dipankar, Sarthok Sircar, S. B. Talla, K. Venkatasubbaiah, V. Lakshmanan, V. V. S. N. Vijay, Kuldeep Singh Lonkar, Amrita Mittal, V. K. Suman, S. Unnikrishnan, N. A. Sreejith and S. Usman.

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While I have been busy with work, my family provided an ideal environment at home and their unstinting support and encouragement made this a labour of love. Their understanding and support during the formative stage of this manuscript was very vital. I specifically like to acknowledge the sacrifices they had to make, so that I could work unhindered despite many odds. My wife, Soma and our adorable children, Soumyo and Aditi, to whom I dedicate this work.

I must also record my sincere appreciation for all the work done for manuscript preparation by Ms. Baby Gaur and Ms. Shashi Shukla, many times over to meet changing needs. Ms. Gaur has typed most of the text, prepared figures and spent endless hours, outside the call of duty in preparing the manuscript. Without the dedication and devotion to work shown by all involved, this book would not be in the present form. Finally, I wish to also acknowledge Cambridge University Press for publishing this work. With all wonderful help obtained from many, I humbly assume responsibilities for all mistakes in this book and welcome suggestions for correcting these, as well as invite any other critique.

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