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Lars Petter Røed

Atmospheres and Oceans on Computers

Fundamental Numerical Methods for Geophysical Fluid Dynamics

Springer

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Preface

The central purpose of this book is to give the reader an insight into the fundamental issues involved in putting oceans and atmospheres on computers. In short, it describes the numerical solution of the partial differential equations (PDEs) governing the motion of atmospheres and oceans, and geophysical fluids in general. The presentation is geared toward students and researchers who aim to understand the physical content of the equations used in the various models and gain experience of the numerical methods used to solve these equations. Much of the formulation is general, hence applicable to any model. Moreover, it is hoped that this book will be useful to students who wish to become forecasters. In this capacity, they will no doubt find themselves analyzing results generated by model simulations and comparing them with observations. In doing so, and knowing something about the model's inner workings, they will be in a better position to provide feedback to model developers on what is realistic and what is not so realistic about the results.

Apart from a brief discussion of spectral methods, commonly applied when solving atmospheric problems, this book focuses on finite difference methods. Present research and development has evolved beyond finite difference methods (e.g., finite element methods), but the simplicity of the finite difference method is useful in a pedagogical treatment of the subject. Moreover, the finite difference methods are still the most commonly applied approach to atmospheric and ocean science.

It is assumed that the reader has little or no prior knowledge of or experience in the use of finite difference methods, so these are explained in some detail. Furthermore, details are provided on how to develop a set of instructions to enable the computer to do the arithmetic.[1] In this way, the full highly nonlinear PDEs that govern the motion of geophysical fluids may be solved. Hence, putting atmospheres and oceans on computers enables an understanding of their global circulation, and the possibility of predicting it. Moreover, it provides an insight into the nonlinear processes that govern their behavior. It is therefore hoped that this book will be a useful source of information for forecasters and researchers alike in their daily work.

[1]This set of instructions is commonly referred to as the model code.

What This Book Is and What It Is Not

Certain topics in the modelling of atmospheres and oceans may appear complex and esoteric, or even magical, to some students. This may lead to a growing distance between those scientists who analyze results from model simulations and observations and those who deal with the model's inner workings. In an endeavor to reduce this gap, the present treatment focuses on the fundamental issues involved in putting atmospheres and oceans on the computer. For this reason, no fully fledged models are presented. On the contrary, the treatment is limited to some of the fundamental balance equations inherent in models of geophysical fluids, such as the advection, diffusion, and rotating shallow water equations. Moreover, we shall discuss numerical methods that work and others that do not, giving reasons in the latter case.

To familiarize the reader with what it takes to develop a numerical model of atmospheres and oceans, and to develop a code that works, we present computer problems to be solved by the reader at the end of each chapter. These computer problems are always associated with the content of the given chapter. They also contain some analytical work to give the reader a better appreciation of the physics involved in each problem. The reader is therefore encouraged to solve these computer problems as they go along.

Some of the models used to forecast atmospheric or oceanic weather are so-called limited area models (LAM). As their name suggests, LAM models cover a limited geographical area, and therefore open boundaries are present at which there are no natural boundary conditions to replace the governing equations (Røed and Cooper 1986). This means that the governing equations are valid at such boundaries, and conditions must be developed that avoid deteriorating the solution in the interior of the LAM domain. More often than not the LAM model is embedded in a global model, or at least one that covers a much larger geographical area, and under these circumstances, the LAM model is nested. Since nested LAM models are commonly used in day-to-day weather forecasting operations, for both atmospheres and oceans, a chapter is included on how to develop sound conditions or nesting techniques at open boundaries (Chap. 7), and there is a section on two-way nesting (Sect. 10.5).

When a model code is developed to emulate the motion of the atmosphere or the ocean, the aim is often to provide a tool that helps us to understand a certain process, or to provide a model to forecast the geophysical fluid's future states. Hence, the model code must provide results that imitate the behavior of the geophysical fluid in question. Consequently, a model developer must be well versed in physics as well as numerics. The former is needed to judge whether the solution provided by the model code is indeed an approximation of the physical reality, and the latter to ascertain whether the model code yields a stable and true solution of the governing PDEs. The book therefore differs from a book on geophysical fluid dynamics. At the same time, it also differs from a book on numerical methods to solve PDEs. We thus include the physics required to understand why some numerical methods work and some do not.

