PARTICLES IN THE COASTAL OCEAN
THEORY AND APPLICATIONS

The coastal ocean comprises the semi-enclosed seas on the continental shelf, including estuaries and extending to the shelf break. It is the focus of many serious concerns, including coastal inundation by tides, storm surges, or sea level change; fisheries and aquaculture management; water quality, health, and pollution; harmful algal blooms; siting and planning of facilities (e.g., power stations); ports and harbor development and maintenance; and accident response. Prediction and modeling of particle motion within these areas is critical to understanding and management of these phenomena and activities. This book summarizes the state of the art in modeling and simulation of the transport, evolution, and fate of particles (physical and biological) in the coastal ocean.

This is the first book to provide a unified development of key concepts that have been scattered under several topical headings – Lagrangian, ensemble, kinetic, Monte Carlo, site-specific, and individual-based modeling methods. These modeling methods have diverse applications in the coastal ocean including sediment motion, oil spills, and larval ecology.

Particles in the Coastal Ocean is an invaluable textbook and reference work for advanced students and researchers in oceanography, geophysical fluid dynamics, marine and civil engineering, computational science, and environmental science.

This work is dedicated to Charles B. Officer, who befriended me as a colleague, early. He discovered more with pencil and paper than the rest of us could do with big machines. He sets a standard that few can match.

Daniel R. Lynch
Hanover

PARTICLES IN THE COASTAL OCEAN

THEORY AND APPLICATIONS

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CAMBRIDGE
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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
Information on this title: www.cambridge.org/9781107061750

First published 2015

Printed in the United States of America

A catalog record for this publication is available from the British Library.

Library of Congress Cataloging in Publication Data

ISBN 978-1-107-06175-0 Hardback

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Color plates follow page 206.

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Daniel R. Lynch is MacLean Professor of Engineering at Dartmouth College and Adjunct Scientist at the Woods Hole Oceanographic Institution (WHOI). He holds degrees from the Massachusetts Institute of Technology and Princeton University. He has published extensively on simulation methods in coastal oceanography and is coeditor of the American Geophysical Union (AGU) volume *Quantitative Skill Assessment for Coastal Ocean Models* (CES 47, 1995) and a companion volume, *Skill Assessment for Coupled Physical-Biological Models of Marine Systems* (JMS 76, 2009). He co-founded the Gordon Research Conference in Coastal Ocean Modeling; was Executive Director of the Regional Association for Research on the Gulf of Maine; and served on the Executive Committee of the US Global Ocean Ecosystem Dynamics (GLOBEC) Northwest Atlantic Program (National Oceanic and Atmospheric Administration [NOAA] and National Science Foundation [NSF]). Sabbatical and other visiting leaves include WHOI, the Institut de Mecanique de Grenoble, the Institute of Ocean Sciences, and the University of Bergen.

Lynch is a NSF Presidential Young Investigator, received the B.H. Ketchum Award for interdisciplinary estuarine studies, and is a Fellow of the American Society of Civil Engineers. He developed the Numerical Methods Laboratory at Dartmouth, around the theme of interdisciplinary computational engineering, and authored the graduate text *Numerical Solution of Partial Differential Equations for Environmental Scientists and Engineers* (Springer, 2005).

Recent investigations focus on Sustainability, Natural Resources, and Professional Education. Included are visiting appointments at the University of Notre Dame (Melchor Visiting Chair); the School of Philosophy at the Catholic University of America; and the Woodrow Wilson School of Public and International Affairs at Princeton. He is coeditor of the special issue *Professions and the Common Good* (ACCU 2006) and a contributor to the *Civil Engineering Body of Knowledge for the 21st Century* (ASCE 2008). He authored the undergraduate text *Sustainable Natural Resource Management for Scientists and Engineers* (Cambridge University Press, 2009).

