Chapter 12. DATA ASSIMILATION FOR MODELING AND PREDICTING COUPLED PHYSICAL–BIOLOGICAL INTERACTIONS IN THE SEA

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1. Introduction

Data assimilation is a modern methodology of relating natural data and dynamical models. The general dynamics of a model is combined or melded with a set of observations. All dynamical models are to some extent approximate, and all data sets are finite and to some extent limited by error bounds. The purpose of data assimilation is to provide estimates of nature which are better estimates than can be obtained by using only the observational data or the dynamical model. There are a number of specific approaches to data assimilation which are suitable for estimation of the state of nature, including natural parameters, and for evaluation of the dynamical approximations.

Progress is accelerating in understanding the dynamics of real ocean biological–physical interactive processes. Although most biophysical processes in the sea await discovery, new techniques and novel interdisciplinary studies are evolving ocean science to a new level of realism. Generally, understanding proceeds from a quantitative description of four-dimensional structures and events, through the identification of specific dynamics, to the formulation of simple generalizations. The emergence of realistic interdisciplinary four-dimensional data assimilative ocean models and systems is contributing significantly and increasingly to this progress.

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Dynamics evolves the state of a natural system forward in time. The state variables (e.g., velocities, temperature, concentration densities of plankton, nutrients, particles) are functions of four-dimensional space–time, classically referred to as fields. A dynamical model to approximate nature consists of a set of coupled nonlinear prognostic field equations for each state variable of interest. The fundamental properties of the system appear in the field equations as parameters (e.g., viscosities, diffusivities, body forces, rates of Earth rotation, grazing, mortality). The initial and boundary values of the state, which are necessary for integration of the equations, may also be regarded as parameters by data assimilation methods. In principle, the state and parameters of the system can be estimated directly by observations and measurements. Given the state of the system at one time, a future state can be estimated by a model prediction. In practice, directly observing and measuring the state and parameter of a physical–acoustical–optical–biological-chemical-sedimentological ocean system is extremely difficult because of sampling, technical, and resource requirements.

Data assimilation provides a powerful methodology for state and parameter estimation via the melding of data and dynamics. It makes feasible such estimates on a substantial and sustainable basis. The general process is schematized in Fig. 12.1. Sensor data are linked to state variables and parameters and transformed as appropriate for the dynamical model via measurement models. Dynamics interpolates and extrapolates the data. Dynamical linkages among all the state variables and parameters allows all of them to be estimated from observations of some of them (i.e., those more accessible to existing techniques and prevailing conditions). Error estimation and error models play a crucial role. Using data assimilation schemes, data and dynamics are melded, often with weights inversely related to their relative errors. The melding is based on an assimilation criterion involving a cost or penalty function. The final estimates should agree with the observations and measurements within data error bounds and should satisfy the dynamical model within model error bounds. There are many important feedbacks in the generally highly nonlinear *ocean observing and prediction system* (OOPS) schematized in Fig. 12.1, which illustrates the system concept and two feedbacks. Prediction provides the opportunity of efficient sampling schemes adapted to real-time structures, events, and errors. Data collected for assimilation also used for ongoing validation can identify model deficiencies and lead to model improvements.

There are many special purposes and different methods that lead to specific versions of the system of Fig. 12.1, and identifying the most suitable ones for biophysical applications requires research. Data assimilation must play several critical roles in the development, design, assessment, and operation of interdisciplinary observing and prediction systems, including, importantly, the control of loss of predictability associated with highly nonlinear coupled biological–physical dynamics. Most germane to the central topic of this volume is the use of data assimilation in dynamical hypothesis testing and the inference of real ocean dynamical processes from data. Data-model misfits or residuals can be used to evaluate different model formulations. Dynamically adjusted data can be used for balance-of-terms studies involving higher spatial derivatives. Furthermore, many essential biological oceanographic rate parameters are presently not directly measurable in situ, and data assimilation is necessary for their estimation.

Some important aspects of state estimation and parameter estimation are exem-

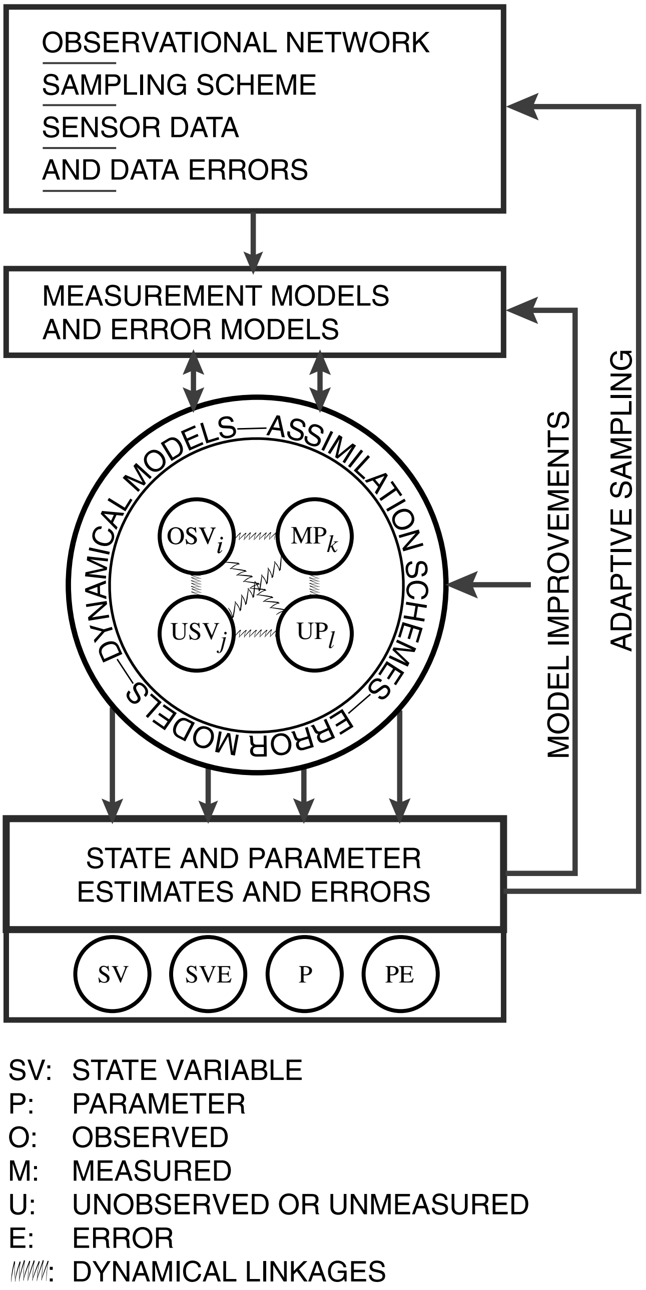


Fig. 12.1. Schematic of the linkages and feedbacks for the process of data assimilation within an ocean observing and prediction system (OOPS). Arrows represent the most common direction for the flows of information. The arrow between the measurement models and dynamical models is double because measurement models can include operators that map state variables and parameters to the sensor data (e.g., interpolations, derivatives, or integrals of state variables/parameters) and operators that transform sensor data into data appropriate for the model scales and processes (e.g., filtering, extrapolations, or integrals of sensor data). The legend at the bottom explains abbreviations.

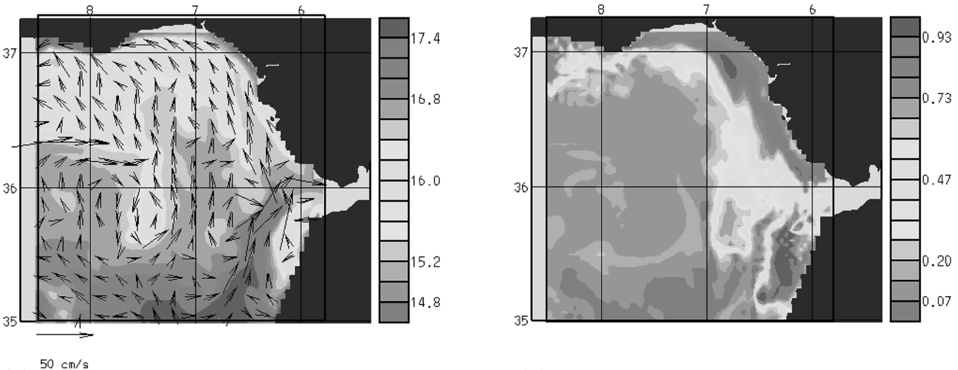
plified via an operational real-time interdisciplinary forecast and a highly idealized predator–prey model, respectively. The operational forecast carried out in March 1998 for NATO naval maneuvers in the Gulf of Cadiz in the northeast Atlantic Ocean, west of the Strait of Gibraltar, is illustrated in Fig. 12.2. The Harvard Ocean Prediction System (HOPS; Section 3.8) was utilized in conjunction with an observational network managed by the NATO SACLANT Undersea Research Centre (Robinson et al., 1999; Robinson and Sellschopp, 2000). Platforms included satellites, aircraft, and ships. Both state-variable fields and associated error fields were forecast, and the error fields were used to design adaptive sampling patterns. For naval operations, the temperature field is important because of its effect on acoustic propagation, and the chlorophyll field is important because it is related to the phytoplankton field that affects bioluminescence, which can be used to detect ship movements.

The simple predator (y)–prey (x) model used to illustrate parameter estimation consists of two coupled nonlinear ordinary differential equations in time (Fig. 12.3) assuming spatial homogeneity (Lawson et al., 1995). There are six internal parameters (a_i, $i = 1$ to 6) representing net growth–death rates, self-interactions and predator–prey interactions, and two initial condition parameters. For a chosen set of parameters, a "true" simulated time series is obtained by model integration, which is then subsampled to provide a data set for assimilation in a model run with imperfect parameters. The true parameters are retrieved iteratively: the model is run forward in time, the adjoint model is run backward in time, and the parameters are adjusted to minimize the penalty function, which consists of the sum of the squared differences between the run estimates and true data. All eight parameters are recovered successfully and accurately.

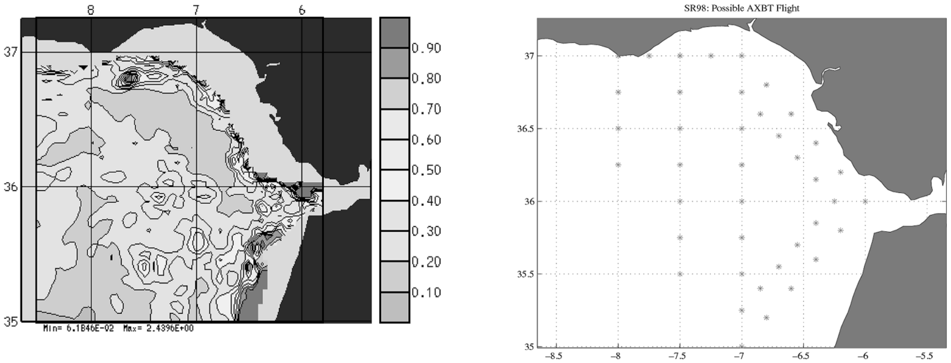
Data assimilation is now being extended to interdisciplinary oceanography from physical oceanography, which has derived and extended methodologies originating from meteorology and engineering for over a decade and a half (e.g., Mooers et al., 1986). In physical oceanography it is now an established technique that is utilized routinely for research and applications. Three books (Bennett, 1992; Malanotte-Rizzoli, 1996; Wunsch, 1996) introduce and overview the topic. A recent review (Robinson et al., 1998) discusses fundamental concepts, introduces the mathematical basis of the range of specific methods under common generic assumptions and uniform notation, and summarizes research progress. That review (hereafter referred to as RLS98) is intended to provide context and background for the present chapter. In particular, the first two sections, on basic concepts, goals, and methods, may be helpful.

There is considerable potential for data assimilation to contribute powerfully to understanding, modeling, and predicting biological–physical interactions in the sea (GLOBEC, 2000). However, the complexity and scope of the problem will require substantial computational resources, adequate data sets, biological model developments, and dedicated novel assimilation algorithms. The complexity also requires that special care be exercised (e.g., to avoid spurious dynamics due to assimilation shocks and to ensure global rather than local minima of penalty functions).

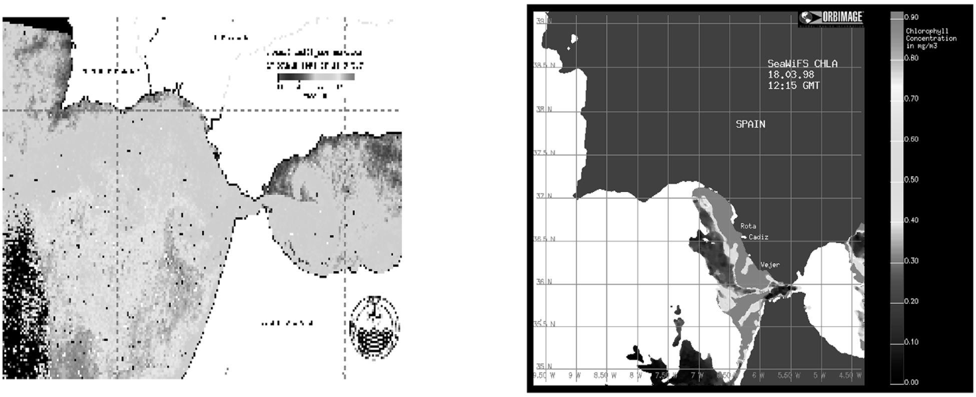
Subsequently in this chapter, in Section 2 we discuss interactive processes, scales, data, models, and methods; Section 3 illustrates assimilation concepts and research issues in terms of detailed case studies; in Section 4 we then overview progress to data more comprehensively but with less detail for individual studies and discuss the prospectus for future progress; and in Section 5 we summarize.



(a) Temperature forecast 21 Mar. 1998 **(b) Chlorophyll forecast 21 Mar. 1998**



(c) Temperature forecast error (100m) **(d) Adaptively designed sampling**



(e) SST from AVHRR 17 Mar. 1998 **(f) Chlorophyll from SeaWiFS 18 Mar. 1998**

Fig. 12.2. See color insert. Real-time multidisciplinary forecast for the Gulf of Cadiz and Strait of Gibraltar: (*a*) melded estimate of forecast temperature with data assimilation; (*b*) melded estimate of forecast chlorophyll with data assimilation; (*c*) forecasted error associated with the estimated field of (*a*) carried out by ESSE methodology (e.g., Lermusiaux and Robinson, 1999); (*d*) sampling track adaptively designed from the forecast and forecast errors; (*e*) remotely sensed sea surface temperature field; (*f*) remotely sensed (SeaWiFS) chlorophyll field. (From Robinson et al., 1999.)