Organization

This book is organized into eleven chapters and one appendix. It is assumed that the book will not be read cover to cover. Thus, each chapter is more or less independent from the rest. To enhance this independence, each chapter starts with a brief introduction and ends with a summary and a few remarks. This organization allows the reader to read the book in a somewhat arbitrary manner, and it is hoped that this will enhance the book's readability and accessibility, both as a monograph and as a reference for students and researchers. Moreover, one or more computer problems are suggested at the end of each chapter. Students and readers are encouraged to do these problems, and the exercises to test their progress. Equally important, it is hoped that by performing the computer problems students will obtain some hands-on experience in programming and visualization of results. By solving the problems, it is also hoped that students will gain an appreciation of the inner workings of an numerical weather prediction (NWP) or an numerical ocean weather prediction (NOWP) model.

To motivate the reader, and for later reference, Chap. 1 starts by describing how the diffusion, advection, and shallow water equations relate to the full equations governing the motion of the atmosphere and ocean. This requires a recapitulation of the governing equations (Sect. 1.1) and the boundary conditions (Sect. 1.2). The chapter continues by discussing the basic approximations commonly made in meteorology and oceanography (Sects. 1.3 and 1.4), which lead to simplified systems of equations. For instance, Sect. 1.5 shows how to derive the shallow water equations, and Sect. 1.6 the quasi-geostrophic equations. The assumptions and approximations needed to obtain them are highlighted. Readers who are well versed in these matters may skip this chapter without loss of continuity.

The diffusion, advection, and shallow water equations belong to a class of equations known as partial differential equations (PDEs). Consequently, Chap. 2 provides a rather detailed account of the way various types of PDEs relate to the advection–diffusion equations and the shallow water equations, and exposes the different physics inherent in elliptic (Sect. 2.1), parabolic (Sect. 2.2), and hyperbolic (Sect. 2.3) PDEs. At the heart of the finite difference methods are Taylor series. Consequently, Sects. 2.5 and 2.6 are devoted to the basics of Taylor series and how to use them to construct finite difference approximations of the various derivatives entering the governing equations, respectively. This involves a discussion of truncation errors and accuracy (Sect. 2.7). It is convenient at this stage to introduce the reader to the notation used throughout the book (Sect. 2.8). The following sections describe some important and useful mathematical concepts such as orthogonal functions (Sect. 2.9), Fourier series (Sect. 2.10), and Fourier transforms (Sect. 2.11). Again readers who are well acquainted with the above may skip this chapter without loss of continuity, except for the part on notation.

Most of the problems associated with geophysical phenomena are time marching problems, which is the subject of Chap. 3. The focus is not on how to solve them, but rather on some of the properties, e.g., conservation of mechanical energy, inherent in the diffusion (Sect. 3.2), advection (Sect. 3.3), and shallow water equations (Sect. 3.4). These are properties that should carry over when solving them numerically, and are therefore useful in assessing model performance. Checking whether these properties are adhered to is part of the quality assurance procedure outlined in some detail in Chap. 11, at the end of this book.

The bulk of the book is contained in the next three chapters, i.e., Chaps. 4, 5, and 6. They lay out various schemes whereby, respectively, the one-dimensional versions of the diffusion, advection, and shallow water equations may be solved numerically by finite difference methods, e.g., the forward-in-time centered-in-space (FTCS) scheme and the centered-in-time centered-in-space (CTCS) leap-frog scheme.

