Computational Methods for Geodynamics

Computational Methods for Geodynamics describes all the numerical methods typically used to solve problems related to the dynamics of the Earth and other terrestrial planets, including lithospheric deformation, mantle convection and the geodynamo.

The book starts with a discussion of the fundamental principles of mathematical and numerical modelling, which is then followed by chapters on finite difference, finite volume, finite element and spectral methods; methods for solving large systems of linear algebraic equations and ordinary differential equations; data assimilation methods in geodynamics; and the basic concepts of parallel computing. The final chapter presents a detailed discussion of specific geodynamic applications in order to highlight key differences between methods and demonstrate their respective limitations. Readers learn when and how to use a particular method in order to produce the most accurate results.

This combination of textbook and reference handbook brings together material previously available only in specialist journals and mathematical reference volumes, and presents it in an accessible manner assuming only a basic familiarity with geodynamic theory and calculus. It is an essential text for advanced courses on numerical and computational modelling in geodynamics and geophysics, and an invaluable resource for researchers looking to master cutting-edge techniques. Links to online source codes for geodynamic modelling can be found at www.cambridge.org/zadeh.

Alik Ismail-Zadeh is a Senior Scientist at the Karlsruhe Institute of Technology (KIT), Chief Scientist of the Russian Academy of Sciences at Moscow (RusAS) and Professor of the Institut de Physique du Globe de Paris. He graduated from the Baku State and Lomonossov Moscow State Universities before being awarded Ph.D. and Doctor of Science degrees in geophysics from RusAS. He lectures on computational geodynamics at KIT, Abdus Salam International Center for Theoretical Physics in Trieste, and Moscow State University of Oil and Gas, while his research interests cover crust and mantle dynamics, basin evolution, salt tectonics and seismic hazards. Professor Ismail-Zadeh is the recipient of the 1995 Academia Europaea Medal and the 2009 American Geophysical Union International Award, and is Secretary-General of the International Union of Geodesy and Geophysics.

Paul Tackley is Chair of the Geophysical Fluid Dynamics Group in the Institute of Geophysics, Department of Earth Sciences, Swiss Federal Institute of Technology (ETH Zürich). He received an MA from the University of Cambridge and an MS and Ph.D. from the California Institute of Technology before taking up a position in the Department of Earth and Space Sciences and Institute of Geophysics and Planetary Physics at the University of California, Los Angeles. He became a full professor there before moving to ETH Zürich in 2005, where he currently teaches courses in geodynamic modelling. Professor Tackley's research involves applying large-scale three-dimensional numerical simulations using state of the art methods and parallel supercomputers to study the structure, dynamics and evolution of the Earth and other terrestrial planets. He has served as an associate editor for various journals and is on the editorial board of *Geophysical and Astrophysical Fluid Dynamics*.

Cover illustration (front): upper images by M. Armann show numerical simulations of thermo-chemical convection in a stagnant- or episodic-lid planet such as Venus, with (left) composition ranging from basalt (red) to harzburgite (blue) and (right) potential temperature (simulations by M. Armann and P.J. Tackley); lower images by T. Nakagawa show numerical simulations of thermo-chemical convection in a mobile-lid planet such as Earth; isosurfaces show cold (blue) and hot (red) temperature anomalies and (green) basaltic composition (simulations by T. Nakagawa and P.J. Tackley).
(back): the images by I. Tsepelev show (top) the time snapshots of the thermal evolution of the descending slab (blue, dark cyan and light cyan mark the surfaces of different temperature anomalies) and pattern of mantle flow (arrows illustrate the flow's direction and magnitude) beneath the south-eastern Carpathians. The model evolution is restored numerically using the quasi-reversibility method for data assimilation (Ismail-Zadeh *et al.*, 2008).