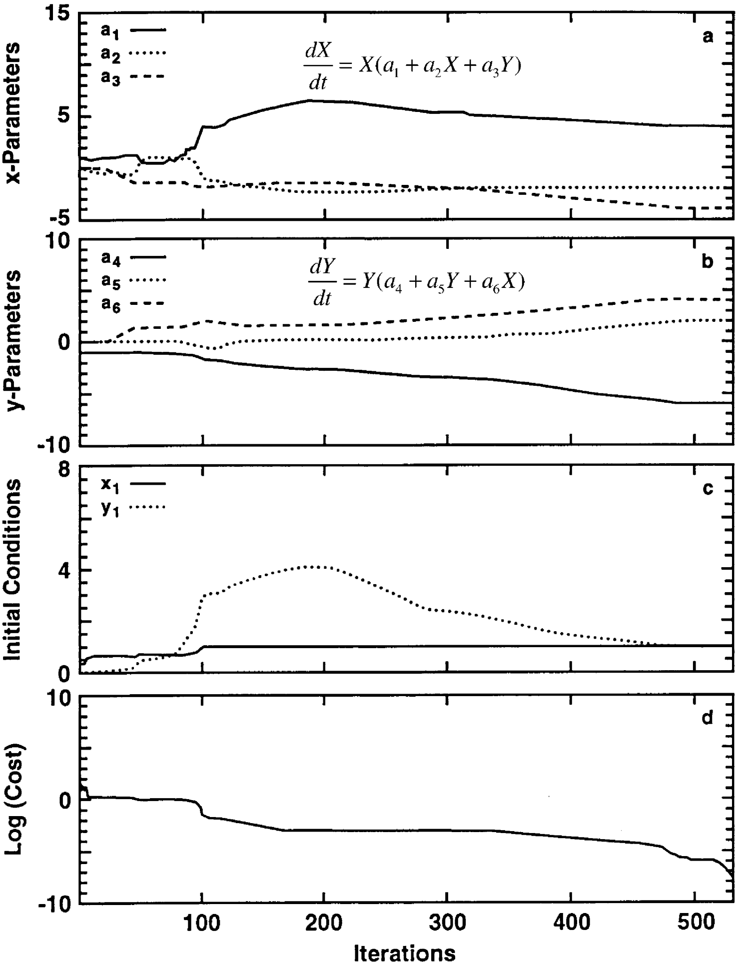


Fig. 12.3. Predator–prey model. Recovery of the (*a*) prey equation 5 coefficients; (*b*) predator equation 6 coefficients, (*c*) initial conditions for the prey X_1, and (*d*) logarithm of the cost function. (Adapted from Lawson et al., 1995.)

2. Processes, Concepts, and Methods

In this section we overview the broad range of biophysical phenomena to which data assimilation is applicable and the systematics of such application, and discuss research issues associated with models, data sets, assimilation procedures, and validation. Fundamental overall research issues relate to the essentially unknown observability, modelability, predictability, and controlability of marine ecosystems. The case studies of Section 3 and overall review of Section 4 illustrate the research issues introduced here.

2.1. Processes and Scales

Interactive biophysical processes in the ocean occur over a great range of space and time scales, and many must be characterized by multiple scales. Some scales characterizing biological structures and events arise from pure biological dynamics, some are directly imposed by physical dynamics, and some are generated by essentially interactive dynamics. Examples are the rapid bloom of phytoplankton in the presence of plentiful light and nutrients, the entrapment of an ecosystem in an eddy, and the formation of an offshore plankton plume in a coastal upwelling system. A number of studies have produced interesting diagrams and schematics of coupled phenomenological scales, which are summarized by Hofmann and Lascara (1998). However, the multiscale aspect of oceanic phenomena must be borne in mind. A physical example is an open-ocean free jet (e.g., the Gulf Stream). It is large scale downstream, jet scale cross-stream, mesoscale in its meandering, submesoscale in ring formation events, depth scale barotropically, thermocline scale baroclinically, and has surface and bottom boundary layers. One thread of organization of biophysical processes in this volume runs from smaller-scale to larger-scale processes. Processes range from turbulence and individual predator–prey encounters to climate change and evolution of the ocean–atmosphere system itself. Some of the most energetic processes occur at intermediate scales, and statistically mesoscale interactive processes can importantly mediate large-scale phenomena.

2.2. System Concept

A system approach that synthesizes theory, data, and numerical computations is essential for rapid and efficient progress in modern interdisciplinary ocean science (Robinson et al., 1999). The concept of ocean observing and prediction systems (OOPS) for field and parameter estimation has only recently crystallized in ocean science and technology. There are three major components of an OOPS: an observational network; a suite of interdisciplinary dynamical models; and data management, analysis, and assimilation schemes.

Generally, multiple interactive scales require compatible observational and modeling nests, and efficiency requires a well-chosen mix of sensors and platforms. During the last decade the first such systems were assembled, constructed, and applied to various applications in a few regions of the world ocean (RLS98; Section 4.2). The architecture of an advanced system concept structured around databases (LOOPS: Littoral Ocean Observing and Prediction Systems; Patrikalakis et al., 1999; Robinson and the LOOPS Group, 1999) is schematized in Fig. 12.4. The LOOPS system is modular, based on a distributed information concept, providing shareable, scalable, flexible, and efficient workflow and management. The system approach to complex interdisciplinary ocean science now shares many common or analogous problems with aspects of computer and information science, complex system science, and optimization technology which can contribute to advanced system methodology in oceanography.

2.3. Models

The Navier–Stokes equations of fluid dynamics (conservation of momentum and mass) together with thermodynamics and radiative transfer theory define the physical hydrodynamical, acoustical, and optical state variables for the ocean continuum and also provide fundamental nonlinear dynamical prognostic model equations for their evolution. The problem lies in determining appropriate approximate forms for processes and scale ranges of interest. This involves closure hypotheses for the parameterizations of scales that are smaller or larger than the scales explicitly represented in

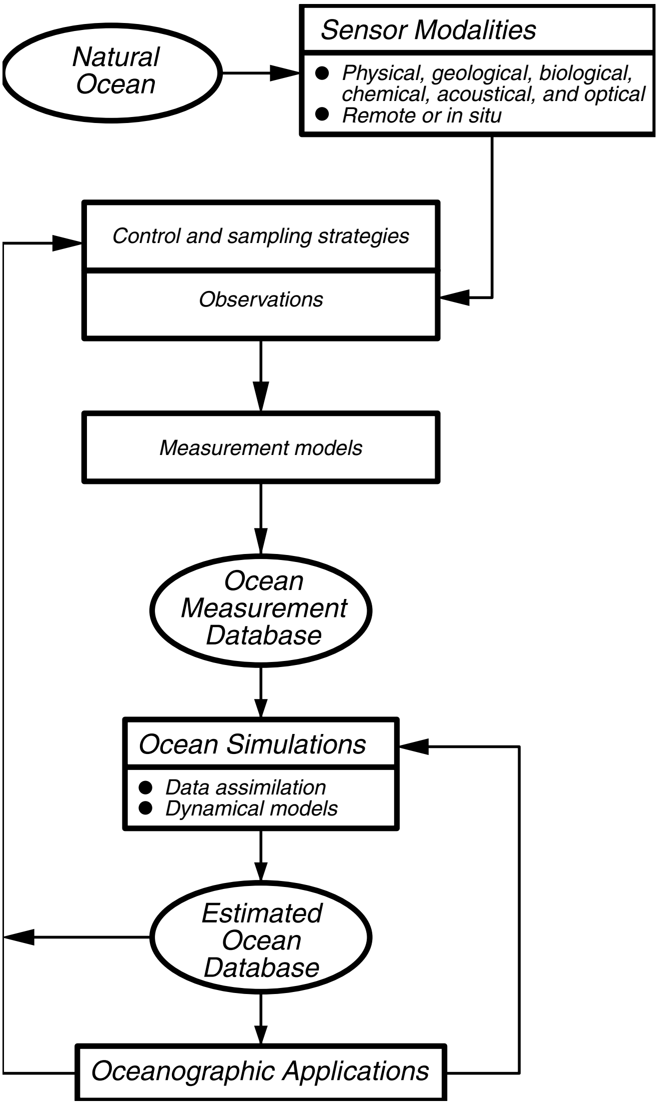


Fig. 12.4. Schematic of the architecture of the Littoral Ocean Observing and Prediction System (LOOPS).

the approximate dynamics [e.g., for the hydrodynamics, Reynolds stresses, and open boundary conditions: Kundu (1990), McComb (1991) and Frisch (1995)].

A similar fundamental dynamical underpinning does not exist for biogeochemical–ecosystem models (hereafter referred to simply as biological models). There are fundamental a priori problems in the definition of the biological continuum, the definition of biological state variables, and the formulation of the basic biological dynamical model equations, which precede the challenging tasks of approximation and parameterization (Platt et al., 1997; see also Chapter 13). General dynamical equations for n biological state-variable fields $\phi_i(\mathbf{r}, t)$ are of the form

$$\frac{\partial \phi_i}{\partial t} + \mathbf{v} \cdot \nabla \phi_i - \nabla \cdot (K_i \nabla \phi_i) = B_i(\phi_1, \ldots, \phi_i, \ldots, \phi_n) \qquad (i = 1, \ldots, n) \tag{1}$$

where t is time, $\mathbf{r}$ the three-dimensional position vector, $\mathbf{v}$ the velocity vector, and K_i a diffusivity. The first term on the left is local time change at a point, the second is advection, and the third term is diffusion. The term B_i on the right is the biological dynamics or *reaction*, which represents all the sources and sinks of ϕ_i due to, for example, reproduction, life-stage transitions, natural mortality, predation, chemical reactions and behavior. Universal formulations for all the processes inherent in the B_i do not yet exist and require substantial research, but the B_i are known to be strongly nonlinear. The general form of equation 1 governs the evolution of dynamically active tracer fields in flows and is known as an advective–diffusive–reactive (ADR) equation.

The concept of treating seawater as a physical continuum with regard to the pointwise statement of the conservation of momentum, mass, heat, and salt is established on sound physical and mathematical bases. The smallest test volume accessible to macroscopic instruments still contains very many molecules (Batchelor, 1967), and the infinitesimal limit process of calculus is applicable in the derivation of the differential equation statements of the conservations. The same is true for dissolved biological and chemical material but not necessarily for larger particles and organisms. It is, however, interesting and fundamental to derive conservation equations for the state variables of the concentration densities of these larger inorganic particles and living organisms by averaging over small but finite volumes (Pedley and Kessler, 1990, 1992) and subsequently, to integrate those equations for the field functions $\phi_i(\mathbf{r}, t)$ in specific circumstances and forcings. As for the physics, an intermediate step will often involve approximations for specific processes and dominant scales of interest (e.g., Siegel, 1998). The nonlinearities of the B_i will produce larger-scale averages of smaller-scale correlated fluctuations (generalized biological Reynolds stresses) which will require parameterizations, and eddy diffusivities will generally be anisotropic and spatially heterogeneous.

The basic biological state variables pertinent to the modeling of a marine ecosystem consist of the life stages of all the species interacting in the food web and all the nutrients and detrital products involved. This is generally a very large number of state variables (closer to infinity than to 10) which for intellectual, conceptual, and computational reasons must be reduced by condensation and aggregation (e.g., Iwasa et al., 1989). A set of critical state variables must be defined for modeling a specific problem, and the concept of a minimal set, an optimal set, and a maximal set has been introduced (GLOBEC, 1995; Nihoul and Djenidi, 1998). The minimum set can capture the process qualitatively, the optimal set can capture the process quantitatively, and the maximal set provides the most detail consistent with data, computational, and conceptual constraints. Research on nested hierarchies of models in which a single aggregated state variable is expanded into several state variables (e.g., a zooplankton variable expanded into several types and size classes) is relevant. Here we consistently use the term *state variables*, but note that many biological modelers use the terms *compartments* or *components*.

An alternative to the Eulerian field equations (equations 1) is the Lagrangian approach, in which water particles or parcels are marked at some initial time and the biological dynamics is subsequently followed along flow trajectories. Individual-based models (IBMs) are Langrangian models for concentration densities of life-stage cohorts of organisms (DeAngelis and Gross, 1992). It is, of course, essential that for biophysical process modeling, the coupled physical and biological models be compatible with respect to interactions and scales, and that the biological model be internally consistent. However, hybrid approaches (e.g., Eulerian physics and Lagrangian biology or a Lagrangian predator in an Eulerian prey field) may be utilized effectively.

Finally, we remark that analytical theoretical models and idealized numerical models can complement the most realistic four-dimensional ocean models and provide valuable insights. Scale analyses and the nondimensionalization of the physical and biological equations (O'Brien and Wroblewski, 1973; Platt et al., 1977; Ryabchenko et al., 1997; Robinson, 1997, 1999a) can significantly enhance the impact of data in assimilative studies, especially for parameter estimation. For example, Ekman numbers replace viscosities in the momentum equations and the ratios of the advective rate to selected biological rates, and so on, parameterize equations 1. A particular idealization that has received much attention is the reduction of biological models to lower spatial dimensions. Hofmann and Lascara (1998) present comprehensive tables of coupled models in zero spatial dimensions (time dependence only), one dimension (vertical with time), and two and three dimensions (vertical and horizontal with time).

2.4. Data

Compatibility (e.g., Anderson et al., 2000) is required between the biophysical data sets and the biophysical models into which the data are to be assimilated. There are also strong compatibility requirements among the physical, biological, and chemical subcomponents of the interdisciplinary data sets suitable for assimilation. The specifics of these compatibility constraints are not yet well known or defined, and a substantial research effort is required to understand them. To succeed, such interdisciplinary research requires an increased synergetic effort among physical, biological, and chemical oceanographers. The different specific purposes for which the data are to be assimilated may, of course, impose different specific requirements on data sets. For example, the rigorous verification of a real-time regional ocean prediction system requires dedicated predictive skill experiments with oversampling, whereas the subsequent operation of such a system requires the definition of an efficient minimal data set for desired accuracies. If a purpose of the assimilation is to control deficiencies of a biological model, the model must generally be capable of representing the oceanic process being observed (i.e., it must be generally valid for the process). This concept is illustrated in Section 3.4.

There are essentially three modes of collecting data for ecosystem studies. Laboratory experiments and measurements provide necessary information on the inner workings of organisms (behavior, growth kinetics) and inorganic reactions (composition ratios, reaction rates), usually in pure-culture or isolated species designs (e.g., Giesy, 1980). In situ samplings in the natural open-ocean environment provide data reflecting the complexities of multiple interactions among various material and species, on multiple scales, in response to internal dynamics and external forcings. To build some bridges between laboratory manipulations or microcosms, and real ocean investigations or macrocosms, experiments with artificial enclosures of seawater can be employed (Grice and Reeve, 1982a,b; Harris, 1996). These *mesocosms* aim to sustain representative, naturally proportioned, and viable ecosystems, either free or artificially forced (Gamble and Davies, 1982; Petersen et al., 1999). As of today, they enclose usually about 10 to 10^4 m^3 of seawater, for days to years. They can provide data on aggregated production rates and exchanges between several trophic levels.