Chapter 4 introduces important and general concepts belonging to the world of finite difference methods, e.g., necessary and sufficient conditions for numerical stability (Sects. 4.3 and 4.7), consistent and convergent schemes (Sect. 4.9), explicit and implicit schemes (Sect. 4.8), and numerical dissipation (Sect. 4.5). Section 4.4 offers a comprehensive exposition of von Neumann's stability analysis, used to investigate under which conditions a given scheme is stable. This is then used to investigate the stability of the diffusion equation (Sect. 4.5). Finally, Chap. 4 also includes a section on how to solve an elliptic problem, using Gauss elimination as a direct elliptic solver (Sect. 4.11).

Chapter 5 continues by exploring the one-dimensional advection equations. Besides introducing various schemes, e.g., the leap-frog scheme (Sect. 5.3), the upstream scheme (Sect. 5.9), and the Lax–Wendroff scheme (Sect. 5.11), by which it may be solved, this chapter also introduces pivotal concepts such as numerical dispersion (Sect. 5.5), computational modes (Sect. 5.7), and numerical diffusion (Sect. 5.15). Section 5.16 presents methods and schemes whereby these unwanted properties may be lessened or avoided. Section 5.12 offers an explanation of yet another scheme, the so-called semi-Lagrangian scheme. This is becoming more and more popular in today's models of atmospheres and oceans, and paves the way for introducing the quasi-Lagrangian schemes used to solve the shallow water equations in Chap. 6. Among the computer problems suggested at the end, the reader is encouraged to complete Computer Problem 5.19.1, which gives insight into how dispersion, diffusion, instabilities, computational modes, etc., tend to show up in the results produced by a numerical model.

Chapter 6 treats the shallow water equations, both in linear and nonlinear form. After presenting the nonlinear, rotating shallow water equations, Sect. 6.2 discusses the various assumptions and approximations required to derive the linear shallow water equations. Section 6.3 is devoted to analytic solutions of the linear equations, such as inertia-gravity waves, coastal Kelvin waves, and Rossby waves, and introduces the potential vorticity as a first integral of the shallow water equations. These waves are observed phenomena and manifest themselves, for instance, as tide and storm surges in the ocean. In contrast, the energy contained in the inertia-gravity waves of the atmosphere is so small that it is regarded as noise. The chapter therefore includes a section on the semi-implicit method commonly applied in atmospheric models (Sect. 6.8). Also discussed are staggered grids (Sect. 6.5), originally introduced by Mesinger and Arakawa (1976) to avoid specifying more boundary conditions than allowed. The remaining sections provide details about various useful schemes for solving the shallow water equations. Since the shallow water equations, like the advection equation, are hyperbolic systems, many of the schemes that work for the advection equation also work for the shallow water equations, e.g., the leap-frog scheme, but since they involve more than one dependent variable they also open the way to new schemes, such as the forward–backward scheme and the quasi-Lagrangian scheme. Computer Problems 6.11.1 and 6.11.2 are particularly recommended here.

Chapter 7 is about open boundaries. In a numerical forecasting model, the size of the grid cells determines its resolution. Since computers have a limited capacity, there will always be a trade-off between grid size and geographical coverage. This implies the existence of a computational boundary where the governing equations are still valid, but where the computation stops. At these boundaries, referred to as open boundaries, a condition must still be constructed to replace the governing equations. This is the theme of Sects. 7.3 through 7.6. However, most of today's limited area forecasting models (LAM) are embedded in a global or basin scale model. The open boundary is then an interface between the LAM and the global model, which has a coarser grid size than the LAM. The solution within the limited area must therefore be nested together with the solution of the coarser mesh model without deteriorating the solution within the limited area. When information is passed on solely from the larger scale model to the limited area model, the technique is referred to as one-way nesting. An example of such a technique, widely used in meteorology, is presented in Sect. 7.5. Recently, two-way nesting techniques have also been suggested, in which information goes both ways. Details of the two-way nesting technique are postponed to Sect. 7.10.

