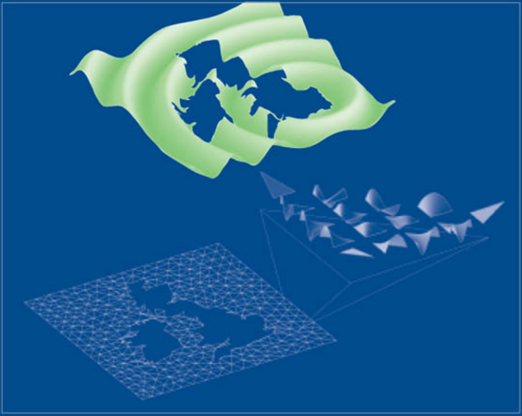
NUMERICAL MATHEMATICS
AND SCIENTIFIC COMPUTATION

Spectral/hp Element Methods for Computational Fluid Dynamics

SECOND EDITION

GEORGE EM KARNIADAKIS
and SPENCER SHERWIN



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Spectral/*hp* Element Methods for CFD

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PREFACE TO SECOND EDITION

There has been significant progress in the development of multi-domain spectral methods both at the fundamental as well as at the application level in the last few years. We have, therefore, undertaken the 'non-trivial' task of updating the book in order to include these new developments. We also wanted to make these methods easier to comprehend and implement by the students, responding directly to the many requests and feedback we received after the publication of the first edition of our book. We are grateful to Oxford University Press, and in particular to the Mathematics and Statistics editor Dr Alison Jones, who gave us this opportunity.

The new developments are primarily in the discontinuous Galerkin methods, in non-tensorial nodal spectral element methods in simplex domains, and on stabilisation and filtering techniques. From the practical point of view, high-order solutions in complex geometries require high-order meshes and high-order post-processing, a subject that is often neglected in the everyday 'production' computing and simulation. Such subjects are now addressed in some detail in this new edition of the book. We have also seen the spectral/*hp* element method applied to less traditional fields, such as seismology, climate modelling, and magneto-hydrodynamics (MHD), and we have included some elements of modelling such applications in this revised version.

Finally, another objective in revising the book has been to provide more details on implementing various aspects of the method. To this end, we have put some emphasis on implementation and technical issues with exercises in the founding Chapters 2 to 5 to aid in implementing basic spectral element solvers, which can be used as building blocks for more complex application codes.

Overall, the book has been increased in new material by almost 50% in order to include all the aforementioned topics.

We would like to thank our many students and colleagues who have provided good critical feedback on the first version of the book. In particular, we would like to thank Drs H. Blackburn, J. Hesthaven, R. M. Kirby, J. Peiró, V. Theofilis, and Z. Yosibash who contributed to the new edition directly by providing plots and other information from their own work. We also want to thank our families who have supported us again during the course of this effort.

Boston, Massachusetts G. E. K.
London, England S. J. S.
Spring 2004

PREFACE TO FIRST EDITION

Our aim in writing this book is to introduce a wider audience to the use of spectral/*hp* element methods with particular emphasis on their application to unstructured meshes. These methods, as their name suggests, incorporate both multi-domain spectral methods (based on a development of original ideas by A. T. Patera) and also high-order finite element methods (based on original ideas of B. A. Szabó). In this book, we provide a unified description of both methods building on previously published works as well as on new material not previously published.

Although spectral methods have long been popular in direct and large eddy simulation of turbulent flows, their use in areas with complex-geometry computational domains has historically been much more limited. For example, in computational aerodynamics, which typically involve the use of unstructured meshes, the preferred methods have been low-order finite element and finite volume methods. More recently, however, the need to find accurate solutions to the viscous flow equations around complex aerodynamic configurations has led to the development of high-order discretisation procedures on unstructured meshes. High-order discretisation is also recognised as more efficient for solution of time-dependent oscillatory solutions over long time periods, for example, in the new field of computational electromagnetics in aerospace design.

Polynomial spectral methods were first introduced in Gottlieb and Orszag [199] and are covered extensively in Canuto *et al.* [86], Boyd [71], and Fornberg [164]. Szabó and Babuška [445] and Bernardi and Maday [45] deal with *hp* finite element and spectral element methods, respectively, and should be consulted for background reading. This book reviews most of the fundamental concepts but does assume the reader has some familiarity with the basic concepts of finite element discretisation and the Galerkin approximation technique.