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Alik Ismail-Zadeh
Karlsruhe Institute of Technology (KIT)
Moscow Institute of Mathematical Geophysics, Russian Academy of Sciences (MITPAN)
Institute de Physique du Globe de Paris (IPGP)

Paul J. Tackley
Swiss Federal Institute of Technology Zurich (ETH)

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To David, Junko, and Sonya
as a sign of deep affection

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Foreword

Geodynamics is the application of the basic principles of physics, chemistry and mathematics to understanding how the internal activity of the Earth results in all the geological phenomena and structures apparent at the surface, including seafloor speading and continental drift, mountain building, volcanoes, earthquakes, sedimentary basins, faulting, folding, and more. Geodynamics also deals with how the Earth's internal activity and structure reveals itself externally in ways both geophysical, its gravitational and magnetic fields, and geochemical, the mineralogy of its rocks and the isotopic composition of its rocks, atmosphere, and ocean. The discipline of geodynamics did not exist until about the early 1970s. The plate tectonics revolution was the impetus for the birth of the subject. Today, geodynamics goes beyond the Earth to consider the interiors and surfaces of other planets and moons in our solar system. While this aspect of the science could be termed planetary dynamics, it involves the same geodynamical processes that shape the Earth, though often with intriguingly different outcomes for the other bodies.

Mathematical modeling, which attempts to understand a phenomenon quantitatively, lies at the heart of geodynamics. In the early years of the subject analytic and semi-analytic methods were sufficient to gain insights into the workings of the Earth's interior. After four decades of progress in the subject it is, generally speaking, no longer possible to address the remaining questions with such simple models. Indeed, it has been necessary for some time now, to employ sophisticated numerical computational models to achieve further understanding of the complex dynamics of the Earth. Accordingly, researchers now entering the field of geodynamics need to acquire the skills to understand the numerical methods upon which computational geodynamics codes are based. An understanding of the methods is required not only for intelligent use of existing codes but also to enable adaptations of the codes and future improvements in them. The present book responds to this need by thoroughly discussing the many different numerical schemes designed to provide approximate solutions to the ordinary and partial differential equations encountered in geodynamical problems and by emphasizing the fundamental principles behind the numerical approaches. It is a book that goes far beyond the black box utilization of numerical tools by providing the student with a deep understanding of the numerical approaches upon which the codes are based.

The book begins with an introductory chapter discussing the basic equations and the boundary and initial conditions of geodynamics followed by general remarks on the numerical approach to their solution. The succeeding chapters discuss all the widely used numerical schemes in detail, finite differences, finite volumes, finite elements, and spectral decomposition. The succeeding two chapters apply these methods to solving linear algebraic equations and ordinary differential equations. The concluding chapters deal with data assimilation, parallel computing, and applications in geodynamics. A number of appendices provide mathematical background.

The authors are distinguished geodynamicists with decades of experience in numerical modeling. They are at the forefront of geodynamical modeling and are responsible for the initial development and continued improvement of state-of-the-art codes. They have written a clear and comprehensive book that everyone working in the field of geodynamics would be well advised to read and keep handy for future reference.

Gerald Schubert
Distinguished Professor of Geophysics and Planetary Physics
University of California
Los Angeles, California
USA

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Preface

The book of nature is written in the language of mathematics
(Galileo Galilei, 1564–1642)

All the mathematical sciences are founded on relations between physical laws and laws of numbers, so that the aim of exact science is to reduce the problems of nature to the determination of quantities by operations with numbers
(James Clerk Maxwell, 1831–1879)

It is impossible to explain honestly the beauties of the laws of nature in a way that people can feel, without their having some deep understanding of mathematics and its methods
(Richard Feynman, 1918–1988)

Great advances in understanding of the planet Earth and in computational tools permitting accurate numerical modelling are transforming the geosciences in general and geodynamics particularly. Research on dynamical processes in the Earth and planets relies increasingly on sophisticated quantitative models. Improved understanding of fundamental physical processes such as mantle convection, lithospheric deformation, and core dynamos in the Earth and terrestrial planets depends heavily on better numerical modelling. Characteristic of this new intellectual landscape is the need for strong interaction across traditional disciplinary boundaries: Earth sciences, applied mathematics, and computer science.

Solid Earth scientists, with few exceptions, rarely achieve mathematical competence beyond elementary calculus and a few statistical formulae. Meanwhile, in some sense it has become a fashion nowadays, when scientists dealing with geodynamics make numerical modelling as their primary research tool. Most of these scientists employ standard commercial software or the codes developed by representatives of the geodynamic community and do not take care of numerical methods and their limitations behind the software and codes. Sometimes numerical results of complicated models, being wrong from a mathematical point of view, can feature the Earth dynamics in a 'realistic' way and can hence lead to wrong physical interpretations. To distinguish between wrong and true solutions, geodynamicists should know more about numerical techniques and their applicability.

