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Volume 592

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Editors

High-Performance Computing of Big Data for Turbulence and Combustion

Springer

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ISSN 0254-1971 ISSN 2309-3706 (electronic)
CISM International Centre for Mechanical Sciences
ISBN 978-3-030-17011-0 ISBN 978-3-030-17012-7 (eBook)
https://doi.org/10.1007/978-3-030-17012-7

This Springer imprint is published by the registered company Springer Nature Switzerland AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Preface

The CISM advanced course on “High-performance Computing of Big Data for Turbulence and Combustion” was held in Udine from May 21 to May 25, 2018. The course was aimed at acquainting participants with present state of art in high-accuracy scientific computing and its future prospects, as applicable to a broad range of areas including fluid mechanics, thermal analysis, and combustion. A substantial part of the course was devoted to efficient implementation of modern Navier–Stokes solution algorithms on future exascale machines, and clever use of the huge database generated by LES and DNS.

This volume includes contributions from the instructors of the CISM course covering virtually all of the topics addressed. Chapters 1 and 2 by T. K. Sengupta, P. K. Sharma, and V. K. Suman are meant to provide basic and advanced general concepts on numerical discretization of convection/diffusion equations, and their application to the study of transitional flows. In Chap. 1, the authors introduce the global spectral analysis (GSA) as a fundamental tool to characterize the behavior of numerical schemes in one and multiple space dimensions. The mathematical formalism is applied to the study of a practical case of focusing instability in the numerical solution of flow in a lid-driven cavity. This chapter shows how GSA links convection–diffusion equation with Navier–Stokes equation for performing very long time simulation with extreme precision, geared toward exascale computing. In Chap. 2, the authors show how the basic notions provided in Chap. 1 translate into practical numerical simulations of transitional and turbulent flows, by also highlighting the necessary numerical resolution requirements as given by GSA. This part includes a thorough analysis of turbulence in spectral space, which is also instrumental for the forthcoming chapters. Two- and three-dimensional routes to turbulence owing to incoming deterministic perturbations are discussed for the canonical flow over a flat plate, and the nonlinear evolution is numerically followed into a state of developed turbulence.

Chapter 3 by S. Pirozzoli is entirely devoted to introducing the reader to the theory and practice of DNS, as applied to both incompressible and compressible flows. The foundations of nonlinear numerical stability analysis are illustrated in Fourier space in terms of the aliasing error, and stabilization techniques relying on discrete preservation of kinetic energy are presented, both in the case of model scalar equations and full Navier–Stokes equations. The important topic of practical implementation of DNS solvers on massively parallel machines is also addressed, and practical suggestions are given to achieve accurate results and fast convergence to a statistically steady turbulence state. Worked out examples include studies of incompressible internal flows, dispersed passive scalars and compressible boundary layer flows.

Chapter 4 by T. Poinsot presents a comprehensive overview of numerical instabilities occurring in high-fidelity simulations of reacting and non-reacting flows, including physical and numerical ones. This part includes an overview of the physics and models in current use for the prediction of turbulent combustion, and of the types of waves which may arise in problems of industrial applications. A series of illustrative LES calculations of realistic burners are presented, with a special eye on careful non-reflecting treatment of numerical boundary conditions to prevent the onset of numerical instabilities. Additional instabilities in turbulent combustion include the case of swirled flames, which may bifurcate to multiple states. The author then devotes a large part of this chapter to possible causes for the growth of errors in LES of reacting flows, which include rounding errors, initial conditions, parallel communications, computational time step, and even machine precision, highlighting significant sensitivity to all of these items, and concluding that mastering instabilities is of crucial importance to fully deploy the predictive capabilities of LES.

Chapter 5 by Mejdi Azaïez, L. Lestandi, and Tomás Chacón Rebollo include a mathematically rigorous treatment of low-rank approximation of large datasets. This subject is becoming a special concern in recent years owing to the growing availability of a huge amount of data from DNS, LES, and RANS made possible by the exponential growth of available computing power. In this chapter, the authors propose shift of paradigm by introducing decomposition to reduced data, presenting an extensive review of current data reduction techniques, and aiming to bridge the gap between the applied mathematics and the computational mechanics communities. By now, classical bivariate data separation techniques are studied in the first part of the chapter, including discussions on the equivalence of proper orthogonal decomposition (POD) in the continuous framework and singular value decomposition (SVD) in the discrete framework. A wide review then follows of modern tensor formats, including Canonical, Tucker, Hierarchical, and Tensor train, along with their approximation algorithms. Whenever possible, links between the continuous and the discrete formalisms are made.

We believe that readers from a wide audience will use and enjoy reading this publication, as each chapter gives insight into a specific tile of the puzzle, so that researcher specialized in numerical analysis, fluid turbulence, combustion, and data analysis will find relevant information for their own specialty. At the same time, we hope that the book as a whole will provide an important reference as it shows how the development in numerical techniques and in physical insight is nowadays intimately connected with fast progress in computer-science-related disciplines, and especially with data analysis. Mastering each and every discipline dealt with in this book will in our intent help to form a new generation of scientists and engineers trained in the multidisciplinary analysis of complex physical phenomena through large-scale computations, which should not only involve brute-force use of machines but also exploit additional insights provided by clever treatment of big data. We expect that in the long term, this different attitude will translate into a better understanding of physical reality and better models, which will, more and more, rely not only on artificial but also on human native intelligence.

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