

Cambridge University Press  
978-0-521-86783-2 - Modeling Methods for Marine Science  
David M. Glover, William J. Jenkins and Scott C. Doney  
Frontmatter  
[More information](#)

---

## 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.

DAVID M. GLOVER is a Senior Research Specialist in the Department of Marine Chemistry and Geochemistry at Woods Hole Oceanographic Institution. He is the author or co-author of 67 published articles, book chapters and abstracts. Dr. Glover's research uses satellite data, model results, and shipboard data to elucidate the mechanisms and processes by which the oceans play a major role in the maintenance of the global climate.

WILLIAM J. JENKINS is a Senior Scientist in the Department of Marine Chemistry and Geochemistry at Woods Hole Oceanographic Institution. He has published 84 peer-reviewed journal and book articles. Dr. Jenkins is the Director of the National Ocean Sciences Accelerator Mass Spectrometry Facility (NOSAMS). In 1983 he received the Rosenstiel Award in Oceanographic Science from the University of Miami and in 1997 he received the Henry Bryant Bigelow Award in Oceanography from the Woods Hole Oceanographic Institution. Dr. Jenkins' interests include studying tracers as applied to oceanic physical, chemical, biological, and geological processes; air-sea and ice-water exchange of gases; ocean biological productivity and its controls; radiogenic and primordial noble gas isotopes in the sea, atmosphere, lakes, ground waters, sediments and rocks; climatic changes in the ocean and its effects on biogeochemical systems; and radiocarbon and the global carbon cycle in the past 60,000 years.

SCOTT C. DONEY is a Senior Scientist in the Department of Marine Chemistry and Geochemistry at Woods Hole Oceanographic Institution. He has authored or

Cambridge University Press  
978-0-521-86783-2 - Modeling Methods for Marine Science  
David M. Glover, William J. Jenkins and Scott C. Doney  
Frontmatter  
[More information](#)

---

co-authored more than 160 peer-reviewed journal and book articles. He was awarded the James B. Macelwane Medal from the American Geophysical Union in 2000 and an Aldo Leopold Leadership Program Fellowship in 2004. He has traveled extensively, lending his expertise to a number of national and international science programs, most recently as inaugural chair of the Ocean Carbon and Biogeochemistry (OCB) Program. He has also testified before both the US House of Representatives and the US Senate. His research interests include marine biogeochemistry and ecosystem dynamics, ocean acidification, the global carbon cycle, climate change, and the intersection of science and policy.

Cambridge University Press  
978-0-521-86783-2 - Modeling Methods for Marine Science  
David M. Glover, William J. Jenkins and Scott C. Doney  
Frontmatter  
[More information](#)

---

# MODELING METHODS FOR MARINE SCIENCE

DAVID M. GLOVER  
WILLIAM J. JENKINS

and

SCOTT C. DONEY  
*Woods Hole Oceanographic Institution*



CAMBRIDGE  
UNIVERSITY PRESS

Cambridge University Press  
978-0-521-86783-2 - Modeling Methods for Marine Science  
David M. Glover, William J. Jenkins and Scott C. Doney  
Frontmatter  
[More information](#)

---

**CAMBRIDGE**  
UNIVERSITY PRESS

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

Cambridge University Press is part of the University of Cambridge.

It furthers the University's mission by disseminating knowledge in the pursuit of education, learning and research at the highest international levels of excellence.

[www.cambridge.org](http://www.cambridge.org)

Information on this title: [www.cambridge.org/9780521867832](http://www.cambridge.org/9780521867832)

© David M. Glover, William J. Jenkins and Scott C. Doney 2011

This publication is in copyright. Subject to statutory exception and to the provisions of relevant collective licensing agreements, no reproduction of any part may take place without the written permission of Cambridge University Press.

First published 2011

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

ISBN 978-0-521-86783-2 Hardback

Cambridge University Press has no responsibility for the persistence or accuracy of URLs for external or third-party internet websites referred to in this publication, and does not guarantee that any content on such websites is, or will remain, accurate or appropriate.