Our motivation to write the book grew steadily from about two decades of experience with students and young scientists in geodynamics (both geologists or geophysicists), who were sometimes disarmed when it comes to understanding of essential features of mathematical and numerical modelling, like how a numerical code works to produce accurate results, which computational methods are behind the codes employed and what is the difference between, let us say, finite differences and finite elements methods, etc. To understand mathematical and computer limitations of numerical modelling, every user should firmly know how the employed numerical methods work for the problems under study. Even though most geoscience students take several semesters of prerequisite courses in maths and/or computer sciences, these students have sometimes little education and experience in quantitative thinking and computation to prepare them to participate in the new world of quantitative geosciences. In order to participate fully in the research of the future, it will be essential for geoscientists to be conversant not only with the language of geology and geophysics but also with the languages of applied mathematics and computers. If all areas of the geosciences are to assimilate into the world of quantitative science, students in geosciences will need a different kind of education than we provide today.

The book *Computational Methods for Geodynamics* bridges two cultures within geosciences (quantitative and qualitative) and assists in solving the problems related to dynamics of the Earth using computational methods. We did not consider filling the gap between geodynamics on the one hand and applied mathematics and computer science on the other hand, but rather to contribute to the understanding of computational geodynamics via basics of numerical modelling, computational methods and challenges in numerical simulations. We believe that this book will complement several excellent textbooks on geodynamics, like *Geodynamics* by Turcotte and Schubert, *Mantle Convection in the Earth and Planets* by Schubert, Turcotte and Olson and *The Solid Earth* by Fowler, in terms of quantitative understanding of geodynamical problems. It will assist students in choosing appropriate numerical methods and algorithms to analyse their research problems (e.g. mantle and lithospheric dynamics, thermal or thermo-chemical convection, geodynamo). This book offers readers the possibility of finding efficient computational methods to be employed in geodynamic modelling (not spending a lot of time in search for the methods in a vast amount of research papers and specialised mathematical books) and seeing examples of how a particular method works for a specific problem. The book can also be of interest to researchers dealing with computational geodynamics as well as to other quantitative geoscientists.

We tried to make the mathematical language of the book not too complicated, and the maths formulations are kept at the level necessary to understand the computational methods. The book is organised into the following parts: fundamental formulations; basic numerical approaches and essential numerical methods; and applications. The first chapter defines the discipline of computational geodynamics and describes the main principles of mathematical and numerical modelling of geodynamic problems. Chapters 2 to 5 describe the finite difference, finite volume, finite element and spectral methods. Chapters 6 and 7 present the basic numerical methods for solving the systems of linear algebraic equations and ordinary differential equations. Chapter 8 is devoted to the methods for data assimilation in geodynamics and presents some applications. The basic concepts of parallel computing are presented in Chapter 9. We discuss how different numerical methods have been used in modelling of various geodynamics problems in Chapter 10.

We have to apologise that the book does not contain all computational methods for geodynamic modelling. We omitted the mesh-free methods, like the discrete element method

(DEM) or the element-free Galerkin method, because these methods are not employed often in modelling of dynamics of the Earth interior and are used mostly to simulate the bulk behaviour of granular material, strain localisation and shear band formations. The reader is referred to some classical works on this topic (e.g. Cundall and Strack, 1979; Liu, 2003) as well as application of these methods to geodynamics (e.g. Hansen, 2003; Egholm, 2007; and references therein).

We have tried to show how mathematical and numerical methods contribute to understanding dynamics of the Earth interior, and how the boundaries between the disciplines are becoming arbitrary and irrelevant. We hope that the book will allow students to learn the languages of the different disciplines in context. Scientists educated in this way, regardless of their ultimate professional speciality, would share a common scientific language, facilitating both cross-disciplinary understanding and collaboration. Mathematics and computational methods provide the best way of understanding complex natural systems, and a good mathematical education for geoscientists is the best route for enabling the most able people to address really important problems in Earth sciences.

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We will be very grateful for comments, inquiries and complaints on the content of the book.