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Thomas H. Gibson · Andrew T. T. McRae · Colin J. Cotter · Lawrence Mitchell · David A. Ham

Compatible Finite Element Methods for Geophysical Flows

Automation and Implementation Using Firedrake

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Preface

The development of simulation software is an important aspect of modern scientific computing, especially in the geosciences. Developing complex numerical code requires a large time investment and a range of knowledge spanning several academic disciplines. Arriving at a physical description of a complex physical system, such as a coupled atmosphere, ocean, and land model, demands acute awareness of domain sciences: meteorology, oceanography, biochemistry, ecology, and rheology. Discretising the governing partial differential equations to produce a stable numerical scheme requires expertise in mathematical analysis, and its translation into efficient code for massively parallel systems demands advanced knowledge in low-level code optimisation and computer architectures. Therefore, development of such software is a multidisciplinary effort and its design must enable scientists across several disciplines to collaborate effectively.

Software projects involving automatic code generation have become increasingly popular in recent years, as these help create a separation of concerns between different aspects of development. This allows for agile collaboration between computer scientists with expertise in hardware and software, computational scientists with expertise in numerical algorithms, and domain scientists such as meteorologists, oceanographers, and climate scientists.

The finite element method is a standard mathematical framework for computing numerical solutions of partial differential equations. It has been widely used in engineering applications for many decades, due to its ease of use on unstructured grids and in complicated geometries. It has become increasingly popular in fluids and solids models within geosciences, and its formulation is highly amenable to code-generation techniques. A weak formulation of the relevant PDEs, together with a mesh and appropriate discrete function spaces, is enough to characterise the problem completely.

The models we present in this book use 'compatible', or 'mimetic', finite element discretisations. While their use in fluids problems is relatively new, compared to the more standard continuous and discontinuous Galerkin methods, their use in other applications can be traced back to the late 1970s. In a geophysical context, these discretisations are a generalisation of the C-grid horizontal variable staggering to a finite element setting. They therefore inherit the C-grid's properties such as good representation of near-grid-scale waves.

The topics in this book are non-exhaustive; the purpose of this text is to provide the reader with an idea for how one might use Firedrake as a base for their own numerical codes. The book is organised in the following way. To establish context, the reader is provided with a gentle introduction to modeling geophysical flows in Chap. 1. This includes summaries of common model hierarchies and desirable properties of numerical models for operational use. Chapter 2 presents the application of finite element modeling for two- and three-dimensional systems. Full discretisations are presented using the framework of compatible finite element methods. Using the Firedrake finite element library is a central aspect of this book, and therefore Chap. 3 is devoted to introduce the reader to basic concepts and examples needed to implement the discretisations summarised in Chap. 2. Both Chaps. 4 and 5 provide numerical implementations of examples using Firedrake in two and three dimensions respectively. In particular, Chap. 5 discusses efficient algorithms for solving the resulting discrete systems, which are essential for real-world operational settings.

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Contents

Chapter 1
Geophysical Fluid Dynamics and Simulation

In this chapter we describe various models for the atmosphere; they will be discretised in the rest of the book. We start by considering models with the fewest approximations and work our way down to simplified models. Model hierarchies have formed the backbone of geophysical fluid dynamics: simpler models are more tractable and easier to analyse, whilst more complex models bring us closer to modelling the real physical system. Moving up and down the hierarchy allows us to trace physical phenomena to mathematical calculations on simpler models. Since the inception of numerical computer simulation, model hierarchies have also been useful as a way to trade off model accuracy with computational cost.

1.1 Hierarchies of Models

The first computer weather forecast on the ENIAC (one of the world's first digital computers) by Charney, von Neumann and coworkers solved a single layer quasi-geostrophic model[1] (Lynch, 2008). Subsequently, as computer power increased, it became possible to move up the hierarchy, making fewer model approximations in more numerically intensive calculations. Numerical weather predictions were made with multilayer shallow water models, hydrostatic compressible Euler models, and finally the non-hydrostatic compressible Euler models which represent the state of the art today (Kalnay, 2003; Bauer et al., 2015; Staniforth and Wood, 2008). Model hierarchies are also very useful in the development of numerical models. One can move down the hierarchy to isolate specific aspects of the model to examine their numerical treatment in a less computationally intensive setting, and then move back up to use this insight. In the development of atmospheric dynamical cores, it is very

[1] We will not cover the quasi-geostrophic model in this book. It is an approximation that filters out acoustic and internal gravity waves, hence allowing a larger timestep, which made the computation feasible on the ENIAC.