David A. Greenberg has been working in Canadian Marine Science since his sessions as a summer student with the Canadian Department of Mines and Technical Surveys in the late 1960s. He received bachelor's and master's degrees in Mathematics from the University of Waterloo (1969 and 1970) and a PhD from Liverpool University (1975). His thesis on modeling Bay of Fundy tides and tidal power set the stage for much of his later work, which includes continued work on tidal power, model development, and application to many theoretical and practical problems. His early work with finite difference models included mesh nesting, transport algorithms, and open boundary limitations. With finite element models he has looked at simulating wetting and drying of intertidal areas, and adapting models from Cartesian coordinates to geographic coordinates for larger domains and constraints on resolution in all ocean models. Processes examined include tidal, wind, density, and boundary-driven circulation; mixing; and sea level rise. Many model configurations have been created for studies in the Bay of Fundy and the adjacent Gulf of Maine, looking at tidal power, biological productivity, sediment transport, paleo tides, and aquaculture parasite and disease transport. Studies outside the Fundy–Maine domain include the tsunami generated from the 1917 explosion in Halifax Harbour, the circulation on the Newfoundland shelf, and the freshwater flow through the Canadian Arctic Archipelago. He continues to work actively in model development and application.

Ata Bilgili received the BSc from the Istanbul Technical University's Faculty of Naval Architecture and Ocean Engineering. He received the MSc and PhD degrees from the University of New Hampshire (UNH) in Ocean and Mechanical Engineering, respectively. His master's and PhD dissertations on Eulerian bed-load transport of coarse sediments and finite element modeling of the tides in the Great Bay Estuarine System in New Hampshire shaped the foundation for his later work. During his postdoctoral studies at UNH and later at Dartmouth College, he worked on improving the tidal models for well-mixed coastal systems with special emphasis on the N2 and S2 tidal components and their residual effects, using both Eulerian and Lagrangian methods. During his residency at Dartmouth College as a Research Assistant Professor from 2001 to 2005, Dr. Bilgili's work concentrated on coding and testing particle tracking methods for the characterization of estuary–ocean exchange and mixing using a statistically significant number of particles on parallel processors. Studies outside this domain included unstructured grid generation for finite element circulation modeling, modeling concentration and dilution of pollutant particles originating from wastewater treatment facilities, and interdisciplinary transfer of modeling products to researchers in the environmental science and education fields. In 2005, Dr. Bilgili started working for the Istanbul Technical University, where he obtained tenure as an Associate Professor of Coastal and Ocean Engineering. His work at this institution includes the application of the techniques developed earlier to wind-dominated coastal systems and the optimization of particle tracking methods on high-performance computing platforms. His additional current interests include the advancement of marine engineering education and environmental contingency planning for ports and harbors.

Dennis J. McGillicuddy, Jr., is a Senior Scientist in the Department of Applied Ocean Physics and Engineering at the Woods Hole Oceanographic Institution. His primary research interest is the interface between the fluid dynamics and the biology of the sea. He has pursued physical–biological–chemical interactions in four contexts: (1) the role of eddies in biogeochemical cycling of the open ocean, (2) impacts of coastal circulation on zooplankton dynamics, (3) the dynamics of harmful algal blooms, and (4) larval dispersal in deep-sea vent communities.

Dr. McGillicuddy received a PhD from Harvard in 1993 and joined the Woods Hole Oceanographic Institution in 1993 as a Postdoctoral Scholar. He was appointed to the scientific staff in 1996. He was a recipient of the Office of Naval Research Young Investigator Award (1998), the American Society of Limnology and Oceanography's Lindeman Award (2000), and the University of Miami's Rosenstiel Award (2008). He is author or coauthor of more than one hundred refereed publications.

Dr. McGillicuddy has been very active in the oversight of large interdisciplinary oceanographic programs on both national and international levels, having served on the scientific steering committees of the Joint Global Ocean Flux Study, the Global Ecosystem Dynamics Program, and the Global Ecology and Oceanography of Harmful Algal Blooms. Dr. McGillicuddy currently serves as Deputy Director of the Woods Hole Center for Oceans and Human Health.

James P. Manning After receiving an undergraduate degree in mathematics (University of Maine, 1979) and a master's degree in oceanography (University of Rhode Island, 1987), James P. Manning has been at NOAA's Northeast Fisheries Science Center for more than 25 years. Given a career largely devoted to building low-cost observing systems with the help of New England lobstermen, there is now an extensive network of individuals who deploy both moored and drifting instrumentation throughout the Gulf of Maine and the southern New England shelf. He also works closely with local ocean circulation modelers, providing them with data for assimilation and validation purposes. At the time of this writing, his web-served archive includes more than 5 million hourly values of moored bottom temperatures and more than a million kilometers of surface drifter tracks. The motivation behind most of these efforts is to describe the physical oceanographic environments of critical offshore spawning grounds. With a melding of data and model simulations, he hopes to help biologists explain the variability in recruitment of larvae and its relationship to the physical conditions.