It is common in today's models of atmospheres and oceans to replace the orthogonal Cartesian coordinate system by a non-orthogonal system, in which the vertical coordinate is replaced by a generalized vertical coordinate such as pressure, isopycnal, or terrain-following coordinates. This is the theme of Chap. 8. Section 8.1 explains in general terms how to transform from a Cartesian coordinate system to a new one. In Sect. 8.2, these "rules" are applied to the governing equation of a non-Boussinesq hydrostatic fluid to gain insight into how the equations transform. Finally, Sect. 8.3 provides an example in which the equation is transformed to a particular terrain-following σ-coordinate system.

Throughout this book, we stick to the mantra: "Make things as simple as possible, but no simpler" (Albert Einstein, 1879–1955). Thus, when developing numerical models to solve the diffusion, advection, and shallow water equations (Chaps. 4 through 6), they are simplified to one-dimensional equations. In reality, all numerical models of the atmosphere and oceans are three-dimensional in space. Hence, to gain insight into how to treat equations with more than one independent variable, Chap. 9 investigates the effect of including more than one-dimension in space. Section 9.1 studies the diffusion equation, and Sects. 9.2 and 9.3 the advection equation and the shallow water equations, respectively. Special consideration is given to the effect on numerical stability.

Chap. 10 presents several topics of a more advanced nature. For instance, Sect. 10.1 shows how to construct higher order spatial schemes. The advection equation is used as a sample equation, and special attention is given to the effect on stability, dispersion, and computational modes. Section 10.2 shows how to treat advection and diffusion when they are combined into an advection–diffusion equation, looking particularly at the effects on the stability of the scheme. Another topic discussed in Sect. 10.3 is nonlinearity, which is an important aspect of the motion of atmospheres and oceans. Again, focus is on the effect of nonlinearity on the stability. We discuss in particular the concept of nonlinear instability. Section 10.4 presents filtering methods like the Shapiro filter, used to avoid nonlinearity causing the model to blow up. Applying such a filter is analogous to adding an artificial eddy viscosity (diffusion term), but filtering has wider applications, because it may also be used to smooth out stable, but noisy results. Moreover, filtering is also an inherent part of the two-way nesting technique presented in Sect. 10.5, which is becoming more and more popular in atmosphere and ocean modelling.

Today's models are complex, consisting of more than a thousand executable statements. Only rarely are the codes making up numerical atmosphere and ocean models written by a single person. They are normally written by a group of people and over many years. Thus, an important aspect of maintaining a numerical model is to ensure its quality. The last chapter of this book is therefore devoted to procedures for assessing the performance of a model (Chap. 11). In particular, the notions of tuned, transportable, and robust models are discussed in Sect. 11.2. These pave the way for the introduction of the detailed quality assurance procedures presented in Sect. 11.3. The crucial elements of these procedures are *model verification*, *sensitivity analysis*, and *model validation*.

Finally, we stress that the use of numerical methods to solve atmospheric and oceanographic problems is to a large degree a "hands-on-experience". It is no use learning how to turn the governing equations into sound finite difference equations without learning how to develop a computer code (a set of instructions) to solve them, how to run them on the computer, and finally how to visualize the results. The first part concerns what is called *programming*. It involves writing the instructions, or "code", in some "language" that the computer understands. The programming language used today in most atmosphere and ocean modelling is FORTRAN. The reason is simply that, when compiled, there is no other language that provides the same speed. To give insight into the fundamentals of the language, a brief introduction to FORTRAN programming is given in Appendix A. To gain familiarity with programming in FORTRAN, the reader is encouraged to solve as many as possible of the problems at the end of each chapter in the sections called "Computer Problems". The reader is also encouraged to solve the exercises at the end of each chapter.

Some Historical Notes

In view of the nonlinear character of the equations they had to solve, it is hardly surprising that scientists and forecasters working in meteorology and oceanography so quickly embraced electronic computers as a tool. It all started in 1946 when the mathematician John von Neumann, then a well-known professor at Princeton University, approached the meteorologist Carl-Gustav Rossby[2] to organize a "Conference on Meteorology". The idea was to acquaint the meteorological community with the Electronic Numerical Integrator and Computer (ENIAC) and the Institute of Advanced Study (IAS) machines, and to solicit their advice and support in designing research strategies. The outcome of the conference was the Princeton Meteorological Project (1947–1953) which was managed by Dr. Jule G. Charney.[3] Among the participants were two young Norwegians, Arnt Eliassen[4] and Ragnar Fjørtoft.[5] The project successfully produced a 24-hour numerical weather prediction in less than 2 hours. This very first attempt to produce a numerical weather forecast was published in 1950 by Charney et al. (1950).