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standard to start with the shallow water equations to focus on horizontal discretisation aspects before moving up the hierarchy.

The hierarchy of models we will build up in this chapter is shown in Figure 1.1. This is just one choice of hierarchy, since for example one can apply the hydrostatic approximation directly to the compressible Euler equations without making Boussinesq/anelastic approximations. Similarly, we do not consider quasi-geostrophic approximations which are valid for rapidly rotating systems; these approximations can be made at any step of our hierarchy.

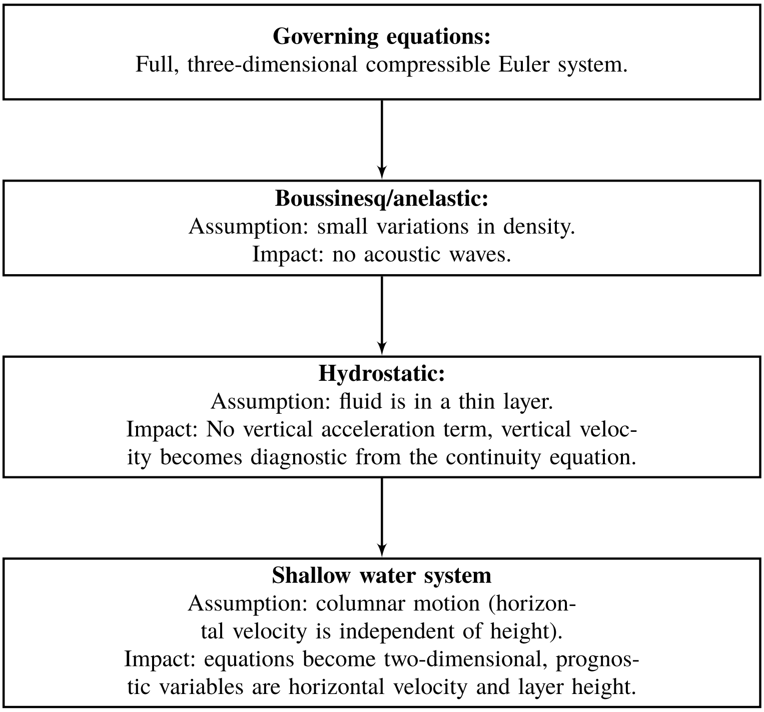

Fig. 1.1 A hierarchy of models illustrating a successive application of various approximations to yield simplified models

1.1.1 The Compressible Euler System

We start by presenting the compressible Euler equations, which have the fewest approximations amongst our hierarchy. We assume that the air is dry (no moisture), inviscid (no viscous forces), and adiabatic (no sources or diffusion of temperature). The governing equations for a dry, inviscid, adiabatic, compressible fluid in a rotating reference frame with angular velocity $\boldsymbol{\Omega}$ may be written in the form

$$\boxed{\begin{aligned} \frac{D\boldsymbol{u}}{Dt} + 2\boldsymbol{\Omega}\times\boldsymbol{u} &= -\frac{1}{\rho}\nabla p - \nabla\Phi, && (1.1)\\ \frac{\partial\rho}{\partial t} + \nabla\cdot(\boldsymbol{u}\rho) &= 0, && (1.2)\\ \frac{D\theta}{Dt} &= 0, && (1.3)\\ p &= P(\rho,T), && (1.4) \end{aligned}}$$

where: $\boldsymbol{u}$ is the fluid velocity, ρ is the fluid density, p is the pressure, and Φ is the geopotential comprising the gravitational and centrifugal potentials (often neglected as it is small compared to the gravitational potential). We use the potential temperature θ, defined as the temperature an air parcel would attain if moved adiabatically to a reference pressure p_R. The ideal gas laws allow us to compute this explicitly:

$$\frac{T}{p^\kappa} = \frac{\theta}{p_R^\kappa} \implies \theta = T\left(\frac{p_R}{p}\right)^\kappa, \tag{1.5}$$

where p_R is a chosen reference pressure, and $\kappa = R/c_p$ is the ratio of the gas constant R and the specific heat at constant pressure c_p. The payoff for this rather complicated formulation is that the potential temperature is constant along Lagrangian trajectories in the absence of diabatic processes.