Cambridge University Press  
978-0-521-86783-2 - Modeling Methods for Marine Science  
David M. Glover, William J. Jenkins and Scott C. Doney  
Frontmatter  
[More information](#)

---

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  
David M. Glover, William J. Jenkins and Scott C. Doney  
Frontmatter  
[More information](#)

---

## Contents

<i>Preface</i>	<i>page</i>	<i>xiii</i>
1	Resources, MATLAB primer, and introduction to linear algebra	1
1.1	Resources	1
1.2	Nomenclature	3
1.3	A MATLAB primer	3
1.4	Basic linear algebra	6
1.5	Problems	13
2	Measurement theory, probability distributions, error propagation and analysis	14
2.1	Measurement theory	14
2.2	The normal distribution	18
2.3	Doing the unspeakable: throwing out data points?	27
2.4	Error propagation	29
2.5	Statistical tests and the hypothesis	31
2.6	Other distributions	33
2.7	The central limit theorem	37
2.8	Covariance and correlation	39
2.9	Basic non-parametric tests	42
2.10	Problems	45
3	Least squares and regression techniques, goodness of fit and tests, and nonlinear least squares techniques	49
3.1	Statistical basis for regression	49
3.2	Least squares fitting a straight line	52
3.3	General linear least squares technique	62
3.4	Nonlinear least squares techniques	68
3.5	Problems	74
4	Principal component and factor analysis	75
4.1	Conceptual foundations	76
4.2	Splitting and lumping	81
		vii

viii	<i>Contents</i>	
4.3	Optimum multiparameter (OMP) analysis	86
4.4	Principal component analysis (PCA)	95
4.5	Factor analysis	104
4.6	Empirical orthogonal functions (EOFs)	109
4.7	Problems	118
5	Sequence analysis I: uniform series, cross- and autocorrelation, and Fourier transforms	120
5.1	Goals and examples of sequence analysis	120
5.2	The ground rules: stationary processes, etc.	122
5.3	Analysis in time and space	123
5.4	Cross-covariance and cross-correlation	131
5.5	Convolution and implications for signal theory	132
5.6	Fourier synthesis and the Fourier transform	135
5.7	Problems	139
6	Sequence analysis II: optimal filtering and spectral analysis	141
6.1	Optimal (and other) filtering	141
6.2	The fast Fourier transform (FFT)	144
6.3	Power spectral analysis	145
6.4	Nyquist limits and data windowing	157
6.5	Non-uniform time series	162
6.6	Wavelet analysis	166
6.7	Problems	169
7	Gridding, objective mapping, and kriging	171
7.1	Contouring and gridding concepts	171
7.2	Structure functions	179
7.3	Optimal estimation	183
7.4	Kriging examples with real data	186
7.5	Problems	192
8	Integration of ODEs and 0D (box) models	194
8.1	ODE categorization	194
8.2	Examples of population or box models (0D)	197
8.3	Analytical solutions	200
8.4	Numerical integration techniques	203
8.5	A numerical example	210
8.6	Other methods	218
8.7	Problems	222
9	A model building tutorial	223
9.1	Motivation and philosophy	224
9.2	Scales	226
9.3	A first example: the Lotka–Volterra model	232



*Contents*

ix

9.4	A second example: exploring our two-box phosphate model	238
9.5	A third example: multi-box nutrient model of the world ocean	245
9.6	Problems	249
10	Model analysis and optimization	250
10.1	Basic concepts	251
10.2	Methods using only the cost function	258
10.3	Methods adding the cost function gradient	264
10.4	Stochastic algorithms	271
10.5	An ecosystem optimization example	274
10.6	Problems	278
11	Advection–diffusion equations and turbulence	280
11.1	Rationale	280
11.2	The basic equation	281
11.3	Reynolds decomposition	282
11.4	Stirring, straining, and mixing	287
11.5	The importance of being non	287
11.6	The numbers game	289
11.7	Vertical turbulent diffusion	293
11.8	Horizontal turbulent diffusion	294
11.9	The effects of varying turbulent diffusivity	296
11.10	Isopycnal coordinate systems	297
12	Finite difference techniques	299
12.1	Basic principles	299
12.2	The forward time, centered space (FTCS) algorithm	300
12.3	An example: tritium and $^3\text{He}$ in a pipe	304
12.4	Stability analysis of finite difference schemes	309
12.5	Upwind differencing schemes	316
12.6	Additional concerns, and generalities	321
12.7	Extension to more than one dimension	323
12.8	Implicit algorithms	329
12.9	Problems	330
13	Open ocean 1D advection–diffusion models	332
13.1	Rationale	332
13.2	The general setting and equations	333
13.3	Stable conservative tracers: solving for $K/w$	334
13.4	Stable non-conservative tracers: solving for $J/w$	338
13.5	Radioactive non-conservative tracers: solving for $w$	340
13.6	Denouement: computing the other numbers	343
13.7	Problems	344