Data assimilation has important roles to play in each of these three modes of scientific experiments, from the rigorous development and verification of models, to the identification of the necessary and sufficient data for parameter estimation and model state predictions. Important feedbacks (Fig. 12.1) are expected to occur, at varied scales and levels of aggregation. Since mesocosm observations are often easy to obtain and intensive, both locally and in budgets (e.g., Banse, 1982), zero- or one-dimensional simplifications of parts of the models B_i (equation 1) can be calibrated, validated, and verified (Section 2.6). Some of these concepts are illustrated in Section 3.3. Similarly, the use of data assimilation in laboratory experiments for marine biology should become widespread in the future.

An efficient mix of platforms and sensors, remote and in situ, is an effective approach not only for individual state variables (e.g., temperature, chlorophyll) but also for the suite of variables composing a compatible set of interdisciplinary data types for coupled biophysical assimilation. Although compatible data sets simultaneously acquired by design are now rare, the promises of coupled biological–physical data assimilation can be realized only by the purposeful acquisition of such coordinated multivariate observations. Several techniques exist to compensate for lack of observations in interdisciplinary data sets and to extend the impact of existing observations; vigorous research is also required in these areas. Multivariate and interdisciplinary correlations, statistical feature models, and structured feature models (e.g., Lozano et al., 1996) provide valuable tools. Missing data for compatible biophysical assimilation can also be estimated off-line of the main simulation or prediction of interest. This approach is illustrated in Section 3.7.

New, advanced measurement techniques for biological fields and parameters present powerful future opportunities for the acquisition of extensive and comprehensive data sets but also present challenging problems of interpretation. Observation of sea surface color from satellites, which was initiated in 1978 from the Coastal Zone Color Scanner (CZCS) and is presently being obtained from the Sea-Viewing Wide Field-of-View Sensor (SeaWiFS), is providing coverage of the surface distribution of biological features essentially unattainable otherwise (McClain et al., 1998). But serious questions remain as the relationship of the observed outgoing surface irradiances to near-surface distributions of chlorophyll, phytoplankton, and inorganic colored materials, and of the relationships of surface distributions to deeper fields (e.g., subsurface chlorophyll maxima). New sensor developments require concomitant research on new measurement models, including, importantly, research on the relationship between sensor variables and dynamical model state variables. For example, direct assimilation of irradiance measurements may be more effective than converting those to chlorophyll and then assimilating them as is done now. Direct use of irradiance measurements will require a more sophisticated bio-optical model component of the biophysical model. In situ measurements of multifrequency acoustics, multispectral optics, and their use simultaneously for biological state variables and parameters is already very promising but requires extensive measurement model research.

Data impact and sensitivity research requires substantial research on skill metrics and error models (Lynch and Davies, 1995; Lynch et al., 1995; Robinson and Glenn, 1999). Their use in quantitative biophysical observation systems simulation experiments (OSSEs; see GLOBEC, 1994) is essential, and OSSEs for automated adaptive sampling research are crucial. There is a need for extensively sampled restricted areas that can serve as test beds for model calibrations, model intercomparisons, parameter estimation, assessment of data requirements, evaluation of data assimilation methods, and other research issues related to biophysical data assimilation.

2.5. Assimilation Methodology

A number of methods developed and used for data assimilation in engineering, meteorology, and physical oceanography are available as starting points for coupled biophysical data assimilation. An overview is presented in Section 3 of RLS98, with an appendix that provides mathematical assumptions and equations for most methods. Details presented there are not repeated here. Most methods are derived directly from estimation theory or control theory. The methods range from simple to complex, but all involve hypotheses that lead to the minimization of an error norm or assimilation criterion to determine the state or parameter values. Optimal application of a method satisfies the criterion exactly, but a suboptimal application does so only approximately. Since assimilation calculations can be costly and time consuming and can strain available or existent computational capabilities, suboptimal methods are often necessary. Twin experiments consist of exercising the assimilation procedure with simulated data of properties usually analogous to those of real data (e.g., Section 1, Fig. 12.3; Malanotte and Young, 1992; Miller and Cornuelle, 1999). This serves to determine if the data and assimilation scheme could work for real data. In identical twin experiments, the model used to create the simulated data is the same as the model used for the assimilation.

The estimation of errors associated with the biophysical model and data available for assimilation is important. The deterministic equations (equation 1) are generally modified and manipulated to equations with stochastic forcings $d\eta_i$ (equation 2a). The ensemble of model parameters (diffusivities, biological rates, etc.), $P_i = \{K_i, R_i, \ldots\}$, are also represented by an equation with stochastic forcings $d\zeta_i$ (equation 2b), where C_i are functionals that describe the deterministic evolution of the parameters with time and space. The state variables ϕ_i are related to the data y_j via measurement models, with stochastic forcings ϵ_j (equation 2c). The assimilation or melding criterion (equation 2d) involves in general the minimization of a functional J of the stochastic or error forcings $d\eta_i$, $d\zeta_i$, and ϵ_j, and of their a priori statistical properties or weights denoted by q_η, q_ζ, and q_ϵ (equation 2d), subject to the constraints of equations 2a to 2c.

$$d\phi_i + \mathbf{v} \cdot \nabla\phi_i \, dt - \nabla \cdot (K_i \nabla\phi_i) \, dt = B_i(\phi_1, \ldots, \phi_i, \ldots, \phi_n) \, dt + d\eta_i \qquad (i = 1, \ldots, n) \tag{2a}$$

$$dP_i = C_i(\phi_1, \ldots \phi_i, \ldots \phi_n) \, dt + d\zeta_i \tag{2b}$$

$$y_j = H_j(\phi_1, \ldots \phi_i, \ldots \phi_n) + \epsilon_j \qquad (j = 1, \ldots, m) \tag{2c}$$

$$\min_{\phi_i, \mathrm{P}_i} J(d\eta_i, d\zeta_i, \epsilon_j, q_\eta, q_\zeta, q_\epsilon) \tag{2d}$$

The three sets of equations 2a to 2c and the assimilation criterion (equation 2d) define the assimilation problem (Fig. 12.1). In equation 2b, the C_i's are often assumed constant (but do not need to be) and equation 2b then simply states that parameters are known a priori up to a certain uncertainty $d\zeta_i$. In equation 2c the measurement model operators are denoted by H_j. These functionals H_j can depend, as do B_i and C_i, on the values of parameters. For example, if the parameter P_i is measured, y_j then represents that measurement and equation 2c is then usually $y_j = P_i + \epsilon_j$. Similarly, if a state variable ϕ_i is measured at the scales of interest, equation 2b is simply $y_j = \phi_i + \epsilon_j$. In equation 2d the functional J is often called the cost, penalty, or objective function. Using equations 2a to 2c to substitute for $d\eta_i$, $d\zeta_i$, and ϵ_j in equation 2d, J is expressed as a function of the unknown state variables ϕ_i and parameters P_i, and known a priori information, the data y_j, and weights q_η, q_ζ, and q_ϵ. The subsequent minimization (equation 2d) subject to equations 2a to 2c by a chosen assimilation scheme leads to optimum estimates of ϕ_i and P_i, denoted by $\hat{\phi}_i$ and $\hat{P}_i$. For state estimation ($\hat{\phi}_i$), we refer to the estimates just before and just after data assimilation as a priori and a posteriori, respectively. For parameter estimation ($\hat{P}_i$), a priori and a posteriori refer to parameter values at the beginning and at the conclusion of the optimization. Data residuals or data-model misfits refer to the differences between the data and model estimated values of the data, $y_j - H_j\ (\hat{\phi}_1, \ldots, \hat{\phi}_i, \ldots, \hat{\phi}_n)$.

If the models or data are used as strong constraints (e.g., model structures and functionality are assumed perfect without errors), the terms $d\eta_i$, $d\zeta_i$, or ϵ_j are null. If the model or data are used as weak constraints, their errors, or the probability distribution of the stochastic forcings, are specified and utilized in the assimilation criterion (equation 2d). We note that these stochastic error forcings $d\eta_i$, $d\zeta_i$, and ϵ_j do not need to have a zero mean, but that equation 2a to 2c can always be written so that they do, by transferring the means to B_i, C_i, and H_j. The assimilation can be understood as a forward or filtering problem, or as a smoothing or inverse problem (Bennett, 1992; Wunsch, 1996; Robinson and Lermusiaux, in press), as is illustrated in Section 3. In simple terms, the parameters or state are said to be observable if their optimum value can be determined from the data and assimilation criterion (equations 2c and 2d). The issue of observability (e.g., Brockett, 1970; Jazwinski, 1970) is important in biophysical estimation, as discussed in Sections 3 and 4. The use of data assimilation methods for biophysical system identification is also described in these sections. Different models 2a to 2c are then intercompared based on criterion 2d. Formal methodologies (e.g., Eykhoff, 1974; Kulhavy, 1996) to do so exist, especially for linear systems, and they should be investigated. In particular, the identification of adequate parameterizations is primordial in ecosystem modeling (e.g., Haney and Jackson, 1996), and in this chapter it is included in the objectives of parameter estimation.

Most minimization criteria 2d are essentially least squares (e.g., error-weighted sum of squared data residuals) or convex optimization problems, which give the conditional mean as optimal estimate if the system is linear or of Gaussian statistics. Some important processes in the ocean (e.g., intermittence and frontal coherence) are inherently non-Gaussian, and methods may need to be extended or developed to deal with these processes, especially when few data are available. This will probably be the case for several important biological processes. However, at this early stage of biophysical assimilation, much is to be learned from the immediate application of existing methods, including the use of simple methods if care is taken to avoid pitfalls such as those illustrated in the following sections.

Biophysical dynamics are generally complex and highly nonlinear, and only data assimilation research will reveal the essential methodological problems and the preferred methods of dealing with them. At this time, research with a variety of methods is desirable, although those that are fundamentally or inherently linear hold less promise. Data assimilation methods and schemes, the structure of dynamical and measurement models, and observational networks and sampling strategies are all interrelated as an overall system (Fig. 12.1). Accuracy, efficiency, optimality, robustness, and stability of the overall system can be achieved only by an iterative development of the system's architecture, components, linkages, and feedbacks.

2.6. *Errors and System Evaluation*

A current topic of data assimilation research in general relates to the representation, attribution, and propagation of errors, and an increased research effort will be required in coming years. The complexity of biophysical processes presents many challenging issues in error modeling. The fact that biophysical data assimilation is in its infancy provides an interesting opportunity to construct such models employing relevant new ideas from the general research effort. A variety of error metrics (equation 2d) need to be explored and defined for specific purposes involved in parameter estimations, simulations, nowcasts, and forecasts. Important examples include penalty functions and weights and predictive skill metrics. Such considerations are essential for the development of effective biophysical observation system simulation experiments and the real-time operation of ocean observing and prediction systems (GLOBEC, 1994). Rigorous system evaluation is time consuming and demanding, and the development of automated schemes for the dual use of data for validation prior to assimilation is desirable.

Dynamical model errors (equations 2a and 2b) can arise from the misrepresentation of dynamical processes, both explicitly and parametrically, the omission of processes, mathematical formulations, and computational algorithms and procedures. Observational errors (equation 2c) can arise from the design and operation of sensors and platforms, sensor and measurement models, and environmental noise. As mentioned above, lack of compatibilities between the models and the data, as well as the biology and the physics, are error sources. Error variances, multivariate correlations, and probability distribution functions are all required. Stochastic processes not represented in the dynamics may be necessary to include in error models (Section 2.5). To reduce the size of the estimation problem, dominant errors need to be identified and represented (e.g., by eigendecomposition of error matrices and projection onto error subspaces) (Lermusiaux, 1997, 1999a,b; Lermusiaux and Robinson, 1999).

For the development of regional biophysical OOPS, the concepts of successive validation, calibration, and verification (Robinson et al., 1996) are useful. Validation demonstrates that the system is generally appropriate for the processes and scales of interest, and calibration tunes the system parameters to the region. Verification requires dedicated predictive skill experiments with oversampling at the scales of interest to establish in real time and quantitatively the predictive capability of the system. Both regionally specific and process generic skill metrics are required. Regionally specific metrics that quantify qualitative regional variabilities (e.g., the bifurcation or not of a current or the occurrence or not of a significant bloom associated with a synoptic event) can substantially reduce verification data requirements. Loss of predictability, which is essentially rooted in nonlinear error propagation and error-scale transfers, ultimately limits predictive capability (RLS98). Since the atmosphere forces the ocean and ocean physics forces ocean biology, there are three sets of nonlinearities involved. The synoptic predictability limit of the atmosphere is *O*(days). The mesoscle predictability of ocean physics due to ocean internal dynamical processes is *O*(days to weeks). However, many dominant nonlinearities and associated predictability limits of regional ecosystems and generic biogeochemical–ecosystem processes are essentially not yet known.

3. Research Concepts and Issues: Case Studies

We present here selected studies and their results chosen to illustrate ideas discussed generally in the preceding section. These case studies precede the overview of Section 4 in order to illustrate in depth interdisciplinary issues, in part as a basis for the understanding of the briefer discussions of individual studies reported there. Each example presents the scientific problem; the data assimilation methodological research concepts and issues; the model, data set, and assimilation scheme; a summary of research highlights; and a discussion of implications for further assimilation research. Two general lines of organization are (1) parameter estimation is followed by state estimation, and (2) idealized, low-dimensional models precede four-dimensional, more realistic models.

3.1. Model Evaluation via Parameter Estimation for the Sargasso Sea

Spitz et al. (1998) address the use of an adjoint method (Bennett, 1992; Wunsch, 1996; RLS98) for the systematic estimation of the parameters of a model for the seasonal dynamics of plankton at a site in the upper mixed layer of the western North Atlantic ocean. The pelagic ecosystem model is the nitrogen-based model of Fasham et al. (1990). The data consist of sparse time series of observations (Fig. 12.5) collected during the U.S. Joint Global Ocean Flux Study (JGOFS) experiments at the Bermuda Atlantic Time-Series Study (BATS) station. Two groups of data assimilation experiments are carried out: identical twin experiments (Section 2.5) to determine if the properties of the BATS data and optimization algorithms permit a successful estimation, and the parameter estimation based on the real BATS data to evaluate the ecosystem model.

The one-dimensional ecosystem model averaged over the mixed layer includes a microbial loop; its seven state variables are the concentrations of nitrate, phytoplankton, zooplankton, ammonium, dissolved organic nitrogen, detritus, and bacteria. The data forcing the model are the monthly mean mixed-layer depths at Bermuda, obtained from the Levitus (1982) climatology, and the incident solar radiation at the ocean surface. The nitrate below the mixed layer and maximum phytoplankton growth rate are free parameters. The BATS ecosystem observations consist of profiles of nitrate, chlorophyll *a* and particulate organic nitrogen concentrations, bacteria cell counts, phytoplankton primary production rates, and bacterial production rates.

