MODELING METHODS FOR MARINE SCIENCE

This textbook on modeling, data analysis, and numerical techniques for marine science has been developed from a course taught by the authors for many years at the Woods Hole Oceanographic Institution.

The first part of the book covers statistics: singular value decomposition, error propagation, least squares regression, principal component analysis, time series analysis, and objective interpolation. The second part deals with modeling techniques: finite differences, stability analysis, and optimization. The third part describes case studies of actual ocean models of ever-increasing dimensionality and complexity, starting with zero-dimensional models and finishing with three-dimensional general circulation models. Throughout the book hands-on computational examples are introduced using the MATLAB programming language and the principles of scientific visualization are emphasized.

Modeling Methods for Marine Science is a textbook for advanced students of oceanography on courses in data analysis and numerical modeling. It is also an invaluable resource as a reference text for a broad range of scientists undertaking modeling in chemical, biological, geological, and physical oceanography.

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CAMBRIDGE UNIVERSITY PRESS

CAMBRIDGE
UNIVERSITY PRESS

32 Avenue of the Americas, New York NY 10013-2473, USA

Cambridge University Press is part of the University of Cambridge.

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www.cambridge.org
Information on this title: www.cambridge.org/9780521867832

First published 2011

A catalogue record for this publication is available from the British Library

ISBN 978-0-521-86783-2 Hardback

This book is dedicated to
Tina, Susan, and Andrea.
They have endured our preoccupations with
loving support, rare good humor,
and infinite patience.

Cambridge University Press
978-0-521-86783-2 - Modeling Methods for Marine Science
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Preface

If you are a student of science in the twenty-first century, but are not using computers, then you are probably not *doing* science. A little harsh, perhaps, and tendentious, undoubtedly. But this bugle-call over-simplification gets to the very heart of the reason that we wrote this book. Over the years we noticed, with increasing alarm, very gifted students entering our graduate program in marine chemistry and geochemistry with very little understanding of the applied mathematics and numerical modeling they would be required to know over the course of their careers. So this book, like many before it, started as a course – in this case, a course in modeling, data analysis, and numerical techniques for geochemistry that we teach every other year in Woods Hole. As the course popularity and web pages grew, we realized our efforts should be set down in a more formal fashion.

We wrote this book first and foremost with the graduate and advanced undergraduate student in mind. In particular, we have aimed the material at the student still in the stages of formulating their Ph.D. or B.Sc. thesis. We feel that the student armed with the knowledge of what will be required of them when they synthesize their data and write their thesis will do a much better job at collecting the data in the first place. Nevertheless, we have found that many students beyond these first years find this book useful as a reference. Additionally, many of our colleagues in the ocean sciences, broadly defined (chemical, biological, geological, and yes, even physical), find this book a useful resource for analyzing or modeling data.

Readers will find this book to be self-contained inasmuch as we introduce all of the concepts encountered in the book, including bringing the reader up to speed on ocean science and physics. Consequently, prerequisites for this book are few. However, exposure to linear algebra, statistics, and calculus sometime in the reader's past will be helpful, but not absolutely required. Additionally, this book uses MATLAB™ as its computational engine and some programming in MATLAB™ is required; for that reason exposure to programming concepts will be helpful as well. We have chosen MATLAB™ (rather than some other mathematics and statistics package) because we find it subsumes arcane details (e.g. data formats) without concealing the process of analysis. There are a number of very useful MATLAB™ `m-files` in this book (some written by us, some donated), which we have made available at `http://www.cambridge.org/glover`, the web page the publisher maintains for this book. These `m-files` are working, practical examples (i.e. code that runs), and each chapter contains detailed problems sets that include computer based assignments and solutions. A fair amount of MATLAB™ instruction occurs throughout the book and in Appendix A, which we call *Hints and Tricks*, so familiarity with MATLAB™ will be helpful but not required as well.[1]

We teach our course in a one-semester blitz divided into three parts. And, yes, taking the course is a little like drinking from a fire hose, but we feel that there is something beneficial about the Zen-like concentration required. The first part of the book deals with the mathematical machinery of data analysis that generally goes under the heading of *statistics*, although strictly speaking some of it is not really statistics (e.g. principal component analysis). The second part deals with the techniques of modeling that we choose to cover in this book: finite differences, stability analysis, and optimization. The third part of this book deals with case studies of actual, published models, of ever increasing dimensionality and complexity, starting with zero-dimensional models and finishing with three-dimensional general circulation models. Our goal is to instill a good conceptual grasp of the basic tools underlying the model examples. We like to say the book is correct, but not mathematically rigorous. Throughout the book the general principles and goals of scientific visualization are emphasized through technique and tools. A final chapter on scientific visualization reviews and cements these principles.