The material contained in this book draws on the ideas and influence of many people, but particular thanks are due to A. T. Patera, S. A. Orszag, and D. Gottlieb, who have advised and collaborated on our research work over the past fifteen years. Much of this book is based on the doctoral thesis of the second author (SJS), as supervised by the first author (GEK). This book has also drawn heavily on doctoral theses of other students supervised by GEK, notably those of R. D. Henderson, I. G. Giannakouros, A. Beskok, C. H. Crawford, T. C. Warburton, I. Lomtev, and J. Trujillo, and also doctoral theses supervised by A. T. Patera, notably E. M. Ronquist, C. Mavriplis, and G. Anagnostou. We would like to thank J. Peiro for his help with the unstructured meshing, and are particularly grateful to our colleagues who provided original figures which we have included in this book. Thanks are also due to those who have given their time and effort to read the proof of this book.

GEK would like to acknowledge the sponsorship of his research program by the Office of Naval Research, the Air Force Office of Scientific Research, the Department of Energy, and the National Science Foundation.

Finally, we would like to thank our wives, Helen and Tracey, for their understanding and patience during the writing of this book. We would especially like to thank Tracey, who was the first person to read the book in its entirety, correcting our grammar and spelling, and also providing a notable contribution to the prose.

Boston, Massachusetts G. E. K.
London, England S. J. S.
Fall 1997

BOOK OUTLINE

In Chapter 1, we present reduced models of the compressible and incompressible Navier–Stokes equations which are used in the various discretisation concepts discussed in the following chapters. The convergence philosophy of spectral and finite element methods, the combination of which provides a dual path of convergence, is also introduced.

In Chapter 2, we present the fundamental concepts that are further developed in the remainder of the book, in the context of a one-dimensional formulation. In doing so, we illustrate the principles and underlying theory behind the construction of the spectral/*hp* element method. In this second revision we have included more details on implementing boundary conditions and used margin identifiers to highlight formulation details, using a '♣' symbol, and implementation details, using a '♦' symbol. We have also added new sections on nodal p-type expansions and on integration errors and polynomial aliasing. The series of exercises included at the end of the chapter solely focuses on developing a one-dimensional spectral element solver.

In Chapter 3, we consider the extension of the one-dimensional formulation to two and three dimensions by the development of expansion bases in standard regions such as triangles or rectangles in two dimensions, and tetrahedrons, prisms, pyramids, and hexahedrons in three dimensions. The construction of these bases uses a unified approach which permits the development of computationally efficient expansions. In this new revision we now formulate the modal basis as solutions to a generalised Sturm–Liouville problem. We also present optimal nodal points, the so-called Fekete points, as well as the electrostatic points on a simplex, and include related approximation results. The exercises at the end of the chapter target construction of multi-dimensional elemental matrices.

Compared to the first revision of the book, Chapter 4 has been restructured with extra emphasis on implementation aspects. In this chapter we complete the multi-dimensional formulation by explaining how the two- and three-dimensional expansions developed in Chapter 3 can be extended into a tessellation of multiple domains. These extensions are decomposed into three sections: local operations such as integration and differentiation; global operations such as the construction of global matrix systems; and pre- and post-processing issues such as boundary representation, high-order mesh generation, and particle tracking. The chapter introduces a matrix formulation to help illustrate the algebraic systems which need to be constructed when computationally implementing the spectral/*hp* method. Formulation of both Galerkin and collocation projections are considered in this manner. The exercises in this chapter include implementation of a two-dimensional spectral/*hp* element solver for a multi-element Galerkin projection.

In this revised version Chapter 5 now considers the diffusion equation; an implicit in time discretisation leads to the Helmholtz equation. This chapter discusses both the temporal discretisation and eigenspectra of second-order operators that dictate time-step restrictions. We also expand on appropriate preconditioning techniques for inversion of the stiffness matrix. The final part of this chapter discusses non-smooth solutions due to geometric singularities and this revised section now includes elements from recent advances in three-dimensional domains. The final exercises section focuses on building on the exercises of Chapters 3 and 4 to implement a two-dimensional standard Galerkin *hp* solution to the Helmholtz problem.