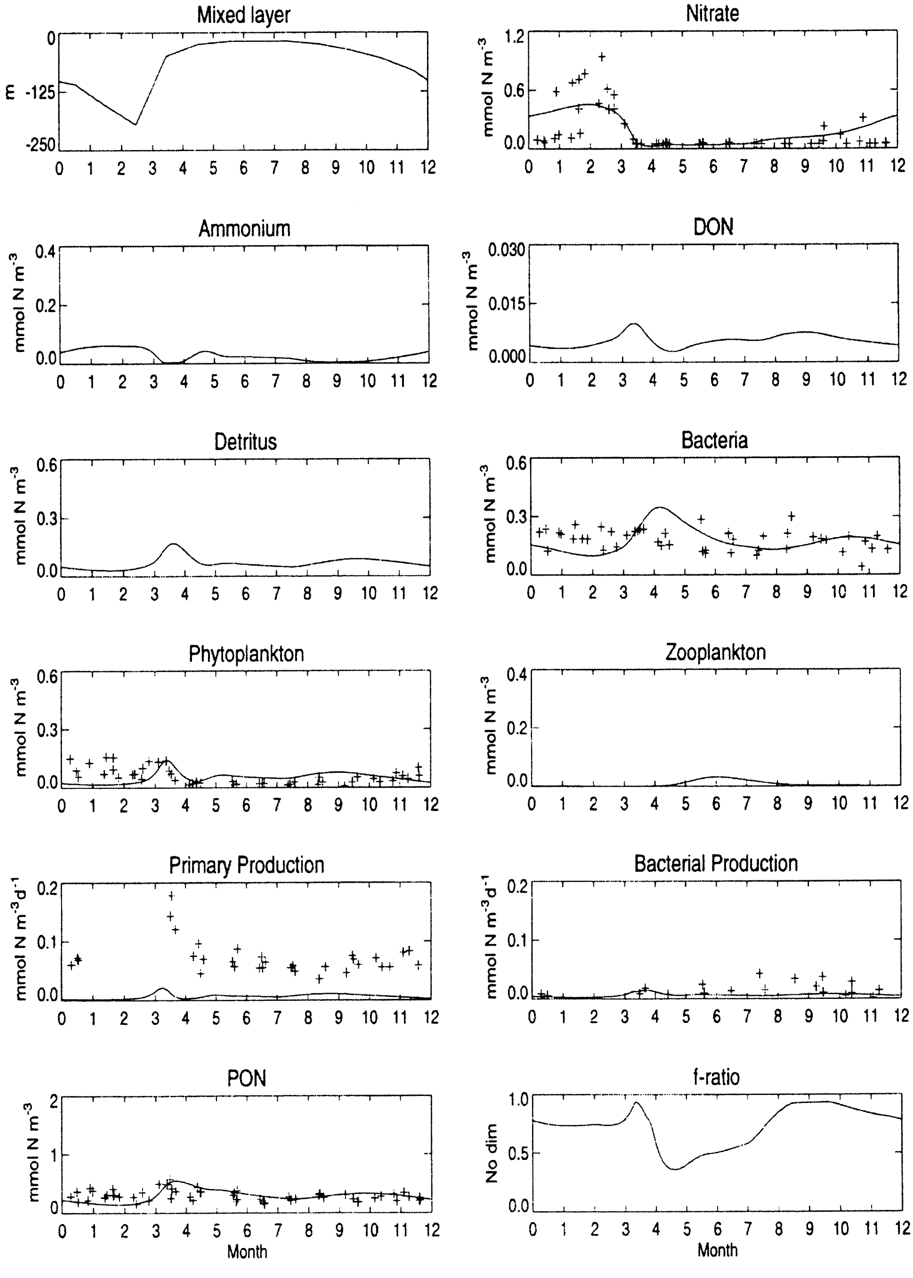


Fig. 12.5. BATS observations between 1998 and 1993 (crosses) and results from data assimilation (solid curves). (From Spitz et al., 1998, Fig. 10.)

Profiles collected at about monthly intervals from 1988 to 1993 are combined into a single year and vertically integrated from the surface to the seasonally varying mixed-layer depth prior to assimilation. These simplifications are based on the assumptions of steady annual cycle and homogeneous mixed layer.

A measurement model (e.g., equation 2c) is constructed based on diagnostic equations and conversion factors. The model phytoplankton nitrogen concentrations are converted to chlorophyll *a* data assuming a linear relationship with constant coefficients. The bacteria cell counts are simply related to nitrogen but given a low weight in the cost function. For the particulate organic nitrogen and phytoplankton primary production rates data, diagnostic equations with constant factors are employed. Bacterial production rates were not used.

The cost function is an error-weighted sum of squared data residuals (Section 2.5). The a priori weight matrices are chosen diagonal. The inverse of the weights are set for each data type, proportional to the time average of the data (Lawson et al., 1995, 1996). Weights for data with large uncertainties are reduced by a factor of 10. An adjoint method is used to minimize the cost function.

For the identical twin experiments, simulated data are generated at the same frequency and type as the BATS data, using the model of Fasham et al. (1990) calibrated for a steady annual cycle at a station northwest of BATS. Five years of model simulations are subsampled at BATS frequencies and combined into one year. This simulated data are assimilated into an independent one-year simulation. Most parameters, but not all, are recovered. To solve this issue, the parameters not recovered are grouped into combinations of parameters (i.e., sums, fractions, or products). Without changing the dynamics, these combinations are then chosen as an alternative parameter set. The twin experiment is redone and all of these combinations are then recovered. The authors note that the parameters to which the dynamics are most sensitive are recovered with fewer iterations.

The BATS data are then assimilated, but the resulting optimized model solution is not close to the data (Fig. 12.5). Primary production is too low in the model. Based on the twin experiments, the data and optimization algorithm are not the probable cause of failure. It is more likely the ecosystem model, imposed as a strong dynamical constraint by the adjoint method (no model errors), and the measurement model and its errors (weights in the cost function), which need to be revised.

For improvements of the ecosystem model, the authors first suggest modifying the primary nitrate forcing from a constant below the mixed layer to a concentration increasing linearly with depth below that layer. This suggestion is based on nitrate profiles at BATS and on previous studies (Fasham and Evans, 1995; Hurtt and Armstrong, 1996). Due to interannual variabilities and episodic physical forcings (e.g., waves, eddies), the assumption of steady annual cycle should also be verified or, we believe, at least imposed as a weak constraint (Section 4.5). In Fig. 12.5, this is shown supported by the sometimes relatively large scattering between data crosses of similar calendar days but different years. For the measurement model, the authors first suggest using nonstatic conversion factors (e.g., chlorophyll *a*/nitrogen ratio in the phytoplankton, which varies seasonally with light intensity) (Hurtt and Armstrong, 1996). More research on N_2 fixation and the diagnostic equations themselves (e.g., the link between the fraction of particulate organic nitrogen that is modeled and its measured total value) may also be useful.

The results of Spitz et al. (1998) show that twin experiments can guide the removal of parameter dependencies by indicating useful groupings and can reveal reasons for unsuccessful real data assimilation. The authors also suggest that the model structures of Fasham et al. (1990) need to be modified to allow a fit of the BATS data (Section 4.4). In addition, issues related to low-dimensional biophysical dynamics, error models, and data manipulations are also important. In particular, the effects of combining multiyear data directly into a single assimilation year should be assessed (e.g., Sections 4.4 and 4.5).

3.2. Model Complexity for the Subarctic Pacific

Matear (1995) illustrates that data assimilation can quantitatively determine the nature of the dynamics and ensure that the complexity of a model is consistent with the information contained in the data using simulated annealing (RLS98) to estimate model parameters and their uncertainties. The consistency of three oceanic mixed-layer ecosystem models of varying complexity with long-term biological data collected at a site in the subarctic Pacific (Station P) are compared. The models are nitrogen-based and aim to describe the seasonal variation of the phytoplankton biomass and production. Horizontal advection and diffusion are neglected based on Frost (1991). The mixed layer is assumed to be homogeneous and to overly an abiotic layer. The vertical forcing is limited to the observed evolution of the mixed-layer depth, and its biological effects are parameterized differently for motile or nonmotile variables (Evans and Parslow, 1985).

The simplest model governs nitrate, phytoplankton, and zooplankton (NPZ) in the mixed layer, based on Evans and Parslow (1985). This three-component model contains 14 parameters. The next model divides zooplankton into two size classes (mesozooplankton and microzooplankton), so as to ensure that only microzooplankton grazing can prevent a bloom of phytoplankton (Frost, 1987). This four-component model requires 18 model parameters. The final model, based on Fasham et al. (1990), includes a microbial loop which has been observed to be significant for the plankton dynamics in the northeast Pacific. It contains seven components and 25 parameters.

The daily data are averages of relatively high frequency observations collected at Station P over several years. Some of these averaged data force the models directly (the annual cycles of solar radiation, mixed-layer depth, mixed-layer temperature, and nitrate concentration below the mixed layer). The remainder of the averaged data constrain model parameters (phytoplankton, rate of primary production, nitrate, and mesozooplankton concentrations) (Fig. 12.6A-1, A-2, A-4 and Fig. 12.7B-4).

For each model, the goal is to estimate the parameters that minimize an error-weighted sum of squares (Section 2.5) comprising daily data residuals (data misfit penalty), differences between state variables on the first and last days of the year (steady-state seasonal cycle penalty), and differences between the final and a priori parameter values (a priori parameter penalty). The a priori error variances for the data (Fig. 12.6A-1, A-2, A-4, and Fig. 12.7B-4) are estimated from data variability, from the uncertainty of converting sensor to data values (e.g., Fig. 12.6, from A-5 to A-1), and from the differences between data processed by two sources. The a priori error variances for the parameters are derived from earlier applications of the models.

Simulated annealing generates a sequence of estimates such that new estimates with lower cost are always accepted, while new estimates with higher cost are accepted with a certain probability. This direct, global method can address strong nonlinearities, but its computational requirements are large. For all three models, the observability (Section 2.5) of the parameters is estimated locally, based on the number of parameters that are resolved independently. This is obtained from the off-diagonal elements of the a posteriori error correlation matrix. In all cases, at most 10 model parameters are resolved, which is always less than the number of unknown parame-

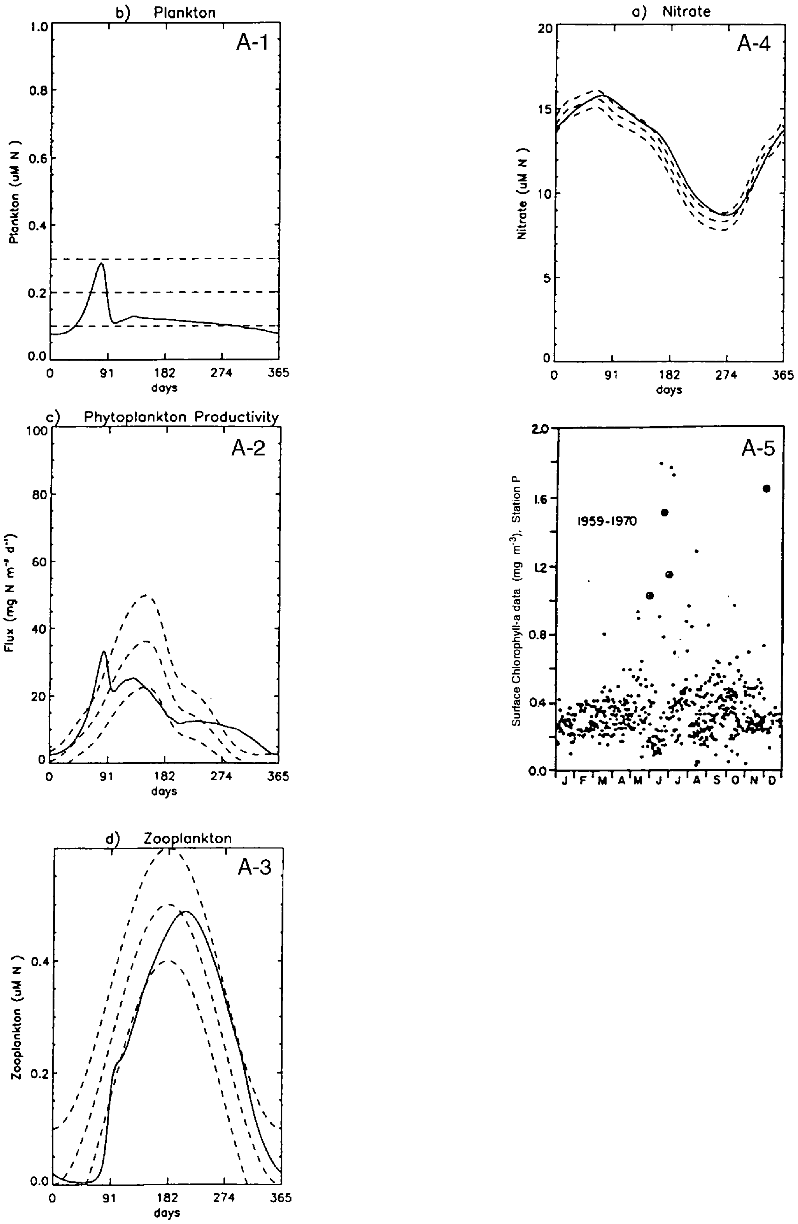


Fig. 12.6. Optimized solution for the three-component model (solid curves), compared with data (dashed curves) and data error estimates (± 1 standard deviation uncertainties, dashed curves). On (A-1), phytoplankton concentration; (A-2), net phytoplankton productivity; (A-3), zooplankton concentration; (A-4), nitrate concentration; (A-5), chlorophyll *a* concentration data, as measured at Station P. The averaged data assimilated are nitrate, phytoplankton, and the phytoplankton productivity. The weak “feature model–like” constraint for the zooplankton is here also represented as a dashed line, with ± standard deviation uncertainties (A-3). Note that the phytoplankton data assimilated (A-1) are constant. (Adapted from Matear, 1995.)