This book makes a very nice basis for a one- or two-semester course in data analysis and numerical modeling. It begins with data analysis techniques that are not only very useful in interpreting actual data, but also come up again and again in analyzing model output (computa). This first "third" of the book could also be used in a one-semester data analysis course. It begins with an introduction to both MATLAB and singular value decomposition via a review of some basic linear algebra. Next the book covers measurement theory, probability distributions, and error propagation. From here the book covers least squares regression (both linear and nonlinear) and goodness of fit (χ^2). The next analysis technique is principal component analysis which begins with covariance, correlation, and ANOVA and ends with factor analysis. No data analysis course would be complete without a treatment of sequence data starting with auto- and cross-correlation, proceeding through Fourier series and transforms, and optimal filtering, and finishing up with, of course, the FFT. We finish the data analysis third of the book with a chapter on gridding and contouring techniques from simple nearest neighbor methods to objective interpolation (kriging).

The middle third of this book is the transitional segment of any course that attempts to bring together data analysis techniques and numerical modeling. However, this portion of the book can also be used as part of a more traditional course on numerical modeling. We begin with integration of ordinary differential equations and introduce some simple but useful zero-dimensional models. At this point we pause for a chapter and present a tutorial on model building, practical things one needs to consider no matter how simple or complex the problem. We then demonstrate how the parameters in such models can be optimized

[1] MATLAB is a registered trademark of The MathWorks, Inc., of Natick, MA 01760, USA. In order to avoid the appearance of crowded redundancy we are dropping the TM from the name, but when we write MATLAB we are referring to the trademarked product.

with respect to actual data. When the problems become too complex to be expressed as ordinary differential equations we use partial differential equations, and a discussion and practical introduction to the advection–diffusion equation and turbulence is presented. Next the concept of finite differences is developed to solve these complex problems. In the final chapter of this middle section we cover the important topics of von Neumann stability analysis (Fourier resurfaces), conservation, and numerical diffusion.

We find that, at this point, the students are primed and ready to tackle some "real" models. However, this final third of the book could be used to augment a modeling survey course, although, to get the most out of such a survey the students would need to be well versed in numerical modeling techniques. The book takes the reader through a series of models beginning with simple one-dimensional models of the ocean that rely heavily on lessons learned in the earlier, nonlinear regression section. There are also one-dimensional models of the upper sediment and a very thorough exposition of a one-dimensional, seasonal model of the upper ocean water column. This last section of the book transitions to two-dimensional gyre models and culminates with a chapter on three-dimensional, general circulation models. Up to this point all of these models have been "forward" models. The final third of the book wraps up with "inverse" models. Here we introduce the concepts of inversion and data assimilation and return to the lessons learned from the singular value decomposition chapter at the beginning of the book. It is followed by three-dimensional inversions involving two-dimensional slices of the ocean.

There are certainly many "mathematical methods" books on the market. But this book is the only one we know of that attempts to synthesize the techniques used for analyzing data with those used in designing, executing, and evaluating models. So, where on one's bookshelf does this volume fit in? It goes in that gap that exists between your copies of Stumm and Morgan's *Aquatic Chemistry* and Broecker and Peng's *Tracers in the Sea* on one side, and Pedlosky's *Geophysical Fluid Dynamics* and Wunsch's *The Ocean Circulation Inverse Problem* on the other. Although we are, and our examples reflect this, oceanographers, we feel that scientists in other fields will find our explanations and discussions of these techniques useful. For while the density, pressure, and nature of the problem being analyzed and/or modeled may be vastly different from the ones commonly encountered in the pages of this book, the mathematics remain the same.

Over the years we have had a great deal of help (particularly from our students, who take great pride and pleasure in finding mistakes in our notes) in pulling together the information found between the covers of the book you hold in your hand. We thank each and every one of our students, friends, and colleagues who have contributed to the betterment of this work. However, at the end of the day, we take full responsibility for the accuracy of our work, and deficiencies therein are our responsibility.