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# Mathematical and Computational Models of Flows and Waves in Geophysics







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Gerardo Hernández-Dueñas • Miguel Angel Moreles Editors

# Mathematical and Computational Models of Flows and Waves in Geophysics



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### Preface

This volume proposes an integral approach to studying the geophysics of Earth. It is motivated by a variety of phenomena from nature with deep and direct impacts in our lives. Such events may evolve across a large range of spatial and time scales and may be observed in the ocean, the atmosphere, the volcanic surface, as well as underground.

The physical laws dictating the evolution of such phenomena lead to the unifying theme of this manuscript, that is, the mathematical and computational modeling of flows and waves. Consequently, the underlying models are given in terms of partial differential equations (PDEs) whose solutions are approximated using numerical methods, thus providing simulations of the aforementioned phenomena, which are to be given the appropriate geophysical validation and interpretation.

The outline of the book is as follows. The first chapter considers rapidly rotating convectively driven flows in extreme parameter regimes, which are of relevance in geophysical and astrophysical settings. The underlying model is the rapidly rotating Rayleigh-Bénard convection (RRRBC) primitive equations. It is well known that laboratory explorations and direct numerical simulations of the governing equations are limited. Consequently, alternative methodologies are required. For instance, the chapter introduces an asymptotic reduction based on small Rossby (Ro) number. The resulting equations, the non-hydrostatic balanced geostrophic equations (NHBGE), form a closed system in which the small parameter Ro no longer appears. The asymptotic procedure eliminates the impediments to using the primitive equations to describe geophysical and astrophysical flows. In particular, the reduced equations describe four important dynamical regimes: cellular convection, convective Taylor columns, convective plumes, and geostrophic applications. The latter connects the chapter that follows.

Chapter 2 deals with interactions of the ocean and the atmosphere, with emphasis on wave theory. The chapter is concerned with some important applications related to the influence of ocean surface waves on present challenging issues. One particular issue is the gas transfer across the interface and its potential impact on climate and its changes. Another one is the upper ocean dynamics and the behavior of surface currents and drift, greatly associated with transport of pollutants and objects on the sea surface. It is noteworthy that the chapter develops the underlying theory, complementing it with data to provide insightful information on the air-sea transfer mechanisms. The aim is to obtain the best knowledge in that respect, in order to be able to predict in the most appropriate fashion the ocean-atmosphere exchange processes of greenhouse gases for instance, and in due course to predict climate and its changes through the use of powerful numerical models.

As illustrated by the first two chapters, in recent decades, computational resources have made possible the simulation of complex phenomena. While the first chapter delves into the mathematical physics to understand geophysical flows, the second chapter relies on data and observation. Both use numerical methods to complement their respective theses. It is apparent that an in depth knowledge of these methods is essential. Thus, Chap. 3 provides a state-of-the-art contribution for one of such methods. Namely, the work proposes a second-order accurate and robust numerical method for the conservative level-set approach, which is applied for capturing the interface between two fluids. The first two chapters include problems of this sort. The exposition will appeal to a numerical specialist, and specifics of the method are included. For instance, the time integration is based on a method that allows the selection between complete explicit and implicit first-order time formulations or a second-order Crank-Nicolson (implicit) method. The space discretization is based on a finite-volume method on prisms elements consisting of unstructured triangular grids on the horizontal directions and several layers in the vertical. Numerical results for three-dimensional simulations require significant computational time to be carried out. Thus, the entire code is developed in parallel. The parallelization of the algorithm is based on a domain decomposition into several sub-domains in the horizontal direction, one for each parallel process, and a parallel solution of the linear system using a multi-color SOR (MSOR) method.

The second part of the book deals with problems associated to solid Earth. In Chap. 4, granular flows in volcanic environments are considered. As a primer, continuum models can be used for modeling this flow phenomenon. However, unlike the equations governing Newtonian fluids, such as the Navier-Stokes equations, granular models may require additional terms that take into account frictional and collisional loss of energy both between particles and between the medium and its substrate. Also, they fail to describe phenomena inherent to the granularity of the medium, such as particle-size segregation and high-speed ejection of individual particles. This failure can be of crucial importance when assessing hazard maps for locations prone to rock avalanches and pyroclastic density currents. Consequently, the chapter focuses instead on the description of discrete models. These models take into account the mechanics of individual particles and are used to explain the behavior of granular flows. This approach uses molecular dynamics (MD) algorithms, which first calculate the sum of forces experienced by each of the individual grains, and afterwards solve the equations of motion with an appropriate integrator. The basics of the method are fully described. An application to active volcanoes is presented.

Preface

Chapter 5 addresses geophysical exploration of underground resources. The exploration of a region of interest requires the measurements of several geophysical datasets which need to be interpreted for characterization. A scheme for cooperative inversion of seismic and gravity measurements is presented. The seismic method has been particularly successful, becoming the basis for other state-of-the-art methods such as full waveform inversion (FWI). FWI is a powerful seismic-imaging method used to estimate a seismic-velocity model such that the discrepancies between observed and synthetic seismograms are minimized. The gravimetric inversion method is an inversion method (GI) for density estimation. This method is well known for estimating structures with horizontal changes of mass distribution. The solution is straightforward using Gauss-Newton minimization to obtain a density model inverting the square matrix on a single step. This method is widely used by geophysicists because of its fast convergence. However, it is computationally expensive and unfeasible for large-scale problems. Full-waveform inversion (FWI) and gravimetric inversion (GI) are carried out in tandem. First, FWI is used to estimate a seismic-velocity model. Then, using Gardner's density-velocity relationship, GI is performed to update the density model. Again, using Gardner's velocity density relation, a velocity model is obtained and the process is iterated. For FWI, minimization is approximated by a gradient-based algorithm. To compute the gradient, the adjoint state method is used. For the reader's convenience, gravimetric and waveform forward modeling are introduced, as well as the numerical methods of solution. Results are illustrated with the well-known Marmousi model, a highly nontrivial benchmark problem in the literature.

The last chapter deals also with wave phenomena. The motivation is the use of electromagnetic methods in geophysics exploration to map the resistive structure of the subsurface using instruments that work at low induction numbers (LINs). These methods have been successfully applied to archaeological studies, groundwater characterization, contaminant migration, and mineral alteration mapping. To interpret electromagnetic measurements, the electric and magnetic fields are computed by solving numerically the Maxwell's equations in the low induction-number domain. The geophysical applications under study lead to high scale computations. Consequently, the differential forms of Maxwell's equations are solved using the parsimonious finite-difference method. Such method is implemented in Fortran and parallelized with OpenMP.

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