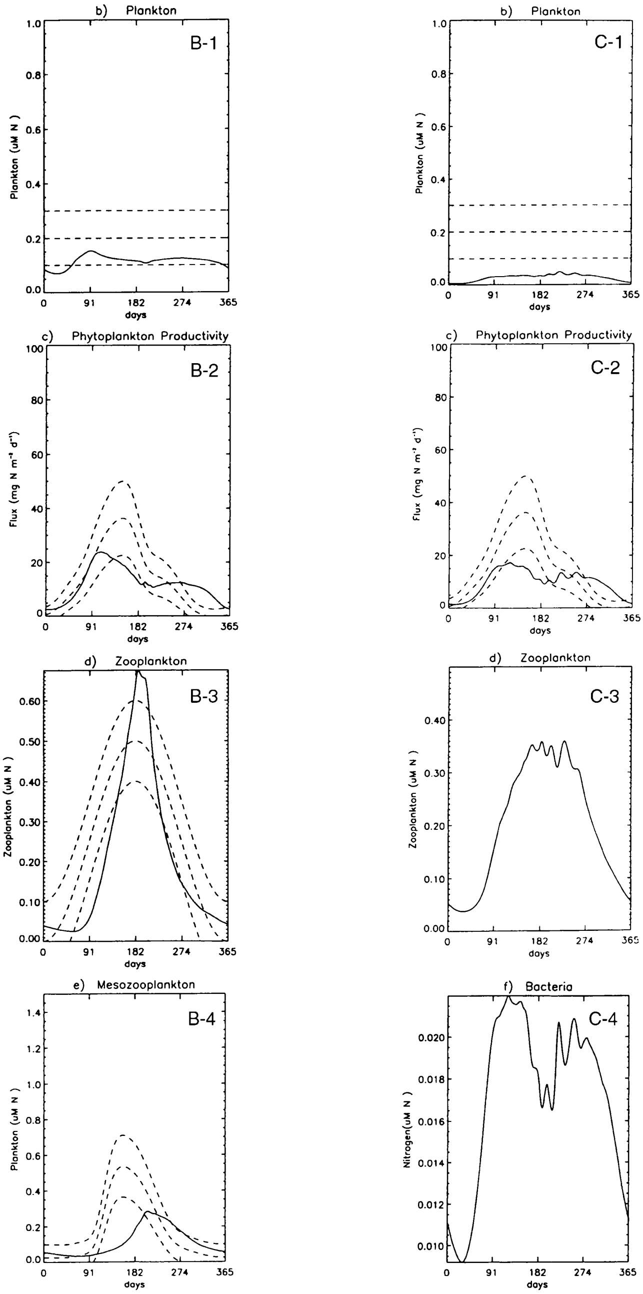


Fig. 12.7. As for Fig. 12.6, but for the four-compartment (B-1 to B-4) and seven-compartment (C-1 to C-4) models. The nitrate concentrations of these two models are relatively similar to those of Fig. 12.6; they are not shown. The mesozooplankton (B-4) is the additional state variable in the four-compartment model and the mesozooplankton data (B-4) are only used with this model. Dashed curves lines on (B-3) show the weak feature model constraint (as on Fig. 12.6). In the seven-compartment model, there is no such weak constraint on the zooplankton (C-3), but there is one on the *f*-ratio (not shown). The bacteria concentration (C-4) illustrates the microbial loop. (Adapted from Matear, 1995.)

ters. For all models, linear combinations of parameters can thus lead to cost function values similar to that at the optimum (i.e., the optimal parameters are numerically not unique). Overall, some a posteriori data residuals are larger than the a priori standard data errors (Fig. 12.6A-1 to A-4, Fig. 12.7B-1 to B-4, Fig. 12.7C-1, C-2); some parameters also have a posteriori errors larger than the a priori ones.

The optimized NPZ model is able to reproduce most patterns and magnitudes of the three types of data assimilated. However, its zooplankton is too high when compared to the few microzooplankton data available at Station P. To utilize this independent information, a weak constraint on the zooplankton (Fig. 12.6A-3) is added to the cost function. With this constraint, the fit is relatively good (Fig. 12.6), but the number of unresolved parameters remains unchanged. The four-component model (Fig. 12.7B-1 to B-4) also fails to produce adequate microzooplankton without the weak constraint (Fig. 12.7B-3). Considering errors, the uncertainties on the parameters comparable to these of the NPZ model are increased; model complexity thus increases more than the information extracted from the mesozooplankton data. In addition, for acceptable zooplankton estimates (Fig. 12.7B-3, B-4), some of the parameters related to their growth and mortality rates seem unrealistic. The author concludes that the four-component structure is inconsistent with the data and thus requires modifications (e.g., nonlinear and/or temperature-dependent rates). The seven-component model (Fig. 12.7C-1 to C-4) produces acceptable concentrations of zooplankton (Fig. 12.7C-3) without the weak, "feature model–like" (Section 2.4) constraint. However, it requires such a constraint for its *f*-ratio estimate (ratio of new production to total production) to agree with the few summer *f*-ratio data available at Station P. Considering errors, the parameters comparable to those of the two other models have larger a posteriori error variances and correlations; fewer parameters are resolved. Since very limited data on ammonium and bacteria are available, it is also difficult to validate the corresponding estimates (e.g., Fig. 12.7C-4).

The analysis of Matear (1995) shows that data used for assimilation can limit the dynamics that can consistently be included in an ecosystem model. The three-component model seems to suffice for explaining the data, but even in this simplest case, several parameters are not uniquely determined and some a posteriori errors are too large. To justify the seven-component model, additional data are necessary to constrain the microbial loop. Data assimilation is, in fact, shown to help identify the missing data sets. In general, all the relevant data available should be used, even if the relations between state variables and data are not simple. To ensure estimates in accord with independent data, a weak, feature model–like constraint was added. Weak data constraints could also have been applied via biological correlations (e.g., the sparse mesozooplankton data could then constrain both the three- and seven-component models, even though these models do not have a mesozooplankton variable). Similar statements apply to the few *f*-ratio data. For all models, several of the optimized parameters are found to be either too small or too large when compared to a priori knowledge. Error models for the biological dynamics might be useful for this type of research.

3.3. *Model Structure for Coastal Mesocosm Experiment*

A promising approach to improving the understanding of ecosystems, and so develop accurate models of such systems, combines data assimilation with mesocosm experiments (Section 2.4). The recent work of Vallino (2000) aims to apply this approach in a coastal environment. Mesocosm data are utilized to assess a class of biological models and estimate their parameters. Different optimization algorithms are intercompared, a relatively detailed measurement model is employed, and some of the problems with the structure of current food web models (e.g., static parameters and the lack of robustness), are illustrated.

The four mesocosms considered examine how food web communities in coastal zones process and utilize the input of terrestrial organic material. The four enclosures contain 7 m^3 of seawater augmented with various combinations of dissolved inorganic nitrogen and dissolved organic matter. The data consist of approximately daily measurements of particulate and dissolved organic carbon, particulate organic and dissolved inorganic nitrogen, chlorophyll *a*, net primary and bacterial productivities, and the light extinction coefficient. The dynamical model is a zero-dimensional pelagic model similar to that of Fasham et al. (1990) but with a fairly complex treatment of organic matter production and consumption. It employs 10 state variables and involves 29 parameters (governing growth kinetics and organic matter decompositions), three of which are measured. With the initial conditions, this leads to 36 free (nonmeasured) parameters.

The main goal is to estimate the parameter values that minimize an error-weighted sum of squared data residuals (Section 2.5); the model structure is a strong constraint and there are no a priori parameter penalties. Parameters are here directly constrained to a bounded space and nondimensionalized. A measurement model (equation 2c) is constructed to link the 10 state variables to the eight types of discrete data. Its error component involves absolute and relative error variances: data error covariances are assumed null, but data errors are set correlated in time to ramp in the discrete data slowly and reduce assimilation shocks (Robinson, 1996; Lermusiaux, 1999a; Anderson et al., 2000). The observability of the parameters is estimated locally, based on the rank, singular values, and resolution matrix of the Hessian matrix at an optimum (Tziperman and Thacker, 1989; Wunsch, 1996). This local analysis indicates that the initial carbon and nitrogen detritii, the carbon/nitrogen ratio of phytoplankton exudate, and the decomposition rate of detritus are not well resolved.

Twelve optimization routines are tested, ranging from local gradient-based, simplex, and quasi-Newton methods, to global simulated annealing and genetic algorithms (e.g., RLS98). While some routines do not perform well, several local routines perform more or less as well as global routines. An interesting result is that the 12 sets of optimum parameter values found by the 12 routines are scattered throughout the bounded range of acceptable values (Fig. 12.8). This scattering occurs even though most routines converge to similar final values of the cost function. The dynamics of the fits differ. Some are smooth fits, others are rapid oscillations in between data points (Vallino, 2000). Overall, several a posteriori data residuals are larger than the a priori standard measurement errors (equation 2c).

The results above indicate that either the data are not sufficient, the assimilation schemes are not adequate, the dynamical model should be a weak constraint, or the dynamical and measurement models, including their a priori errors, should be improved. To investigate some of these possibilities, the author carries out an identical twin experiment. Data are extracted daily from a model simulation of a mesocosm. The corresponding cost function is reduced using three different routines. All recover most parameters and lead to good fits of the simulated data. Since the data type and resolution are as for the actual oceanic mesocosm, the data are overall sufficient and the optimization routines adequate. It is the models and the strong dynamical constraint that are probably inadequate.

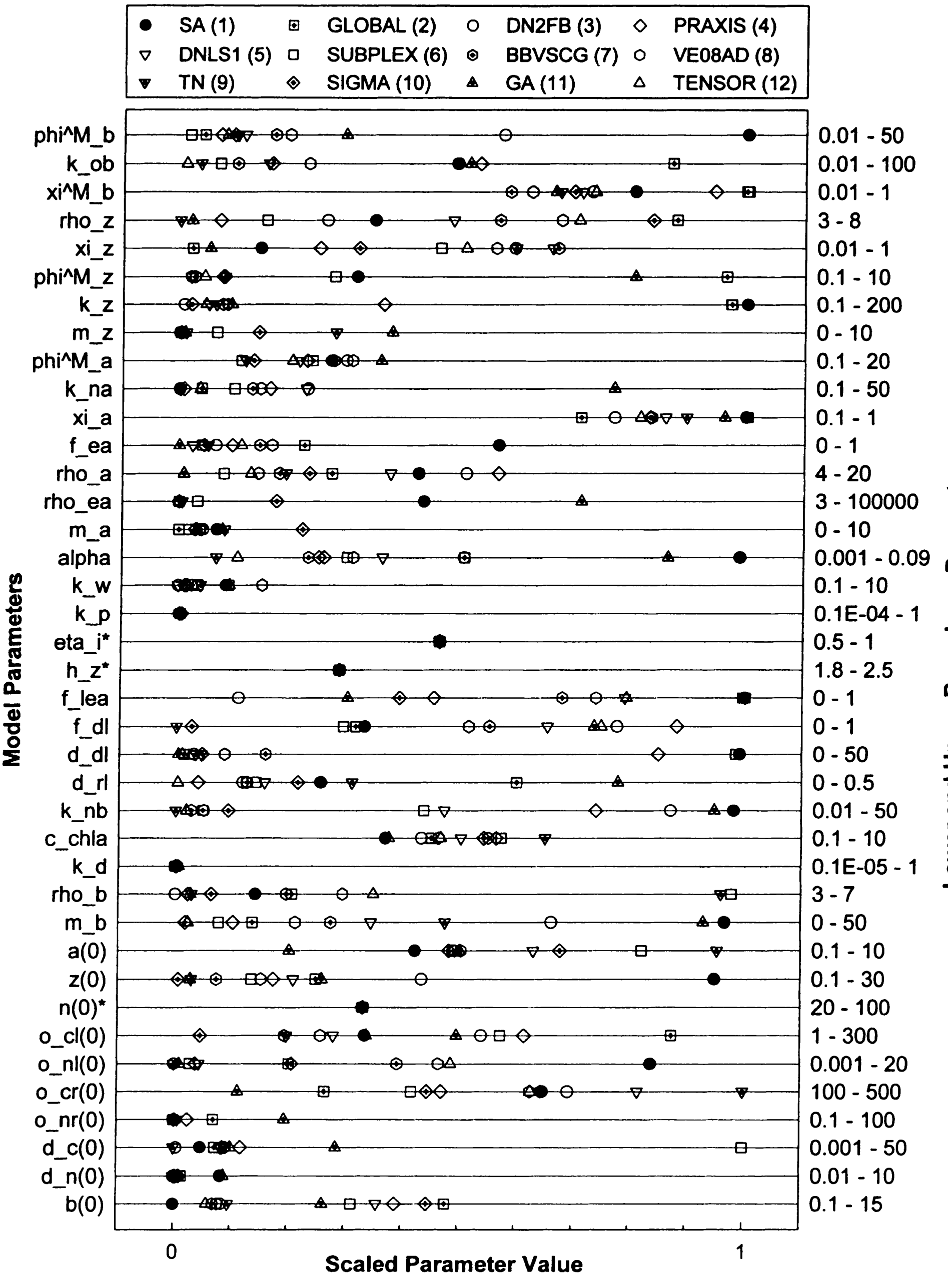


Figure 12.8. Optimized, scaled (0 to 1) parameter values associated with each of the minima located by the 12 optimization routines (abbreviated routine names and their symbols are on top of the figure). Model parameters (left ordinate) and their absolute parameter bounds (right ordinate) are described in Vallino (2000). Parameters marked with an asterisk (left ordinate) were held constant during the data assimilation. (From Vallino, 2000.)

The author argues that model structures are probably inadequate because of aggregation and parametrization uncertainties. The large number of optima (Fig. 12.8) appears related to the strong sensitivity of aggregated models to parameters and initial conditions (Beckers and Nihoul, 1995). This sensitivity results from the strong nonlinearities (e.g., growth rates varying with biomass). Another reason discussed is the assumption of static parameters. Parameters can vary with the local environment in coastal regions, and the parameters fitted for one mesocosm are not adequate for the other mesocosms. To address these two issues, the author considers a simpler, first-order kinetic model and a model with a dynamic carbon/nitrogen ratio of phytoplankton. However, these two models do not improve the fit to data. The author thus suggests alternative directions for improvements. Since accurate modeling of all organisms and their interactions is unlikely and not practical, aggregation into a few trophic or functional groups (Totterdell et al., 1993) is necessary. However, aggregation should involve models for the growth kinetics of aggregated consortia of species. The structures of such models do not necessarily mimic these of single-species models; they should be derived from multiple-species interactions. More abstract models (e.g., starting from mass or energy conservation) may also be useful and should be investigated (Platt et al., 1981).

Based on the findings of Vallino (2000), several issues and research directions can be identified. One of them is error model research (Section 2.6) (e.g., the relaxation of the strong dynamical constraint and the assessment of a priori errors in the measurements, parameters, and model structures). Another is the compatibility of the sampling (e.g., data type, coverage, time and space scales) with the ecosystem under study (Section 2.4). Data assimilation can reduce parameter uncertainties and thus reveal structural errors should the model with optimized parameters still fit the data poorly. Since mesocosm data can be seen as a zero- or one-dimensional limit of regional oversampling, mesocosm data assimilation may allow the verification of some structures of zero- or one-dimensional simplifications of biological dynamical models.

3.4. *Model and Data Compatibility for the Equatorial Pacific*

In a study of biological–physical interactions in the central equatorial Pacific, Friedrichs (1999) and Friedrichs and Hofmann (2001) have used an adjoint method (e.g., RLS98) to obtain realistic fields for dynamical inferences. This research illustrates the necessity for a biological model to be valid for the general representation of the coupled process studied in order for data assimilation to be possible (Section 2.4). It also demonstrates the importance and utility of both scale analysis for model formulation and nondimensional analysis in parameter estimation. A number of physical scales and forcings were studied, including low-frequency circulations in both the absence and presence of an El Niño event and a tropical instability wave (TIW) (Qiao and Weisberg, 1995; Yu et al., 1995).