In Chapter 6, we focus on the scalar advection equation and develop a Galerkin discretisation using the techniques described in Chapter 4. We then include an extended presentation of the discontinuous Galerkin formulation for advection equations. Similar to Chapter 5, we also review eigenspectra of the advection operators in both two and three dimensions which are relevant for explicit time stepping. A further new addition is the discussion on two forms of a semi-Lagrangian method for advection (strong and auxiliary forms) that could potentially prove very effective in enhancing the speed and accuracy of spectral/*hp* element methods in advection-dominated problems. A further new section on stabilisation techniques is then introduced that discusses filters, spectral vanishing viscosity, and upwind collocation. This new material is important as it relates directly to the robustness of the method, especially in marginally resolved simulations.

In Chapter 7 (previously Chapter 5) we introduce and discuss the topic of non-conforming elements for second-order operators. This chapter has been extended to include a comprehensive presentation of the discontinuous Galerkin method with a comparison of different versions from theoretical, computational, and implementation standpoints.

In Chapter 8, we present different ways of formulating the incompressible Navier–Stokes equations based on primitive variables, that is, velocity and pressure, as well as velocity–vorticity algorithms. We consider both coupled, splitting, and least-squares formulations for primitive variables, and in this revision we now discuss both the Uzawa coupled algorithm and a new substructured solver. The discussion on primitive variables time-splitting has been rewritten to include recent theoretical advances in the pressure-correction and velocity-correction schemes as well as the rotational formulation of the pressure boundary condition. Whilst an important issue for primitive variable formulation is the efficient incorporation of the divergence-free constraint, an analogous problem for the velocity–vorticity formulation is the accurate imposition of the boundary conditions which is also discussed. The final section is devoted to nonlinear terms; it includes a discussion of spatial and temporal discretisation with focus on the semi-Lagrangian method for the incompressible Navier–Stokes equations.

In Chapter 9, we discuss numerical simulations of the incompressible Navier–Stokes equations. First, we present exact Navier–Stokes solutions that can be used as benchmarks to validate new codes and evaluate the accuracy of a particular discretisation. In the current revision this section has been restructured, with more benchmark solutions, to emphasise verification and validation of spectral/*hp* element solvers. A new section on three-dimensional stability (biglobal stability) is also included—spectral/*hp* elements are particularly effective in this field. The chapter continues by discussing some aspects of direct numerical simulation (DNS) and large-eddy simulation (LES). The issue of stabilisation at high Reynolds number is then presented using the concepts of dynamic subgrid modelling, over-integration, and spectral vanishing viscosity. A new parallel paradigm based on multi-level parallelism is introduced that can help realise adaptive refinement more easily; the final section includes a heuristic refinement method for Navier–Stokes equations.

Chapter 10 has been expanded to consider not only compressible Euler and Navier–Stokes equations but general hyperbolic conservation laws. This is an area in which high-order methods have had little success in the past. The principle issue is how to effectively use the high-order expansions of the spectral/*hp* method whilst honouring the inherent monotonicity and conservation properties of the analytic system. We consider different ways of dealing with these fundamental issues for both the Euler and the Navier–Stokes equations. A new section for the shallow water equations is also included and the section on the discontinuous Galerkin method has been rewritten. Finally, the last section discusses modelling of plasma flows, i.e., the so-called magneto-hydrodynamic (MHD) equations.

Finally, the appendices provide details on Jacobi and Askey polynomials as well as numerical integration and differentiation which are essential building blocks of the spectral/*hp* element techniques. A full description of commonly used expansion bases is provided, which now includes nodal points for non-tensorial electrostatic and Fekete point distribution in simplex domains. The final appendix also details Riemann solvers commonly used in the solution of the Euler equations.

CONTENTS

NOMENCLATURE

Sets

$\Re$	Real numbers
$\bigcup$	Set union
$\bigcap$	Set intersection
$\emptyset$	Empty set
$\in$	Is a member of; belongs to
$\notin$	Is not a member of; does not belong to
$\subset$	Is a subset of
$\not\subset$	Is not a subset of

Expansion basis notation

ϕ_{pq}, ϕ_{pqr}	Expansion basis
$\psi_p^a, \psi_{pq}^b, \psi_{pqr}^c$	Modified principal functions
$\widetilde{\psi}_p^a, \widetilde{\psi}_{pq}^b, \widetilde{\psi}_{pqr}^c$	Orthogonal principal functions
$h_p(\xi)$	One-dimensional Lagrange polynomial of order p
$L_i^{N_m}(\boldsymbol{\xi})$	Two-dimensional Lagrange polynomial through N_m nodes $\boldsymbol{\xi}_i$
P_i	Polynomial order in the ith direction
Q_i	Quadrature order in the ith direction
$x_1, x_2, x_3, \boldsymbol{x}$	Global Cartesian coordinates
$\xi_1, \xi_2, \xi_3, \boldsymbol{\xi}$	Local Cartesian coordinates
η_1, η_2, η_3	Local collapsed Cartesian coordinates
$\chi_i(\xi)$	Local Cartesian to global coordinate mapping