x	<i>Contents</i>	
14	One-dimensional models in sedimentary systems	346
14.1	General theory	346
14.2	Physical and biological diagenetic processes	350
14.3	Chemical diagenetic processes	353
14.4	A modeling example: CH <sub>4</sub> at the FOAM site	356
14.5	Problems	363
15	Upper ocean 1D seasonal models	365
15.1	Scope, background, and purpose	365
15.2	The physical model framework	369
15.3	Atmospheric forcing	371
15.4	The physical model's internal workings	376
15.5	Implementing the physical model	380
15.6	Adding gases to the model	387
15.7	Implementing the gas model	393
15.8	Biological oxygen production in the model	402
15.9	Problems	407
16	Two-dimensional gyre models	409
16.1	Onward to the next dimension	409
16.2	The two-dimensional advection–diffusion equation	412
16.3	Gridding and numerical considerations	419
16.4	Numerical diagnostics	426
16.5	Transient tracer invasion into a gyre	433
16.6	Doubling up for a better gyre model	442
16.7	Estimating oxygen utilization rates	449
16.8	Non-uniform grids	451
16.9	Problems	452
17	Three-dimensional general circulation models (GCMs)	453
17.1	Dynamics, governing equations, and approximations	454
17.2	Model grids and numerics	463
17.3	Surface boundary conditions	469
17.4	Sub-grid-scale parameterizations	474
17.5	Diagnostics and analyzing GCM output	479
18	Inverse methods and assimilation techniques	489
18.1	Generalized inverse theory	489
18.2	Solving under-determined systems	494
18.3	Ocean hydrographic inversions	499
18.4	Data assimilation methods	506
19	Scientific visualization	516
19.1	Why scientific visualization?	516
19.2	Data storage, manipulation, and access	518

Cambridge University Press  
978-0-521-86783-2 - Modeling Methods for Marine Science  
David M. Glover, William J. Jenkins and Scott C. Doney  
Frontmatter  
[More information](#)

---

<i>Contents</i>		xi
19.3	The perception of scientific data	521
19.4	Using MATLAB to present scientific data	526
19.5	Some non-MATLAB visualization tools	530
19.6	Advice on presentation graphics	532
Appendix A Hints and tricks		537
A.1	Getting started with MATLAB	537
A.2	Good working practices	539
A.3	Doing it faster	541
A.4	Choose your algorithms wisely	543
A.5	Automating tasks	544
A.6	Graphical tricks	545
A.7	Plotting oceanographic sections	547
A.8	Reading and writing data	549
<i>References</i>		552
<i>Index</i>		564

Cambridge University Press  
978-0-521-86783-2 - Modeling Methods for Marine Science  
David M. Glover, William J. Jenkins and Scott C. Doney  
Frontmatter  
[More information](#)

---

## 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<sup>TM</sup> as its computational engine and some programming in MATLAB<sup>TM</sup> is required; for that reason exposure to programming concepts will be helpful as well. We have chosen MATLAB<sup>TM</sup> (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<sup>TM</sup> *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<sup>TM</sup> instruction occurs throughout the book and in Appendix A, which we call *Hints and Tricks*, so familiarity with MATLAB<sup>TM</sup> will be helpful but not required as well.<sup>1</sup>

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 ( $\chi^2$ ). 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

<sup>1</sup> 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.