The Meteorology Project marked the beginning of the scientific field known as Numerical Weather Prediction (NWP). An important basis for the rapid development of NWP in the 1950s and 1960s was the deterministic paradigm stated by Vilhelm Bjerknes[6] at the turn of the century. In his famous 1904 paper Bjerknes, stated that (Bjerknes 1904):

> If it is true, as most scientists think, that the atmospheric state at any time can be developed from its earlier state using physical laws, then it follows that a necessary and sufficient condition for a rational solution to the problem of weather forecasting is a sufficiently accurate knowledge of the present atmospheric state, and a sufficiently accurate knowledge of the equations that govern the development of the atmosphere from one state to the next.

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[2]Carl-Gustaf Arvid Rossby (1898–1957) was a Swedish-born American meteorologist. He was the first to explain the large-scale motions of the atmosphere in terms of fluid mechanics. He identified and characterized both the jet stream and the long waves in the westerlies that were later named Rossby waves.

[3]Jule Gregory Charney (1917–1981) was an American meteorologist. As part of his Ph.D. work, he developed a set of equations for calculating the large-scale motions of planetary-scale waves (the quasi-geostrophic vorticity equations). He gave the first convincing physical explanation for the development of midlatitude cyclones, known as the baroclinic instability theory.

[4]Arnt Eliassen (1915–2000) was a Norwegian meteorologist who pioneered the use of numerical analysis and computers for weather forecasting. His early work was done at the Institute for Advanced Study in Princeton, New Jersey, together with John von Neumann. He received the Carl-Gustaf Rossby Research Medal in 1964 and the prestigious Balzan Prize in 1996 "for his fundamental contributions to dynamic meteorology that have influenced and stimulated progress in this science during the past fifty years".

[5]Ragnar Fjørtoft (1913–1998) was an internationally recognized Norwegian meteorologist. He was part of the Princeton team that performed the first successful numerical weather prediction using the ENIAC electronic computer in 1950. He was also a professor of meteorology at the University of Copenhagen and director of the Norwegian Meteorological Institute.

[6]Vilhelm Friman Koren Bjerknes (1862–1951) was a Norwegian physicist and meteorologist who did much to develop the modern practice of weather forecasting.

Another important basis was the later attempt by Lewis Fry Richardson[7] to compute a 6-hour weather forecast by hand. He did this by first casting the governing equations into finite difference form using numerical methods (Richardson 1922). Afterwards, while serving with the Quaker ambulance unit in northern France during World War I, he solved the finite difference equations using only pen and paper.

Although Bjerknes did not mention it, the statement quoted above is also true when forecasting oceanic "weather", that is, the growth and fate of meanders, jets, and eddies, the latter being the ocean's high- and low-pressure systems. Oceanic lows and highs are, however, much smaller than their atmospheric counterparts. Hence, the power and capacity of the early computers was insufficient to make oceanic forecasts in the 1950s and early 1960s. However, as computer power and capacity grew,[8] computers and numerical methods were also more commonly used to solve the equations governing oceanic motion. The first published results from numerical experiments using a basin scale ocean model appeared in Bryan and Cox (1967).[9] This started the scientific field of Numerical Ocean Weather Prediction (NOWP) in the late 1960s. In fact, the capacity and power of today's computers are suitable for forecasting oceanic weather, at least for limited areas. Furthermore, it is interesting to note that NWP and NOWP are among the major scientific fields pushing computer technology to its very limits.

