PREFACE

The central purpose of this book is to contribute to a rationalization of the physical, mathematical, and numerical foundations of computer models used to understand and predict the global ocean circulation. The presentation is geared toward students and researchers in ocean and climate science who aim to understand the physical content of the equations used in ocean models and to become exposed to methods for solving these equations. Much of the formulation is general, and so applicable to any ocean model. However, for purposes of presenting concrete examples, attention is focused on z-coordinate models and generalizations based on isomorphisms with the z-model structure. In their traditional construction, z-models represent the most common model class used to simulate the global ocean climate system. Future ocean model research and development certainly will evolve beyond the limitations of z-models (see Chapter 6). Nonetheless, their maturity and popularity, and the ease of generalizations beyond them, warrant a thorough discussion. Furthermore, their relative simplicity aids in the pedagogical treatment of the subject.

It is hoped that this book can partially fill a niche in the literature whereby a (mostly) first principles presentation of ocean climate models is given, with discussions extending from fundamental ocean fluid mechanics to detailed parameterization and discretization issues. This aim is to be distinguished from a book on ocean *modeling* or a book on ocean *physics*. To do justice to ocean modeling, a book must provide extensive discussions of simulations and their relation to Nature's ocean. To do justice to ocean physics, we would need to remove much of what remains fundamental to the model builder yet which can be characterized as "ocean model engineering." Further discussions of theoretical solutions and phenomena would also be required of such a book.

To the student, some topics in ocean model fundamentals can appear complex and esoteric. This point has contributed to what is arguably a growing distance between scientists who analyze numerical ocean model simulations and scientists who understand details of the model's inner workings. The two groups ideally should be working hand-in-hand, so that model users who compare simulations to observations can provide feedback to educate model builders about what is realistic, and not so realistc, regarding the simulations. Likewise, model builders must communicate to the user certain of the model's fundamental aspects, and its limitations, so as to lend perspective and experience to the user.

When the model user knows little of the model fundamentals, and the model builder is detached from observations of Nature's ocean, models stand the chance of losing credibility, and large-scale observations can lack a rational mechanistic description. This situation is unhealthy for the science.* It is hoped that this book provides the climate science student and/or researcher with a digestible presentation of ocean models so as to assist in removing their mystery and opacity. In the end, this book will be worth the effort (to read and to write) if it helps to reduce the distance between model builder and model user.

WHAT THIS BOOK IS AND IS NOT

The scientist who builds an ocean model aims to provide a tool facilitating the understanding of ocean physics. Ideally, the numerical tool is congruent with physical reality, and so the model builder must be well versed in ocean physics. By exposing a selection of fundamental physical issues that arise when building an ocean model, this book may allow the student to garner a better appreciation, if not an improved understanding, of the underlying notions and methods forming the foundation of models.

To assist in providing a readable book, presentations are self-contained and generally start from a basic physical perspective. To garner the most from the discussions, some patience and persistence is asked of the reader since many of the discussions are dense. This is perhaps the most important prerequisite for making it through this book from cover to cover. As with most treatments of continuum mechanics, some level of mathematical sophistication, fully explained in the text, proves useful to present physical and mathematical results cleanly and in a generality necessary for developing global ocean models. To help with such material, a working knowledge of classical mechanics, vector calculus, and basic fluid mechanics, each realized from undergraduate physics courses and/or graduate studies in the geosciences, is useful.

This book is not a text on oceanography, geophysical fluid dynamics, or numerical methods. Hence, there are no problem sets given, no computer simulations described, and only very few theoretical solutions presented. Furthermore, little mention is made of ocean observations, and knowledge of basic numerical methods is assumed. For more complete treatments of these subjects, the reader is referred to one or more of the many excellent texts and monographs in the literature. A selection of these, familiar to the author, includes the following.

- Pickard and Emery (1990) and Tomczak and Godfrey (1994) present observational descriptions of the ocean and so introduce the reader to the phenomenology that a computer model aims to simulate.
- Gill (1982), Apel (1987), Pedlosky (1987), Cushman-Roisin (1994), Pedlosky (1996), Mellor (1996), Salmon (1998), and Pedlosky (2003) discuss various aspects of geophysical fluid dynamics and theoretical physical oceanography.
- Washington and Parkinson (1986), Trenberth (1992), Peixoto and Oort (1992), Chassignet and Verron (1998), Haidvogel and Beckmann (1999), Kantha and Clayson (2000a), and Kantha and Clayson (2000b) introduce the reader to various aspects of climate physics and climate modeling.