Given some velocity field $\boldsymbol{u}$, we denote the material derivative by $\frac{D}{Dt}$. For a field F, $\frac{DF}{Dt}$ is given by the instantaneous time rate of change of F, plus a contribution from the spatial variation of F as a result of being moved by $\boldsymbol{u}$,

$$\frac{DF}{Dt} \equiv \frac{\partial F}{\partial t} + (\boldsymbol{u}\cdot\nabla)F. \tag{1.6}$$

If the material derivative is zero, then the field is materially conserved following the motion of the fluid. Thus we interpret the above equations as material derivatives of various fluid quantities, especially after noticing that

$$0 = \frac{\partial\rho}{\partial t} + \nabla\cdot(\boldsymbol{u}\rho) \equiv \frac{D\rho}{Dt} + \rho\nabla\cdot\boldsymbol{u}. \tag{1.7}$$

Equation (1.4) closes the system of equations by relating pressure to the other thermodynamic variables. In the case of the atmosphere, the equation of state for an ideal gas is typically used, i.e.,

$$P(\rho,T) = \rho RT, \tag{1.8}$$

where R is the gas constant for dry air.

It is fairly common to use an alternative formulation of the pressure gradient term

$$\frac{1}{\rho}\nabla p = c_p\theta\nabla\Pi, \tag{1.9}$$

where Π is the Exner pressure given by the equation of state

$$\Pi = \left(\frac{R\rho\theta}{p_r}\right)^{\frac{\kappa}{1-\kappa}}. \tag{1.10}$$

One of the reasons for making this change is that it is then fairly simple to incorporate the thermodynamic effects of moisture into the pressure gradient term. The situation is more complicated in the case of the ocean, where the equation of state additionally depends on salinity. In this book we shall concentrate on the dry adiabatic case, but the techniques developed here are directly extensible to model the moist atmosphere, and the ocean.

These equations also need boundary conditions. In this book we shall mostly restrict ourselves to slip boundary conditions $\boldsymbol{u} \cdot \boldsymbol{n} = 0$ where $\boldsymbol{n}$ is the vector normal to the boundary. Another important boundary condition is the free surface boundary condition, $p = p_A$ (where p_A is an external reference pressure). In this case, the boundary surface must move with the velocity $\boldsymbol{u}$ at the boundary.

We note for later that (1.2) is an expression of local mass conservation; integration over a control volume V leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho \,\mathrm{d}\boldsymbol{x} + \int_{\partial V} \boldsymbol{u} \cdot \boldsymbol{n} \,\mathrm{d}S = 0, \tag{1.11}$$

where $\boldsymbol{n}$ is the outward pointing unit normal vector to the boundary ∂V of V. This shows that the rate of change of total mass in V is balanced by fluxes through the boundary ∂V.

At this point, it is worth discussing various approximations to the Coriolis term $2\boldsymbol{\Omega} \times \boldsymbol{u}$. For a model on the sphere, $\boldsymbol{\Omega}$ is aligned with the polar axis. A common approximation is the *traditional approximation*, under which the vertical part of this force is neglected (since it is small compared to the gravitational force). For a coordinate system whose origin is at the centre of the sphere, we write $\hat{\boldsymbol{r}} = \boldsymbol{x}/|\boldsymbol{x}|$ for the unit vector pointing away from the origin. Then the traditional approximation replaces $\boldsymbol{\Omega}$ with $f\hat{\boldsymbol{r}}$, where $f = \boldsymbol{\Omega} \cdot \hat{\boldsymbol{r}}$. Under this approximation, the Coriolis term vanishes at the equator and is maximum at the poles. We call f the Coriolis parameter.

For both mathematical simplicity and in the study of various models, a patch of the planetary surface can further be approximated by a plane that is tangent at one point. We consider two common treatments of the Coriolis parameter:

1. *f-plane approximation*: $f \equiv f_0$ is taken to be constant-valued. This approximation is used frequently in the case of highly idealised flows. A notable consequence is that Rossby waves, which depend on variations in f, do not occur in models using this approximation.
2. *β-plane approximation*: Since f depends on variations in latitude, an f-plane approximation may not be appropriate when considering flows over large length scales. The β-plane approximation improves on this by considering leading-order variations: $f = f(y) = f_0 + \beta y$.