Alfredo L. Aretxabaleta is a physical oceanographer working at the USGS Science Center in Woods Hole, MA. He received a BS in Marine Sciences from the University of Las Palmas de Gran Canaria in Spain in 1998 and a PhD in Marine Sciences from the University of North Carolina at Chapel Hill (UNC-CH) in 2005. While at UNC-CH, he was part of the USGLOBEC real-time forecasting team, and he worked on the development of a coastal observing system for the Southeast United States. He then worked as a postdoctoral investigator at the Woods Hole Oceanographic Institution on the physical processes affecting harmful algal blooms ("red tides") in the Gulf of Maine and Bay of Fundy, as part of the US EcoHab and BoHab projects. Then he worked at the Institut de Ciencias del Mar (Barcelona, Spain) on the development and improvement of the first satellite measuring salinity from space (SMOS, Soil Moisture and Ocean Salinity of the European Space Agency). Currently, Aretxabaleta is working with the US Geological Survey in Woods Hole on sediment transport problems in the coastal ocean, ranging from cohesive sediment behavior to resuspension of material from the bed. His main interest is the implications of the physical processes in the ocean for problems of interdisciplinary nature such as the behavior of biological organisms or the transport of pollutants and/or sediment. Aretxabaleta has collaborated in teaching introductory-level classes on physical oceanography and the modeling of marine and Earth systems. He is also one of the authors of the book *Project Earth Science: Physical Oceanography* of the National Science Teachers Association.

Cambridge University Press
978-1-107-06175-0 - Particles in the Coastal Ocean: Theory and Applications
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Preface

This is a book about the coastal ocean; specifically, about simulating particle motion within it. It unifies essential ideas, for a multidisciplinary group of scientific professionals.

We take as given realistic computer fields for the primary variables: velocity, pressure, temperature, salinity, and turbulence. These fields are becoming available for wide use, in site-specific realizations that account for detailed forcing and topography. Emerging are some biogeochemical fields in some cases: nutrients, light, plankton. This is our *virtual environment*. Though imperfect, it has reached a high level of realism, and it is continuously improving.

Our subject is the transport, evolution, and fate of particles in these environments. For simple particles, physical motion is of fundamental concern. For chemically active particles, one adds reaction, transformations, and interaction with bounding surfaces. For living particles, one adds suspension, growth, death, transformation, behavior, and reproduction. Nonlinear physical–biological interaction is implied and natural.

The material is culled from 20 years of research projects. A diverse collection of ideas has emerged, variously titled *Lagrangian*, *ensemble*, *kinetic*, *Monte Carlo*, *site-specific*, or *individual-based* methods. They share the common theme of simulating many small units (particles) individually, allowing variability to develop among them without prior aggregation. Current computing power makes broad operational use possible.

To date there is no single source that unifies these ideas for the audiences intended. Our book fills that gap. Included are basic ideas about applied probability; random walk; interpolating and navigating general computational meshes and data products; and Monte Carlo simulation methods. Applications include drifters, sediment motion, oil spills, and larval ecology.

Overall, our intention is to facilitate the analysis of coastal ocean phenomena using simulation of *particle dynamics*. The notion of *trajectory* is general – the physical and biochemical history experienced by an individual *particle in motion*. The work is configured as a teaching and reference source, suitable for year-4 and beyond university students and for working professionals.

Acknowledgments

We have benefited over the years from collaboration with many individuals. In particular, we are grateful for the enormous contributions of Francisco Werner, Charles Hannah, Christopher Naimie, Charlie Miller, Craig Lewis, Jeff Proehl, John Loder, Fred Page, Brian Blanton, Keston Smith, Justin Ip, and Ruoying He in developing the ideas covered here.

Special thanks go to Malcolm Spaulding for generous assistance with Chapter 10.