*In an ideal world, those who focus on the elements of ocean model design and construction should spend time at sea, and those who regularly go to sea should learn more about models and use them to help rationalize datasets.

- The books and reviews by Haltiner and Williams (1980), O'Brien (1986), Bryan (1989), Durran (1999), and Randall (2000) describe numerical methods of use for geophysical fluid dynamics.

- The book edited by Siedler et al. (2001) is noteworthy for its many lucid contributions by leading experts. This book affords the reader a clear view at the state-of-the-art in ocean observations, theory, and modeling.

Given the above caveats about what is not contained in this book, it would be remiss not to admit that there are numerous further topics missing that arguably should be present in a monograph on ocean models. Their absence is due to the author's physical and mental limitations, rather than any reflection on their lack of importance. It is hoped that this book nonetheless serves as a useful complement to other presentations, and that it provides a stepping-stone for future expositions which may fill the many holes contained here.

It is worth commenting a bit here on the level of technical sophistication employed in this book. As discussed above, the aim is to rationally and systematically formulate the equations to be used by numerical ocean climate models. As these models are posed in a spherical geometry, it is necessary to make some use of notions from non-Euclidean geometry. This is facilitated by general tensor analysis. Hence, this book generally does not shy away from the use of tensor analysis where it is needed, yet a conscious effort is made to use more familiar vector calculus notation when sufficient. Overall, it is hoped that the mathematical treatment is self-contained enough to allow the interested reader to become proficient in the tools of tensor analysis. However, those uninterested in such details can readily jump across places where tensor gymnastics are employed, without too much loss of continuity.

This book maintains the premise that *physical, mathematical, and numerical details matter when formulating the algorithms of ocean climate models.* This perspective prompted the author to exploit many of the tensor analysis tools discussed above, as well as ideas from functional methods to discretize the elliptic transport operators appearing in certain subgrid scale (SGS) schemes. However, the approach requires defense since there remains a large degree of uncertainty in the SGS schemes appropriate for ocean climate simulations. The neutral physics and horizontal friction operators discussed in Parts 4 and 5 are prime examples.

A large degree of physical uncertainty may argue for the use of a somewhat "impressionistic" approach regarding the level of detail warranted to formulate the mathematical and numerical aspects of ocean models. However, the perspective taken in this book is that it is precisely because of the large physical uncertainty that modelers should pay a great deal of attention to mathematical and numerical details. Doing so gives a more solid technical foundation to the algorithms, thus allowing the scheme's physical ideas to more clearly translate into rational behavior from the simulation. Importantly, mathematical and numerical rigor does not translate into physical rigor (nor is the complement true). Nor should it be construed as providing weak physical ideas with a sheen of legitimacy. Instead, such attention to detail attempts to provide a sound venue from which to better represent any physics, or lack thereof, available from the scheme. Doing so provides the physical modeler with a better tool for understanding.

Quite generally, what is argued for in this book is an increased level of *honest* *algorithm* development in ocean climate models. By this is meant that physical, mathematical, and numerical details should be exposed, and a sincere attempt should be made to rationally address and document them. Furthermore, assumptions and uncertainties should be clearly articulated rather than obscured. This may prove no more successful in improving the simulations than an impressionistic approach. However, there are cases where less rigorous methods have proven less successful. Additionally, more rigor and honesty will promote an improved facility to reason why simulations from various models agree, or differ, from one another, and in so doing assist in reducing uncertainty in model predictions.

ORGANIZATION

This book is organized into parts, each of which have multiple chapters. It is assumed that the book will *not* be read cover-to-cover. Consequently, the contents of each part are written so that they can largely be read independently. Chapters likewise aim for such independence, though less so. This organizational style allows the book to be useful for those reading it in a more or less arbitrary manner, so long as some of the basics are appreciated. It is hoped that this approach enhances the book's readability, accessibility, and utility as both a monograph and reference to students and researchers.

Chapter 1 starts the book with an introduction to ocean climate models. It is here that we are exposed to some reasons why ocean models are of primary importance for climate science. This chapter also helps to motivate the more fundamental, and by necessity mathematical, development presented in subsequent chapters.