The biological model was a one-dimensional (vertical) ADR model (equation 1) depth averaged over the euphotic zone (Friedrichs and Hofmann, 2001). The dynamics for the biological state variables (phytoplankton, zooplankton, nitrate, ammonium, and detritus) is schematized on Fig. 12.9. Iron limitation of primary productivity was parameterized by a feature model (Section 2.4) in the euphotic zone tied to deeper observations. The physical diffusions and advections were input from calculations based directly on time series observations from moorings. Scale analyses indicate that diffusions were negligible compared to advections, that vertical advections were important for all state variables, and that horizontal advections were also important

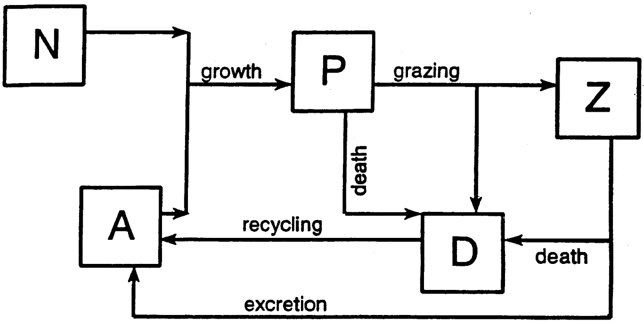


Fig. 12.9. Schematic of the biological components [phytoplankton (P), zooplankton (Z), ammonium (A), nitrate (N), and detritus (D)] and biological interactions included in the equatorial Pacific ecosystem model. (Adapted from *Deep-Sea Research II*, **48,** M. A. M. Friedrichs and E. E. Hofmann, Physical control of biological processes in the central equatorial Pacific, pp. 1023–1069, copyright 2001, with permission from Elsevier Science.)

for the two nutrients. The study was centered at (0°N, 140°W) and data for physical forcings and biological assimilations were taken from moorings from the Tropical Atmosphere Ocean (TAO) project and from two cruises (TS1, TS2) that occurred during the U.S. Joint Global Ocean Flux Study (JGOFS) Equatorial Pacific Process Study (EqPac) in 1992. TS1 occurred during the 1991–1992 El Niño and TS2 after the El Niño event. The control variables for the adjoint assimilation were nondimensionalized and scaled to order unity to facilitate minimization of the penalty function.

The marine ecosystem model requires the specification of 16 parameters, and a sensitivity analysis revealed that the model results were relatively insensitive to certain parameters and that many model parameters were highly correlated. Based on the results of this preliminary sensitivity analysis, six parameters (phytoplankton and zooplankton growth rates, phytoplankton and zooplankton mortality rates, the half-saturation coefficient for iron uptake, and the rate of nutrient recycling) were allowed to vary within permissible ranges determined by information gleaned from the EqPac cruises.

Fifty forward model simulations were performed in which values of these six parameters were randomly chosen for each simulation to be within the permissible ranges. These results (Fig. 12.10) demonstrate how small changes in parameter values can result in large differences in simulations. Even when conservative estimates of the uncertainties associated with these parameters were made, several model state variables had variations of a factor of 5 to 10. In an effort to select the optimal values for these parameters, biogeochemical data from the two EqPac cruises were assimilated.

In one experiment, 50 assimilative runs were performed in which data from the TS1 cruise were assimilated starting with the same 50 random parameter sets used to generate the forward model results of Fig. 12.10. This experiment identified a minimum of the cost function (parameter set A; Fig. 12.11) that reduced the model-data misfit for the independent TS2 data, below the mean misfit obtained for the 50 forward model simulations.

When a second experiment was conducted in which all the TS2 data but no TS1 data were assimilated (not shown), the cost function did not converge in over 200 assimilation runs. This intriguing result implies that although the ecosystem model structure is consistent with conditions during which the TS1 data were collected (the

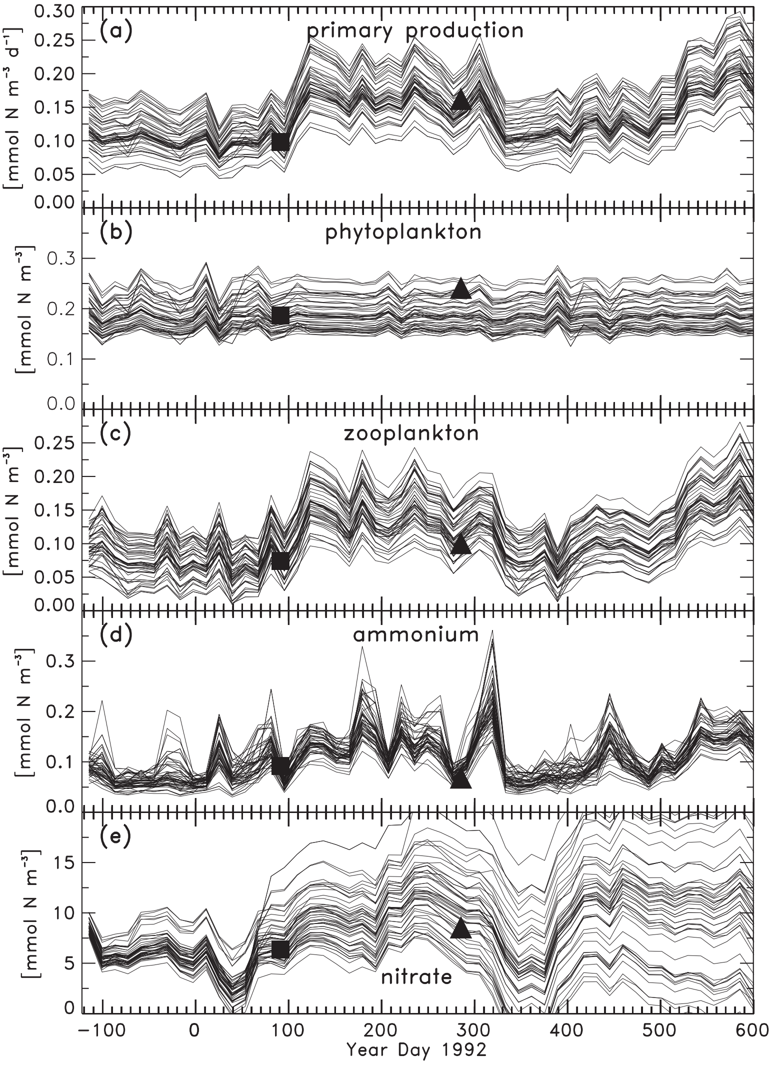


Fig. 12.10. Fourteen-day averaged time evolution (beginning on 9/1/91) of 50 forward model simulations, generated using 50 randomly selected sets of parameter values that fall within reasonable ranges (*a*) primary production, (*b*) phytoplankton, (*c*) zooplankton, (*d*) ammonium, and (*e*) nitrate. Average values from the TS1 (square) and TS2 (triangle) cruise data are shown for comparison. All quantities are depth-averaged over the euphotic zone. (Adapted from Friedrichs, 2001.)

1991–1992 El Niño), it is inconsistent with conditions during which the TS2 data were collected.

Environmental conditions during the TS1 and TS2 cruises differed dramatically. Not only was the thermocline relatively deep during TS1 and shallow during TS2, characteristic of the El Niño/non-El Niño time periods, respectively, but also a tropical instabilty wave (TIW) passed by 0°N, 140°W during the TS2 cruise. In order to determine the cause of the failure of the TS2 assimilation experiment, the portion of the TS2 data set that was collected during the passage of this wave was removed

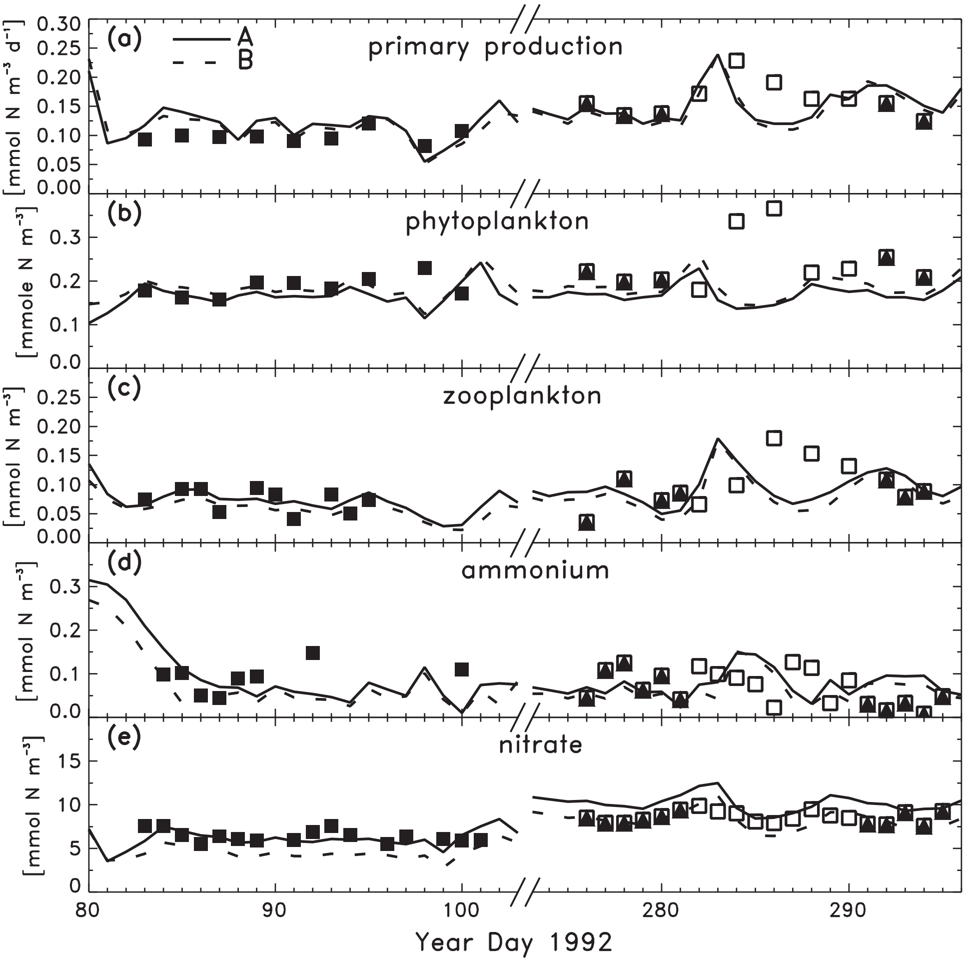


Fig. 12.11. Simulated time distributions of (*a*) primary production, (*b*) phytoplankton, (*c*) zooplankton, (*d*) ammonium and (*e*) nitrate obtained using two optimal parameter sets recovered from the assimilation of the TS1 data set (parameter set A; solid line) and a subset of the TS2 data set (parameter set B; dotted line) using the adjoint method. The TS1 data (filled squares), TS2 data (open squares) and the subset of the TS2 data (filled triangles) are shown for comparison. (Adapted from Friedrichs, 2001.)

from the TS2 data, and the assimilation process was repeated. In this experiment the cost function did converge and a parameter set (B; Fig. 12.11) was obtained that improved the model-data misfit for the independent (TS1) data set.

These results suggest that the initial TS2 assimilation experiment was unsuccessful because the model structure was inconsistent with ecosystem changes associated with the TIW. The large change in species composition observed during the passage of this wave (Bidigare and Ondrusek, 1996) is the most likely cause of this inconsistency. In this way, the adjoint assimilation of the EqPac data reveals that although the model structure is consistent with both El Niño and non–El Niño conditions, it breaks down during the passage of instability waves, which are believed to be associated with significant changes in species composition.

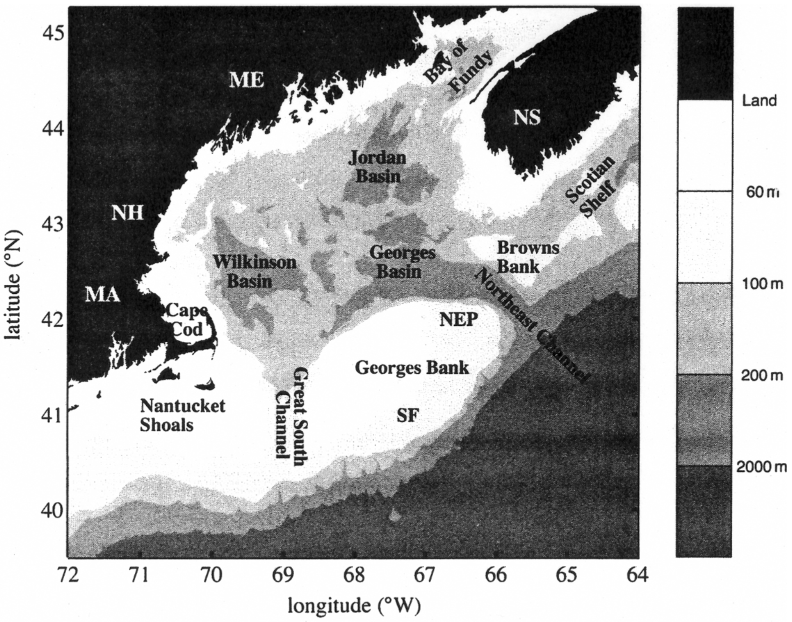
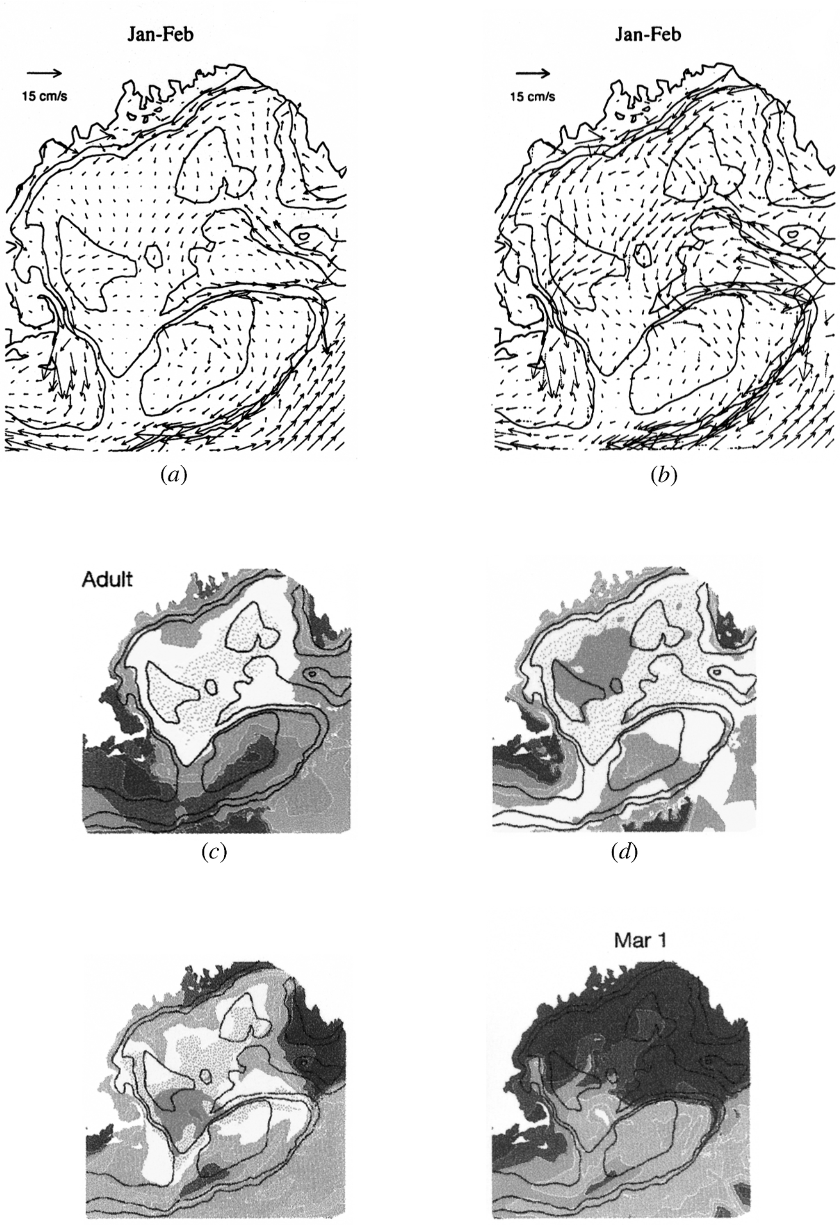


Fig. 12.12. Schematic of the bottom topography of the Gulf of Maine and Georges Bank. NEP, Northeast Peak; SF, Southern Flank. (From Lynch et al., 1998, Fig. 1.)