The atmosphere and the ocean form a coupled system exchanging momentum, heat, and moisture. This was recognized early on in climate modelling, and the very first climate models were thus coupled atmosphere–ocean models (an excellent review can be found in Edwards 2011). With the ever-growing capacity of computers, coupled atmosphere–ocean models are also developed with NWP/NOWP in mind (see, e.g., Warner et al. 2010). In this undertaking, sea ice and wave models are also taken into account. Thus, in the not too distant future, fully coupled models will probably be the standard prediction tool for making weather forecasts of atmospheres and oceans in one sweep. In light of this, anyone aspiring to become a meteorologist, an oceanographer, or a climatologist must have a sound knowledge of and insight into the fundamental methods used to develop reliable numerical methods for solving oceanographic and meteorological problems.

[7]Lewis Fry Richardson (1881–1953) was an English mathematician, physicist, meteorologist, psychologist, and pacifist who pioneered modern mathematical techniques of weather forecasting.

[8]Growth in computer power and capacity has been almost exponential since the 1940s.

[9]Kirk Bryan (Jr.) (b. 1929) is an American oceanographer who is considered to be the founder of numerical ocean modelling. Starting in the 1960s at the Geophysical Fluid Dynamics Laboratory, Bryan worked with a series of colleagues to develop numerical schemes for solving the equations of motion describing flow on a sphere. His work on these schemes led to the so-called Bryan–Cox code, used for many early simulations, and it also led to the Modular Ocean Model currently used by many numerical oceanographers and climate scientists.

Readers who are interested in a full account of the history, personalities, and ideas behind the successes of NWP and NOWP are encouraged to read the excellent book published recently by the mathematicians Ian Roulstone and John Norbury (Roulstone and Nordbury 2013).

Caveats and Concerns

It should be emphasized that the numerical solutions returned by the computer depend on the method used. The computer is very good at producing numbers based on the instructions it receives. The numbers may look reasonable, even when they provide a false solution. When developing a model code, or making use of an existing model code of the atmosphere and/or ocean, it is important to be able to judge whether the given numerical method yields the "true" solution to the PDEs. The essence of this book is about acquiring just such knowledge.

As already mentioned, most processes in the ocean and atmosphere are highly nonlinear, so more and more research in NWP and NOWP relies on sometimes hugely complex computer codes. It is a growing concern that many of these codes are written and amended by scientists who are not necessarily skilled programmers. This concern is corroborated in a statistical survey by Hannay et al. (2009), which states "the knowledge required to develop and use scientific software is primarily acquired from peers and through self-study, rather than from formal education and training". Even though the numerical methods may be sound, the codes themselves may be rather poorly written from a skilled programmer's point of view. Only rarely do these codes undergo rigorous testing. Hence, model codes may inadvertently contain errors that are potentially damaging to the results.

Another serious concern is that computers always produce results in terms of numbers. These numbers may look reasonable, but in reality be totally false due to the use of unsound numerical methods. Such results may even lead to wrong conclusions. In fact, there are examples in the literature where a numerical solution is interpreted as a new physical phenomenon, which is later shown to be a pure artifact produced by an incorrect numerical method. It is therefore important to understand why some methods are sound and some unsound for a specific problem. Likewise, it is important to acquire knowledge of the "quality" of the computations. In light of these concerns, a chapter is added at the end of the book to give insights into quality assurance procedures that can be used to assess the quality of a specific model (Chap. 11).

Many of the numerical methods employed today have been developed historically to solve atmospheric problems. Nevertheless, these methods also work when solving oceanographic problems, simply because the *dynamics* of the two systems are very similar. In a numerical context, there is therefore no need to treat meteorology and oceanography separately, in particular regarding the more fundamental methods. A further rationale is, as already mentioned, that atmospheres and oceans are inherently coupled. However, it should be kept in mind though that there are also numerical methods and techniques unique to each of them. In particular this concerns methods relevant to *thermodynamics*. However, the treatment of these issues goes beyond the scope of this book.

Oslo, Norway Lars Petter Røed
March 2017

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[10]http://www.stephenlyle.org/.

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