Part 1 begins the main part of the book by focusing on the equations describing stratified fluid dynamics on a rotating sphere. Chapter 2 introduces some physical ideas underlying a continuum description of the ocean fluid. It also highlights common approximations made in ocean climate models. Chapters 3 and 4 derive the hydrodynamical equations of the ocean fluid. Chapter 5 presents aspects of ocean energetics and thermo-hydrodynamics. Chapter 6 presents some mathematical results applicable to a generalized vertical coordinate description of the ocean. This chapter also highlights some deficiencies inherent in the different model classes now in use for simulating the ocean.

The equations described in Part 1 offer a precise mathematical description of a particular realization of the ocean fluid. To make use of this description requires an infinite level of knowledge about the ocean's state, i.e., the positions and velocities of each fluid parcel, and full information about forces acting on the parcels. In practice, we are always faced with less than infinite information in both space and time. Hence, it is necessary to derive alternative equations via a coarse-graining procedure. That is, we need to determine approximate, averaged, or mean field equations for the coarsened ocean fluid.

Part 2 presents three chapters illustrating various issues with averaged descriptions of the ocean. Chapter 7 begins with a general discussion of subgrid scale processes, with a focus on those contributing to dianeutral transport. Such transport is spread non-uniformly throughout the World Ocean, with most occurring in regions near ocean boundaries. Dianeutral transport plays an important role in affecting the ocean's stratification and vertical distribution of tracers, and this chapter provides an introduction to some of the issues. Chapter 8 is the first of two chapters discussing some formal issues related to averaging the equations. Here, we accept the fact that the precise state of the turbulent ocean is not physically measurable with finite instruments, thus necessitating a statistical approach. In particular, this chapter provides a conceptual and mathematical interpretation of the fields discretized by a z-model. It is argued that these equations represent an ensemble mean, as measured at a fixed point in space-time, of individual realizations of the ocean fluid. The subgrid scales considered in this average are associated with the small-scale dianeutral mixing arising from three-dimensional turbulence. In Chapter 9, we focus on the transport of volume and tracers by mesoscale eddies. This transport, which is mostly two-dimensional and oriented according to *neutral directions*, is the dominant means whereby tracers are stirred within the ocean interior, with tracer gradients ultimately dissipated by small scale mixing processes. The discussion in this chapter motivates a particular interpretation of model variables for those cases where the simulations do not explicitly resolve mesoscale eddies. Furthermore, in this context we see how the choice of vertical coordinate strongly affects the simplicity of the mathematical description of adiabatic transport.

Part 3 presents three chapters on the semi-discrete equations of an ocean model, with focus on those equations used in a z-model. Semi-discrete refers to equations that have some parts discretized, some parts continuous. Chapter 10 begins the discussion with an introduction to issues arising when discretizing the primitive equations. This material is quite terse and is presented mostly to anticipate later discussions given in other chapters. The aim for the remainder of this part is to describe in general terms the equations of a discrete z-model, and to outline methods used to time step these equations. In particular, Chapter 11 discusses the semi-discrete version of the mass and tracer budgets, and highlights the importance of maintaining compatibility between these budgets. Chapter 12 discusses various methods used to march the primitive equations forward in time.

Chapter 9 introduces a framework for thinking about transport in the ocean interior. The parameterization of this transport in ocean models constitutes the *neutral physics* part of the models. Notably, the integrity of z-model simulations has greatly improved since modelers started employing such schemes (for a review, see Griffies et al., 2000a). Part 4 of this book aims to rationalize the neutral physics schemes commonly used in z-models. This aim is far from realized, since so many aspects of subgrid scale closure applied to ocean models are not deductive. Nonetheless, we give it our best shot.

In the first two neutral physics chapters, Chapters 13 and 14, we explore physical and mathematical aspects of neutral physics transport operators. Our focus in these discussions is on neutral physics in the ocean interior, as this has been the emphasis thus far in the literature. In Chapter 15, we consider how modelers handle the neutral physics schemes next to boundaries. This material is relatively fresh and is the subject of intense research. Chapter 16 finishes this part with details of a method for discretizing neutral physics in z-models.

Horizontal friction used in ocean models plays an important role in determining the integrity of the simulations. Additionally, the state of the art in ocean climate model horizontal friction remains at an engineering stage, with modelers encouraged to use horizontal friction largely for purposes of maintaining numerical stability. The more scientifically satisfying situation is to consider horizontal friction as a parameterization of unresolved physical processes, such as in the kinetic theory of gases. However, there is no theory for how to close the momentum equation at scales relevant to ocean climate studies. Hence, horizontal friction used in ocean climate models is *ad hoc*. Indeed, some argue that dissipation of kinetic energy, which all the model implementations of friction aim to do, is an egregiously incorrect basis on which to design the schemes (e.g., Holloway, 1999). Either of these points would remain purely academic, were it not for the importance that friction plays in the simulations. Its details are crucial especially in boundary and/or equatorial regions, where geostrophy breaks down. Hence, it is critical that modelers understand the rationale underlying some of the commonly used schemes, if only to motivate approaches that lead to improvements.