3.5. *Calanus Bloom Process Inference in the Gulf of Maine*

The Gulf of Maine is a semienclosed sea (Fig. 12.12) with major topographic features, including three deep basins and Georges Bank, an important fisheries resource. A dominant copepod *Calanus* (*Calanus finmarchicus*) is believed to play a significant role in the dynamics of the regional ecosystem, and Lynch et al. (1998) have studied biological–physical interactions influencing the annual bloom of this *Calanus*. A general hypothesis is introduced that the mean abundance and distribution of the species is the result of basic animal characteristics combined with the climatological mean physical and biological environment, and specific processes are investigated by a series of idealized and realistic simulations. The data assimilation methodology is assimilation by initialization and nudging. The specific scientific focus is the midwinter initiation of the annual bloom by diapausing populations, and their role in supplying reproducing populations to Georges Bank during spring. At this early stage of coupled assimilation, this study illustrates how simple methods can be used to obtain important results.

The physical dynamical model used was the free surface finite-element primitive equation Dartmouth shelf model (Lynch et al., 1996). The model driven by buoyancy flows, atmospheric fluxes, and tides has been used to construct a bimonthly circulation climatology (Lynch et al., 1997), which was used to advect the copepod in an Eulerian biological model. Simulations were run from January through April with both depth-averaged and near-surface layer advections. The January–February fields are shown on Fig. 12.13*a* and *b*. The biological model was a population dynamics model resolving 16 life stages of the species (egg, six naupliar, six copepodite, and three adult stages). Vertical swimming behavior could allow for aggregation in the



(*a*) (*b*)

(*c*) (*d*)

(*e*) (*f*)

Fig. 12.13. See also color insert for parts (*c*)–(*f*). Biological/physical simulations of *Calanus finmarchicus* population dynamics: (*a*) vertical averaged Lagrangian velocity for January–February; (*b*) average surface layer (top 25 m) Lagrangian velocity for January–February; (*c*) decadally averaged bimonthly adult *Calanus* abundances in the upper 200 m centered on January 1; (*d*) decadally averaged bimonthly adult *Calanus* abundances in the upper 200 m centered on March 1; (*e*) adult *Calanus* abundances on March 1 from G_0 simulation; (*f*) adult *Calanus* abundances on March 1 from G_1 simulation. (From Lynch et al., 1998.)

near-surface layer. Interaction with other biological variables was simply parameterized by mortality and food supply, and limited food supply inhibits egg production. In some simulations the model allowed reproduction of the initial population generation (G_0) to produce the next generation (G_1). The data set for initialization and verification consisted of bimonthly 10-year means (1977–1988) of *Calanus* abundance (adults and three highest copepodites) in the upper 200 m binned into 97 tiles for the Gulf of Maine. The adult bimonthly distribution centered on January 1 and March 1 are shown on Fig. 12.13*c* and *d*.

The results of March 1 for simulations initialized on January 1 are shown on Fig. 12.13*e* for the most realistic G_0 simulation and on Fig. 12.13*f* for a baseline G_1 simulation. The distributions are for total adults in the near-surface layer. The G_0 simulation is regarded as being in reasonable agreement with MARMAP (Mountain and Holzworth, 1989) data, but the G_1 population has developed too rapidly over Georges Bank. The development is slowed in subsequent simulations by assuming food limitation in the Gulf of Maine but not over Georges Bank. The low abundances on Fig. 12.13*f* near the Scotian Shelf, the Bay of Fundy, and the shelf break south of Georges Bank are regarded as not real but caused by inadequate specification of open boundary sources.

General results are summarized and dynamical processes presented in the three-level schematic of Fig. 12.14. Diapausing populations wintering-over in all three deep basins of the Gulf (Fig. 12.12) are assumed to rise into the circulation throughout January and February, and this source is represented by nudging the water column over the basins to maintain initial abundances. Exit from diapause lasts for about two months, and thus the deep source regions provide a persistent rather than impulsive supply of G_0 adults to Georges Bank, arriving with viable egg production having been inhibited by lack of sufficient food.

Research directions discussed by the authors include closing the annual cycle with an extended simulation and a second (G_2) population generation, and the treatment of the Scotian shelf, Bay of Fundy, and shelf-break open boundary condition sources as a parameter estimation problem by data assimilation. The extension of the model to include detailed treatment of primary production and predation is also considered in the context of some of the issues of complexities, computational resources, and data requirements discussed in Section 2, and it is argued that even the densest biophysical data sets available today are sparse relative to requirements, so that data-based modeling is essential for realistic studies of ecosystem dynamics.

3.6. Inverting for Population Dynamics in the Gulf of Maine and Georges Bank

McGillicuddy et al. (1998b) employ an adjoint method to investigate the biophysical mechanisms that control the seasonal variations in abundance of *Pseudocalanus* spp. in the Gulf of Maine and Georges Bank. The copepod *Pseudocalanus* is an abundant zooplankton in the region (different from *Calanus finmarchicus* studied in Section 3.5). The authors postulate that the *Pseudocalanus* variations observed result from the interactions of population dynamics with fluid motions. Even though a broad spectrum of time and space scales are possibly relevant, as a first step, the authors explore the relationships between the seasonal mean physics and seasonal biology, especially the mechanisms controlling the biology at these scales. The biological model employed is a horizontal two-dimensional (three-dimensional vertically

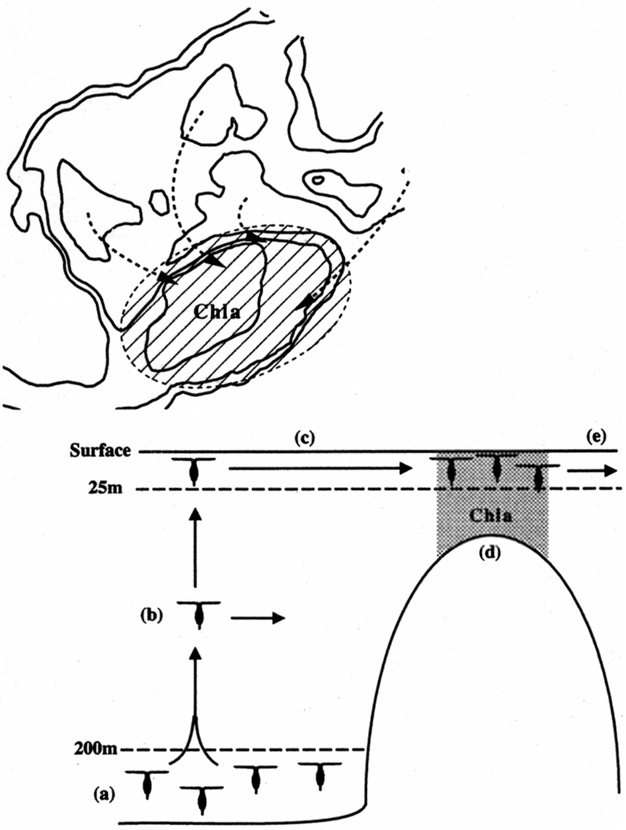


Fig. 12.14. Schematic of final G_1 initiation scenario: (*a*) large source population of diapausing animals in the deep basins of the Gulf of Maine; (*b*) slow bankward transport of rising C5s; (*c*) fast bankward transport of adults in the surface layer; (*d*) reproduction on the bank where food is abundant; (*e*) loss from bank. (From Lynch et al., 1998, Fig. 23.)

integrated) ADR equation (equation 1) for copepod concentration fields in which the specified two-dimensional velocity and diffusivity fields are outputs of a seasonal physical model. An adjoint method is used to directly “invert for the population dynamics,” that is, to estimate the source or reaction term $B_{i=1} = B(x, y, t)$ in the vertically integrated form of equation 1, based on the observed variations in abundance and specified physical fields.

The general circulation of the Gulf of Maine is mainly cyclonic, from east to west, with the Maine coastal current interacting with several topographically controlled gyres and feeding some of the predominant clockwise circulation around Georges Bank (see Fig. 12.13*a* and *b*). This coastal circulation is forced by external atmospheric, Scotian shelf and slope processes, which lead to complex physical dynamics. The numerical circulation used by the authors is obtained from a finite-element model of the flow in the region (Lynch et al., 1996, 1997). The three-dimensional flow is vertically integrated and broken down into six periods of two months. The resulting horizontal climatological transport is specified as input to the two-dimensional ADR model for the copepod concentrations.

Two sets of experiments are carried out to evaluate the effects of the modeled physical fields on passive tracer dynamics (advective-diffusive equation). One set shows that the main domain of interest is not affected by the open boundaries over the two-month time scales of interest. The other focuses on the pathways on and off Georges Bank and the degree of material retention on the bank. At seasonal scales, conditions vary between two extremes. In winter, a significant portion of the bank is diluted in two months, by inflows from the north and outflows to the southwest. In late summer, global stratification and local mixing effects strengthen the clockwise circulation around the bank, increasing retention.

The *Pseudocalanus* spp. concentration fields, $\phi_{i=1} = C_{\text{obs}}$ in equation 1, are obtained from 11 years of data collected during the MARMAP program. The data for the adult stage of *Pseudocalanus* are combined into one year, binned into bimonthly periods and objectively analyzed to lead C_{obs} (Fig. 12.15, first row). For each of the bimonthly periods, the optimization problem is formulated as follows. Given the imposed initial conditions in analyzed copepod concentration $C_{\text{obs}}(x, y, t_0)$, find the reaction term $B(x, y)$ that minimizes the difference between the next set of analyzed concentration $C_{\text{obs}}(x, y, t_1)$ and the concentration at t_1 obtained by integration of the forward ADR model forced by $B(x, y)$ from t_0 to t_1. The model up to the unknown $B(x, y)$ and the objectively analyzed data are thus assumed exact, while the cost function is a final cost (i.e., nonzero only at t_1) (e.g., Wunsch, 1996). An adjoint method is used for the inversion, using the adjoint code of the discrete dynamical model.

The inversion leads to six source terms $B(x, y)$, one for each bimonthly transition. The first three are plotted on (Fig. 12.15, second row), along with the objectively analyzed C_{obs} (Fig. 12.15, first row), and the remaining terms in the ADR equations, averaged over the bimonthly periods (Fig. 12.15, third and fourth rows). Most patterns exhibit relatively strong seasonal and spatial variations. The copepod abundance (Fig. 12.15, first row) shows that for the domain covered by data, from January–February to May–June, concentrations increase, building maxima on Georges Bank and in the coastal waters of the western Gulf of Maine. For the rest of the year, most patterns are maintained, but amplitudes decrease in these two active regions. Copepod tendencies Fig. 12.15, fourth row) are found to be controlled primarily by a balance between the source and advection terms (Fig. 12.15, second and third rows). During January–February to March–April (Fig. 12.15, first column), on Georges Bank, growth dominates but is almost balanced by advection of low concentrations from the Gulf of Maine. In western coastal areas, moderate growth occurs. Two months later (Fig. 12.15, second column), net growth intensifies in these coastal waters. On the bank the tendency is overall positive, with growth and advection still nearly balancing but in a dipolar mode. Growth dominates the dilution by advection on the northeastern side, while southwestward advection of high concentrations from this northeastern crest dominates net mortality on the western side. As the bank becomes more isolated due to the reinforcing clockwise circulation, especially on the northern flank (Fig. 12.15, third column), growth on the northeastern side drops and, overall, abundance on the bank decreases, due to the persisting southwestward advection on its western side and mortality on its southwestern extremity. In late summer (McGillicuddy et al., 1998b), retention is maximum and abundance declines due to mortality. During late fall and early winter, the advection and source terms are closely balanced, maintaining a relatively low abundance. For the western coastal areas, the source term (growth and mortality) is the main control of abundance, except in late

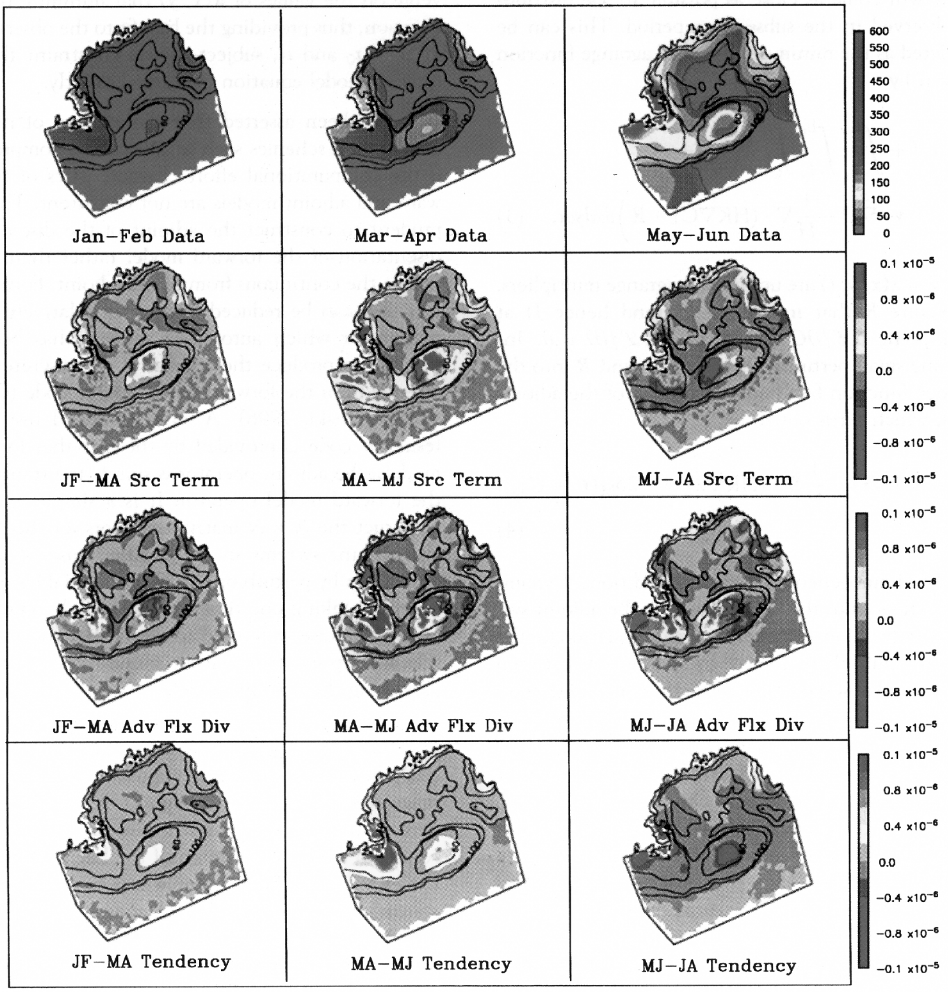


Fig. 12.15. See color insert. Top row: bimonthly climatological *Pseudocalanus* spp. distributions (adults only) objectively analyzed from the MARMAP data (number of animals m–3). Second row: three source terms $B(x, y)$ resulting from three of the six inversions. Each $B(x, y)$ is located directly below the analyzed data used to initialize the experiment. That is, the JF–MA source term results in a forward model integration which matches the March–April analyzed data. Last two rows: two of the remaining terms in the ADR equation, adjective flux divergence and overall tendency, averaged over the period of integration. Fields in the bottom three rows have been normalized to the bottom depth, so the units are "number of animals m–4s–1." (From McGillicuddy et al., 1998b; reprinted by permission of Blackwell Science, Inc.)

spring, when the southwestward advection by the Maine coastal current accumulates organisms in the Massachusetts Bay areas.