Additional thanks to Rick Lumpkin, Jon Hare, and Jeff Pessutti, who provided valuable reviews, and to Vitalii Shermet for providing particle tracking code.

We thank our sponsors: NSF, NSERC, NIEHS, NOAA (OAR, SeaGrant, CICEET, CSCOR), NASA, ONR, the special interagency programs including GLOBEC, ECOHAB, MERHAB, GOMTOX, and NOPP; and others who supported these developments. DJM gratefully acknowledges additional internal WHOI support from the Holger W. Jannasch Senior Scientist Chair.

We thank the National Center for High Performance Computing at the Istanbul Technical University (http://www.uybhm.itu.edu.tr/index.php) for the use of its parallel computer clusters for some of the simulations in this book, under contract number 1001192011.

Acronyms

ACCU	Association of Catholic Colleges and Universities
ADCP	Acoustic Doppler Current Profiler
AGU	American Geophysical Union
ASCE	American Society of Civil Engineers
ASLO	American Society of Limnology and Oceanography
CICEET	Cooperative Institute for Coastal and Estuarine Environmental Technology
CSCOR	Center for Sponsored Coastal Ocean Research
ECOHAB	Ecology of Harmful Algal Blooms
GEOHAB	Global Ecology and Oceanography of Harmful Algal Blooms
GLOBEC	Global Ocean Ecosystem Dynamics
GOMTOX	Gulf of Maine Toxicity Project
IOOS	Integrated Ocean Observing System
JGOFS	Joint Global Ocean Flux Study
LAPCOD	Lagrangian Analysis and Prediction of Coastal and Ocean Dynamics
MERHAB	Monitoring and Event Response for Harmful Algal Blooms
NASA	National Aeronautics and Space Administration
NCCOS	National Centers for Coastal Ocean Science
NEFSC	Northeast Fisheries Science Center
NIEHS	National Institute of Environmental Health Sciences
NSERC	Natural Sciences and Engineering Research Council
NSF	National Science Foundation
NOAA	National Oceanic and Atmospheric Administration
NOPP	National Ocean Partnership Program
OAR	Office of Oceanic and Atmospheric Research
ONR	Office of Naval Research
SG	Sea Grant
SMOS	Soil Moisture and Ocean Salinity
USGS	United States Geological Survey

Definitions and Notation

Vectors and Scalars

Bold indicates vector (e.g., $\mathbf{V}$)
Nonbold indicates a scalar (e.g., ρ)

Eulerian Fields

$\mathbf{x}$ is a geographic coordinate. It can be 2-D or 3-D. Implied is a Cartesian system with scalar parts (x, y, z); if other projections are used, they will be explicitly identified.
Unit vectors are indicated by underlining, for example, $\underline{\mathbf{x}}$.
$\mathbf{v}(\mathbf{x})$ and $\zeta(\mathbf{x})$ are Eulerian fields, respectively a vector field $\mathbf{v}$ and a scalar field ζ.
$\frac{\partial}{\partial x}$, $\frac{\partial}{\partial t}$, ∇, and so forth indicate conventional Eulerian partial derivatives in the $(\mathbf{x}, t)$ domain.

Lagrangian Particle Trajectory and Properties

$\frac{dA_j}{dt} \equiv \dot{A}_j$ indicates a Lagrangian time derivative of A following particle j.
$\mathbf{X}_j(t)$ is a specific location in $\mathbf{x}$, the position of the jth particle at time t.
$\mathbf{V}_j = \dot{\mathbf{X}}_j$.
$\mathbf{V}_j$ is the velocity of particle j: $\mathbf{V}_j(t) = \mathbf{v}(\mathbf{X}_j(t))$.
$M_j(t)$ is the scalar mass of an individual particle j at time t.

Numerical Analysis

$\mathcal{O}(\alpha)$ indicates "small terms of order α," that is, the leading or largest term scales as α.
ΔQ^k indicates the backward difference $Q^k - Q^{k-1}$.

Elements

$\mathbf{x}_i$ is the value of the coordinate $\mathbf{x}$ at node i.
$\phi_i(\mathbf{x})$ is the ith basis function, centered at node i.
ϕ_{ik} is the location of particle k on an element (the value of ϕ_i at point k).
ρ_i is the value of a function ρ at node i.