Given the importance to simulations of horizontal friction, Part 5 is offered as a tutorial for these issues as they are commonly practiced in ocean climate modeling. Chapter 17 focuses on the friction force in the continuum, with mathematics developed in Part 6 of some utility. Chapter 18 then considers how to choose a viscosity to set the friction force's magnitude in an ocean climate model. The issues discussed in these chapters are generic, whereas Chapter 19 finishes this part of the book with a discretization of the horizontal friction operator on a B-grid.

Tensor analysis is not commonly taught in oceanographic or atmospheric science curricula. However, an understanding of general tensor analysis is necessary when formulating the equations of rotating fluid dynamics in a spherical geometry. Hence, tensor analysis is needed by those actually building ocean climate models, and by those aiming to fully understand details of the model's equations. Two chapters are included at the end of the book that aim to develop tensor analysis from a relatively fundamental level, with examples drawn from ocean fluid dynamics. Chapter 20 introduces the basic notions, and Chapter 21 expands on these notions while deriving some key results from calculus on curved manifolds. The presentation is aimed at the reader who has a solid foundation in undergraduate vector calculus. No exposure to Cartesian or general tensors is assumed. The pace may be a bit slow for those who have some exposure to tensor analysis, yet it is hoped that both experienced and inexperienced readers will find something of use here. For those aiming to garner a "just-the-facts" treatment, some attempt has been made to allow one to only briefly read or to skip much of this material. For this purpose, salient points are summarized as needed in the appropriate places throughout the main text, with Section 21.12 offered as a more general summary.

CONCERNING AN EMPHASIS ON SGS PHYSICS

Some comments are offered here to anticipate how the reader may feel after reading the large parts of this book addressing SGS physics. For those who may feel unsatisfied, consider three possible reasons. First, parameterizations of the ocean SGS are based on partially deductive arguments, and a great number of inspired guesses. Describing the subgrid scale, and turbulence in particular, is highly nontrivial and incomplete, both formally and phenomenologically. There are few general principles and few unambiguous observations. Second, as mentioned in many places throughout this book, simulations are dependent on details of the closure schemes. The reader will need to take this point on faith, since no simulations are presented in this book. Griffies et al. (2000a) reviews numerous studies illustrating this point. It is unsettling that simulation integrity depends to a large degree on aspects of the models that are uncertain. Unfortunately, this is the state of the art in ocean modeling. Third, sensible implementations of many closure schemes in a global model require a relatively sophisticated level of mathematical and numerical tools. The reader may feel little motivation for learning the fancy tools, if the physical ideas underlying the tools are only partially complete or even wrong. However, experience has shown that cavalier implementations of closure schemes can produce spurious results, thus rendering a poor or incorrect understanding of what the scheme is physically supposed to be doing in the simulation. Hence, fleshing out whether a scheme makes sense physically for global ocean simulations often requires a nontrivial investment in methods and techniques. Notably, the use of sophisticated mathematical and numerical tools, many of which are described in this book, in no way should be mistaken for sanctioning a physical theory as being sound, robust, or the final word on the subject.

Given the incomplete status of many ideas in ocean subgrid scale closure, one may argue that there is little reason to write a book, or a large part of a book, that places so much energy on documenting schemes now in use. Indeed, with the title to this book using the word “fundamentals,” one may feel this should require it to present notions that are in universal agreement within the ocean science community. Such is not the case for *ocean model* fundamentals, nor is it likely that the community will reach such a state. Ocean scientists thrive on debate. But then why not at least wait until ideas are clarified a bit more? How much more?

Attempts to tie together various strands of understanding can help to reveal those parts of the story that are incomplete or wrong. There are indeed many incomplete stories in this book, and elsewhere in ocean modeling. Some are likely very wrong. Nonetheless, science makes progress when both what is well established, and what is not so well established yet is done in practice, are pedagogically articulated. One goal of this book is to do just that. If this goal is realized, even partially, then some success will have been achieved. Fundamental methods, techniques, formulations, assumptions, and presumptions must be exposed to the point that researchers and especially students can better understand what sorts of problems are in need of being solved and where there are holes in understanding. Oceanography requires such for its evolution into a mature science.