Various constants

N_{dof}	Number of global degrees of freedom
N_b	Number of global boundary degrees of freedom
N_m	Number of elemental degrees of freedom
N_{eof}	Total number of elemental degrees of freedom $N_{\mathrm{eof}} \simeq N_{\mathrm{el}} N_m$
N_Q	Total number of quadrature points $N_Q = Q_1 Q_2 Q_3$
N_{el}	Number of elements
λ	Helmholtz equation constant
e	Element number $1 \leqslant e \leqslant N_{\mathrm{el}}$
i, j, k	General summation indices
p, q, r	General summation indices

Elemental arrays

$\boldsymbol{B}$	Basis matrix
$\boldsymbol{W}$	Diagonal weight/Jacobian matrix
$\boldsymbol{D}_\xi$	Elemental derivative matrix with respect to ξ
$\boldsymbol{\Lambda}(u)$	Diagonal matrix of $u(\xi_1, \xi_2)$ evaluated at quadrature points
$\boldsymbol{M}^e$	Elemental mass matrix

$\boldsymbol{L}^e$	Elemental Laplacian matrix
$\boldsymbol{H}^e$	Elemental Helmholtz matrix
$\boldsymbol{f}^e$	Force vector of the eth element
$\boldsymbol{u}^e$	Vector containing function evaluated at quadrature points
$\hat{\boldsymbol{u}}^e$	Vector of expansion coefficients

Global arrays

$\boldsymbol{W^e}$	Block diagonal extension of matrix $\boldsymbol{W^e}$
$\boldsymbol{f}^e$	Concatenation of elemental vector $\boldsymbol{f}^e$
$\boldsymbol{\mathcal{A}}^\top$	Matrix global assembly
$\boldsymbol{M}$	Mass matrix $(= \boldsymbol{\mathcal{A}}^\top \underline{\boldsymbol{M}^e} \boldsymbol{\mathcal{A}})$
$\boldsymbol{L}$	Laplacian matrix $(= \boldsymbol{\mathcal{A}}^\top \underline{\boldsymbol{L}^e} \boldsymbol{\mathcal{A}})$
$\boldsymbol{H}$	Helmholtz matrix $(= \boldsymbol{\mathcal{A}}^\top \underline{\boldsymbol{H}^e} \boldsymbol{\mathcal{A}})$
$\hat{\boldsymbol{v}}_g$	List of all elemental coefficients $(= \underline{v^e})$
$\hat{\boldsymbol{v}}_l$	Global list of coefficients

Solution domains

Ω	Solution domain
$\partial\Omega$	Boundary of Ω
Ω^e	Elemental region
$\partial\Omega^e$	Boundary of Ω^e
$\partial\Omega_{\mathcal{D}}$	Domain boundary with Dirichlet conditions
$\partial\Omega_{\mathcal{N}}$	Domain boundary with Neumann conditions
$\boldsymbol{n}$	Unit outward normal

Differential operators

∇^2	Laplacian
$\nabla \cdot$	Divergence
$\nabla \times$	Curl

Spaces

$\mathcal{X}$	Space of trial solutions
$\mathcal{X}^\delta$	Finite-dimensional space of trial solutions
$\mathcal{V}$	Space of test functions
$\mathcal{V}^\delta$	Finite-dimensional space of test functions
$\mathcal{P}_P(\Omega)$	Polynomial space of order P over Ω

Operators

$\mathcal{I}$	Interpolation operator
$\mathcal{I}^\delta$	Discrete interpolation operator
$\mathbb{P}$	Projection operator
$\mathbb{P}^\delta$	Discrete projection operator
$\mathbb{L}(u)$	Linear operator in u

Fluid variables

$\mathbf{v}$	Velocity $[u, v, w]^\top$
p	Pressure
$\boldsymbol{\omega}$	Vorticity
ρ	Density
μ, ν	Dynamic, kinematic viscosities