The continuous function $\rho(\mathbf{x})$ is interpolated with the bases:

$$\rho(\mathbf{x}) = \sum \rho_i \phi_i(\mathbf{x}) \tag{1}$$

A_e is the area of element e.

Singularities

$\delta(x)$ is the Dirac delta function. It is zero everywhere but has a removable singularity at the origin, $x=0$. Specifically, $\int \delta(x)\,dx = 1$ if the domain of integration includes the origin; otherwise, the integral is zero.

$\delta_j \equiv \delta(x-x_j)$ is the Dirac delta function, singular at position $x = x_j$.

$\int f(x)\cdot\delta_j\,dx = f(x_j)$. This integral samples the function $f(x)$ at the point x_j.

Random Numbers

Several symbols are reserved for random numbers:

ϵ indicates a random number.
$\mathcal{R}$ indicates a random number.
η indicates a random number.

Generally, an overbar indicates a mean or average, for example, $\overline{F}$. A departure from the mean is indicated by either of two markers, $\widehat{F}$ or $\widetilde{F}$.

Some familiar distributions:

$\mathcal{U}$ is the uniform distribution.
$\mathcal{G}$ is the Gaussian distribution.
$\mathcal{N}$ is the standard Normal distribution: Gaussian with zero mean, unit variance.

The random variable z as generated from the distribution f is denoted $z \sim f$.

Example: $z \sim \mathcal{U}[0,1]$: z is a deviate uniformly distributed on the interval $[0,1]$.
Example: $z \sim \mathcal{G}(a,b^2)$: z is a Gaussian deviate with mean a and variance b^2.
Example: $n \sim Pois(\lambda)$: n is a Poisson deviate with rate λ.

Parameters and Properties of Distributions

f is the probability density function (PDF).
F is the cumulative distribution function (CDF); $F(x) = \int f\,dx$.
E is the Expectation operator: $E(x) = \int x f(x)\,dx$.
μ indicates the expected value (mean) of a distribution: $\mu_\epsilon = E(\epsilon)$.
Var indicates the variance of a distribution; equivalently, its second moment about the mean:

$$Var(\epsilon) = E(\epsilon-\mu_\epsilon)^2 \tag{2}$$

σ indicates standard deviation; $\sigma^2 \equiv Var$.
ρ indicates a (dimensionless) autocorrelation coefficient in a random time series.
$\nu(\mathbf{x})$ is the particle *intensity*, number of particles per unit area.
$P[event]$ is the probability of that event occurring. Example: $P[x \geq 5] = .1$.

Covariance

Cov_{xy} is the expected value of the product of x and y: $Cov_{xy} = E[(x-\mu_x)(y-mu_y)]$.

$C_m(\epsilon)$ is the autocovariance of the discrete, demeaned series $\widehat{\epsilon}$, at points separated by lag m:

$$C_m(\epsilon) \equiv E\left[\widehat{\epsilon}^k\,\widehat{\epsilon}^{k-m}\right] \tag{3}$$

C is symmetric: $C_i(\,) = C_{-i}(\,)$.

$C_0(\epsilon)$ is the same as σ_ϵ^2.

ρ_m is the autocorrelation coefficient, at lag m – the normalized autocovariance: $\rho_m = \frac{C_m}{C_0}$.

Time Series

$\mathcal{R}$ generally indicates a random displacement over Δt. Units: length

$\mathcal{R}_1$ generally indicates a random velocity change over Δt. Units: length/time

$\mathcal{R}_2$ generally indicates a random acceleration change over Δt. Units: length/time/time

$d\mathcal{W}$ is the Wiener increment.

$\Delta\mathcal{W}$ is the Wiener integral $= \int_t^{t+\Delta t} d\mathcal{W} \sim \sqrt{\Delta t}\cdot\mathcal{G}(0,1)$.

$\mathcal{R}_v$ is the Wiener noise input to the AR1 model.

S_v is its size.

$\mathcal{R}_v\,dt = S_v\,d\mathcal{W}$ is the scaled Wiener increment.

$\mathcal{R}_a$ is the Wiener noise input to the AR2 model.

S_a is its size.

$\mathcal{R}_a\,dt = S_a\,d\mathcal{W}$ is the scaled Wiener increment.