OCEAN CLIMATE MODEL DEVELOPMENT

Let us close this preface with some personal reflections on what is necessary for the climate science community to produce the highest quality numerical models. Start by noting the obvious: ocean climate models are not conceived one year, to be then publicly released and supported the next. Instead, they take years, indeed decades, of creative passion and obsession from many scientists and engineers. It is only via patience and persistence that an ocean climate model is successfully realized.

There are many phases of development that an ocean climate model sees. The first phase can be considered a *vision* phase, where model equations are written down and then debated by theorists and modelers alike. Material in Parts 1 and 2 of this book address this phase. Upon arriving at a set of suitable equations, one moves onto the prototype phase, where the continuum equations are discretized and coded into one's favorite computer language (Matlab, Fortran, C, etc.) using various numerical methods. Simplified tests are conducted and analyzed using the prototype model, and modifications made to address problems and limitations. In Parts 3, 4, and 5 of this book, we encounter examples of how to take the continuum equations and cast them into a form appropriate for certain ocean models, and methods are presented to solve these equations. No numerical tests are presented, as this would add much to an already long book.

Assuming that the developer of the prototype model is confident that the model produces a physically relevant simulation, one then moves onto the third and perhaps most taxing phase of ocean climate model development. It is taxing since it requires a significant level of interaction and compromise with other model developers and model users, possessing their own needs and desires. This phase sees the prototype model, which is basically a raw skeleton, become penetrated and surrounded by a tremendous amount of infrastructure and superstructure. These added layers serve many purposes, not the least of which are (A) to allow the ocean model be readily coupled to other component models, such as models of the atmosphere, sea ice, biogeochemistry, etc.; (B) to facilitate the model's use on various computer platforms, each of which possesses idiosyncrasies understood by few but experienced by many; (C) to provide diagnostic capabilities that render the model accessible to scientific probing; and (D) to remain flexible enough so that its algorithms can be modified, tested, and further refined. Only by successfully completing the third phase does an ocean model become appropriate for serious ocean climate studies.

Model documentation is essential during the third phase, and afterward, since multiple users make contact with the model and require clear, complete, and pedagogical treatments of the algorithms. Without this, the model may tend toward becoming a black box, with only a few developers privy to its underlying "knobs and handles." In contrast, models that are well documented allow for easier usage and so present fewer barriers to the developer and nondeveloper alike. Furthermore, honest documentation allows for educated scrutiny from those scientists who may not have the time or ability to penetrate the computer code, but who can provide valuable comments on the methods and fundamentals. This situation clearly advances the state of ocean climate model integrity, and thus advances the climate science field in general.

The final stage of model development comes about when limitations of a particular model become so apparent that new efforts focus on building a new model prototype, thus starting the process over again. The motivation for starting over may come from new paradigms in computer architecture, novel ideas regarding ocean model algorithms, or simply the desire to understand and have control over the details of the model. The magnitude of the redevelopment effort should not be underestimated by those aiming to start over.

Ocean model development as a process flourishes only when there is an intimate marriage between research and development, with each phase of model building requiring an unpredictable amount of time to debate and explore various research avenues. Allowing adequate time requires dedication and support from funding agencies and managers. Absent such, ocean climate model development is handicapped, the integrity of simulations compromised, and the depth of scientific understanding shallow. For this reason, it is critical to maintain a research and development environment that fosters a healthy balance between addressing the exigencies of the moment with visions extending out years and decades. Doing so will help climate modeling to mature into a hard science. Short of this goal, the massive problems of climate science, including anthropogenic climate change, will remain elusive. It is the profound responsibility of leaders in the international climate science field to foster a balanced research and development environment, especially now that the questions of climate change are at the forefront of society's concern, and the signals appear to be rising above ambient levels of natural variability.

DISCLAIMER

Early versions of this book grew from various notes and publications written over many years to document the *Modular Ocean Model* from the Geophysical Fluid Dynamics Laboratory. Hence, elements of this book originate from scientific papers published while the author was a GFDL employee. Reference to these papers is provided at the appropriate place in the text. However, no sentences in this book are taken verbatim from published papers. The material has been extensively reworked, refined, and digested to enhance pedagogical value well beyond that appropriate for technical papers or reports. Additionally, the bulk of this book's writing occupied personal time, and was not part of any official assigned government duty.