Discrete Convolution

Z_i are convolution coefficients. For a discrete (linear) time series Q forced by the series F

$$Q^N = \sum_{j=1}^{N} F^j Z_{N-j} \tag{4}$$

The series Z is the response to unit forcing. The convolution is the superposition of responses to all past influences F.

B^k is the partial sum of convolution coefficients,

$$B^k = \sum_{i=0}^{k} Z_i \tag{5}$$

Introduction and Scope

The Coastal Ocean

The *coastal ocean* comprises the semi-enclosed seas on the continental shelf, including estuaries and extending to the shelf break. Geographically the scope is approximately that of the Exclusive Economic Zone for which nation-states are responsible.

The coastal ocean is the focus of many serious concerns, including coastal inundation by tide, storm, or sea level change; fisheries and aquaculture management; water quality, health, and pollution; harmful algae blooms; facilities siting and planning; ports and harbor development and maintenance; spills and other accidents. All fall within the scope of science, engineering, and development. All demand professional competence in promoting wise and healthy use of this critical region, and in anticipating, monitoring, and responding to events therein.

The Virtual Environment

Computational Circulation Products. A realistic simulated or virtual environment (herein "the environment") is becoming available for scientific and engineering use. This takes the form of site-specific computational products for the baseline physical fields. Simulated particles in these fields offer the possibility of high realism, facilitating advanced analysis.

Equations and Variables. Well-defined equations and variables characterize the coastal ocean. For our purpose, the bundle of "physical" variables includes pressure, velocity, temperature, salinity, light, nutrients, and subgrid or unresolved mixing rates (typically in the form of turbulent energy, mixing length, a stability parameter, and eddy diffusivity). These all share very conventional formulations for their evolution and transport. This scientific foundation has advanced very far and supports the construction of site-specific environments.

Randomness. There will always be unresolved dynamics, and they must be accounted for, both in motion and in biotic development. At the simplest level, there is truncation error, equation error, and forcing uncertainty. These all contribute to a distribution of possibilities for the environment itself. In addition, there is uncertainty about basic biotic rates and their distribution across individuals in the same population. Perhaps most fundamentally, in setting out a gridded calculation and product, the real motion at the subgrid will have at best a statistical description. Particles live in the subgrid, and influences there can only be statistically described. A Monte Carlo approach, historically always anticipated, is now clearly possible for the coastal ocean.

User Groups and Regional Systems. Networked availability of site-specific environments are emerging in the form of regional observation/modeling systems. The Integrated Ocean Observing System (IOOS) provides an international network for these, and some standards. As a class these offer continuous, cooperative improvement. Specific products include site-specific climatologies and data archives, hindcast products, and forecasts. These can support many applications: scientific studies, infrastructure planning, response to emergencies, and so forth.

Technical user groups provide model-family support spanning applications globally. These share a laboratory/university research and demonstration focus. Further practical implementation is a professional matter, to be done by a proper blend of private-sector initiative and public-sector support.

Professional competence demands scientific bundling of the advanced supporting ideas. Accordingly, *our text serves this need.*

The Present Work

Our purpose is to present the basics of a Lagrangian particle-based approach to simulation. We do not seek to construct the virtual environment, but to describe phenomena within it. Required is a basic description of principles: the Lagrangian trajectory in physical–biological space and its statistical nature; the data file standards that are needed to import the detailed environment and to record the simulation results; and enough basic simulation mathematics to make ideas easy to implement in practical programs.

A fundamental assumption is that geometric realism in the coastal ocean demands an unstructured horizontal mesh – so we assume the simplest in this category, the linear mesh (triangles or quadrilaterals). This is not to constrain the sophistication of the fields themselves – neither their interpolation nor their generation. Rather, we seek to liberate the geometrical description of the coastal ocean from any constraints imposed by horizontal mesh. It is a truism that any published field on a structured horizontal mesh structure can be converted to one of triangles for the purpose of particle simulation. So, nothing is lost, but a vast degree of generalization is gained. This is the baseline. We extend the ideas to quadrilateral meshes for generality.

This book is *not* a replacement for conventional descriptions of the coastal ocean or how to simulate it – there are many excellent works in that category. Rather, it is