To evaluate their source term estimates, the authors refer to historical food and predator data. The growth estimates of *Pseudocalanus* do not disagree with data on its food availability. Food is always limiting inside the Gulf of Maine, never limiting on Georges Bank, and sometimes limiting in coastal waters. For mortality, there is possibly less agreement. The period of copepod decline on Georges Bank (May–June to September–October) logically overlaps the period of maximum predator concentrations. However, these predators are not known to be more abundant on the southwestern side of the bank, while inside the Gulf of Maine, the largest predator concentrations are observed when copepods are estimated to grow the most. To explain this, further research is required (e.g., show that mortality rates are controlled by factors other than the abundance of predators).

These results show that the seasonal variability of *Pseudocalanus* is spatially variable as a function of its own growth or mortality, and advection by climatological currents. Diffusion is not important. The ecological scenario proposed is that of two self-sustaining populations, one in the western Gulf of Maine and the other on Georges Bank, separated by a region of the Gulf where food concentrations are too low for the copepods to thrive. This interpretations agrees with some previous results but differs from others. The solution is probably sensitive to the inverse problem formulation. Time-dependent source terms or, in general, more sophisticated biology, as well as error models for the data and biophysical models, should be investigated. Portions of the inverted source terms could, in fact, be due to deficiencies in the physical model. Even though the physical features found important to the biology are robust in climatological studies, time-dependent (storms, internal waves) and three-dimensional stratified mesoscale flows should be included. The effects of life stages may also be important (e.g., the voyage from the western Gulf of Maine to Georges Bank may be possible for the nonfeeding early stages of the copepod). Another specific issue concerns the compatibility of data and dynamics (e.g., the effects of nonlinear interactions on multiple scales in both the data and models). Coupled inversions including ADR equations and data for the food and predators, as well as models and data for the individual *Pseudocalanus* species of possibly different behavior, should be useful. More advanced syntheses, with newer data, models, and assimilation methods (RLS98), should further the understanding.

3.7. Assimilation Methodology for Biophysical Dynamics in the Gulf Stream

In a study of coupled physical and biological processes in the Gulf Stream meander and ring region (GSMR), Anderson et al. (2000) have addressed the issues related to the necessity for assimilation of a comprehensive and compatible biophysical data set for a case in which only sparse in situ observations were available and the necessity of the avoidance of spurious shocks in the assimilation process. In GSMR, mesoscale meanders grow, evolve, and propagate, and submesoscale events include the birth and reabsorption of rings as well as temporary contacts between meanders and rings. Vertical and horizontal advections occur, including upwelling, downwelling and cross-frontal exchanges which can stimulate productivity, enhance biological gradients, and produce plankton patchiness. The scientific context involved the use of data assimilation in order to achieve a simulation adequate to reveal specific real ocean (sub)mesoscale dynamical processes. The simulation was carried out for the nutrient limited conditions of late summer when the large-scale biological fields are slowly varying in time. Specific scientific objectives were (1) to determine what physical and/or biological processes caused a high-phytoplankton patch at the Gulf Stream front observed in the data, and (2) to assess the impact of stream meandering, ring–stream interactions, and winds on vertical velocity, vertical nitrate transport,

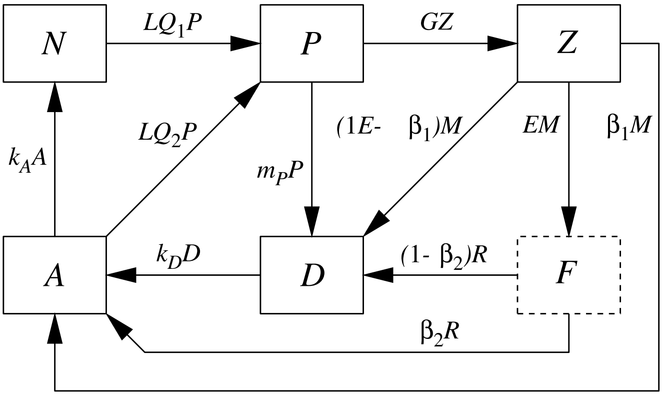


Fig. 12.16. Five-component biological model. The five state variables are nitrate (N), phytoplankton (P), zooplankton (Z), ammonium (A), and dissolved and suspended particulate organic nitrogen (D). Fast-sinking detritus (F) is included but sinks and remineralizes instantaneously, and thus is not an explicit state variable. (Reprinted from *Deep-Sea Research I*, **47,** L. A. Anderson et al., Physical and biological modeling in the Gulf Stream region, I, Data assimilation methodology, pp. 1787–1827, copyright 2000, with permission from Elsevier Science.)

phytoplankton and zooplankton patchiness, primary production and new production, particle export, and cross-stream exchanges of nitrate and phytoplankton (Anderson and Robinson, 2001).

The study was carried out with the Harvard Ocean Prediction System (HOPS) primitive equation (PE) physical dynamical model coupled to a five-state-variable (nitrate, ammonium, phytoplankton, zooplankton, and dissolved plus suspended particulate organic nitrogen) biological model (Fig. 12.16 and equation 1), and data were assimilated via the HOPS optimal interpolation scheme (Robinson, 1996, 1999b). The coupled biophysical dynamical simulation was run for about two weeks, from year day (yd) 272 to 279 of 1988, utilizing data starting at yd 265 from both a Gulf Stream meander coupled biological–physical dynamics experiment (BIOSYNOP/Anatomy of a Meander—BS/AM) (Hitchcock et al., 1993; Lohrenz et al., 1993; Mariano et al., 1996) and a Gulf Stream real-time forecasting project (GULFCAST) (Glenn and Robinson, 1995). The BS/AM in situ data consist of approximately 320 XBTS; 216 CTDs, half of which also measured fluorometry (chlorophyll); a total of 32 nutrient stations; and a few zooplankton measurements, all located in a domain approximately 2° of latitude and 5° of longitude in extent centered at (38°N, 70°W). The GULFCAST data consist of weekly locations of the surface Gulf Stream meandering front and the location and size of all warm- and cold-core rings determined from satellite sea surface temperature and height measurements, located in a domain approximately centered at (37°N, 69°W) and 6° of latitude and 10° of longitude in extent.

The procedure for optimal interpolation (OI) assimilation of compatible biophysical fields is schematized in Fig. 12.17. GULFCAST methodology provides full-water-column three-dimensional estimates for the stream and rings by the use of feature models, or typical synoptic structures for temperatures and salinities located at stream and ring frontal locations (Gangopadhyay et al., 1997). Fields for initialization of the PE model, assimilation, and verification were prepared from objective analyses of the composite BS/AM and GULFCAST temperature and salinity data sets and

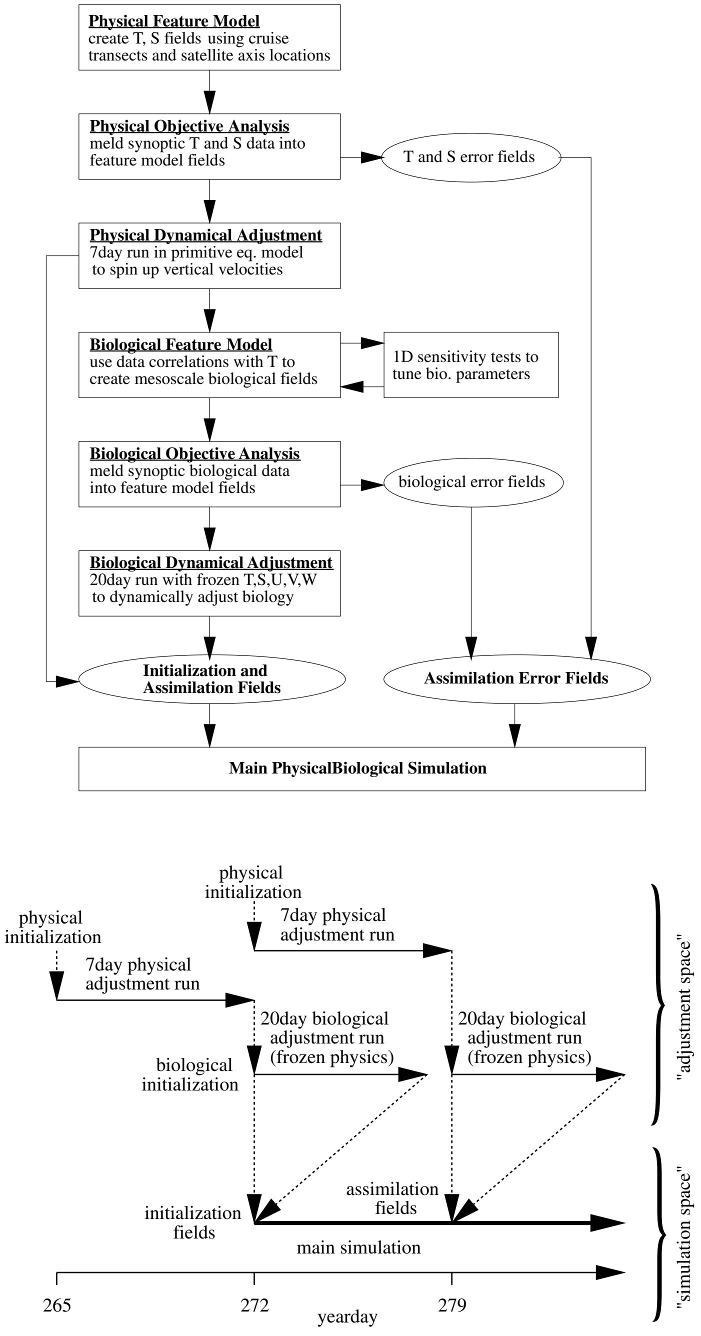


Fig. 12.17. (*a*) Flowchart for creating compatible physical and biological initialization and assimilation fields; (*b*) time chart of compatible physical and biological field generation and assimilation into the main simulation. (Reprinted from *Deep-Sea Research I*, **47,** L. A. Anderson et al., Physical and biological modeling in the Gulf Stream region, I, Data assimilation methodology, pp. 1787–1827, copyright 2000, with permission from Elsevier Science.)

geostrophic velocities (Lozano et al., 1996; Robinson, 1996). Considerable experience exists in forecasting and simulating the physical fields in the GSMR with OI assimilation (Glenn and Robinson, 1995; Gangopadhyay and Robinson, 1997; Robinson and Gangopadhyay, 1997). In general, the smooth evolution of the zeroth-order horizontal flow structures by the primitive equations is negligibly affected by the vertical velocity adjustment shock associated with assimilation. This, however, is not often the case for the biological ADR equations (1), and the vertical velocity adjustment to the update of the horizontal flow must be achieved prior to assimilation into the biological dynamics (Fig. 12.17*a*).

Assimilation of the BS/AM phytoplankton and nutrient data was carried out based on biological objective analyses analogous to the physical analyses. This required the preparation of background full-water-column three-dimensional estimates of phytoplankton and nitrate fields over the larger GULFCAST domain together with dynamically compatible fields for the zooplankton, ammonium, and organic nitrogen. The BS/AM data were used to provide vertical profiles and derive biological-state-variable/temperature correlations and biological/biological correlations. Biological/temperature correlations were then used to construct biological feature model fields for the mesoscale meandering stream and ring structures. Dynamical adjustment among the biological fields themselves and the choice of optimal biological parameters within reasonable constraints is obtained at this stage by zero- and one-dimensional (vertical) dynamical sensitivity runs of the biological diffusive-reactive equations (Fig. 12.16 and equation 1) without advection. Finally, the biological fields are adjusted to the three-dimensional circulation by freezing the velocity fields and running the full ADR equations until relatively large initial time derivatives of the biological fields have decreased and the biology is judged to be time varying in dynamical equilibrium with the physics.

The entire procedure is schematized on the flowchart of Fig. 12.17*a* and the time chart of Fig. 12.17*b*. Note that the vertical velocity adjustment is run for seven days and the final biological adjustment for 20 days, and the concept of *adjustment space* and *simulation space* introduced in Fig. 12.17*b*. Dynamically adjusted biological data for the assimilation day is melded with physical data from seven days earlier dynamically evolved in adjustment space. The compatibility procedure schematized on Fig. 12.17 has some general applicability, but the adjustment times must be chosen appropriately for the dynamics of the region being simulated.

To illustrate the necessity and importance of the compatibility methodology, Fig. 12.18 compares a compatible biological and physical assimilation with the case of the assimilation of physical data only. Although the vertical velocity has been adjusted prior to assimilation, the patches of nitrate maxima on Fig. 12.18 (row 3) are larger and stronger than those on Fig. 12.18 (row 2). Applying the methodology to process studies of the GSMR. Anderson and Robinson (2001) found that in late summer conditions, submesoscale ring–stream interactions rather than mesoscale meandering were the dominant mechanism for generating phytoplankton maxima and patches at the Gulf Stream front and for enhancing cross-frontal exchange. Important research directions for compatibility methodology include the development of objective criteria for establishing the dynamical equilibrium of coupled biophysical fields, data impact and adaptive sampling studies, and the exploration of optimally efficient procedures.

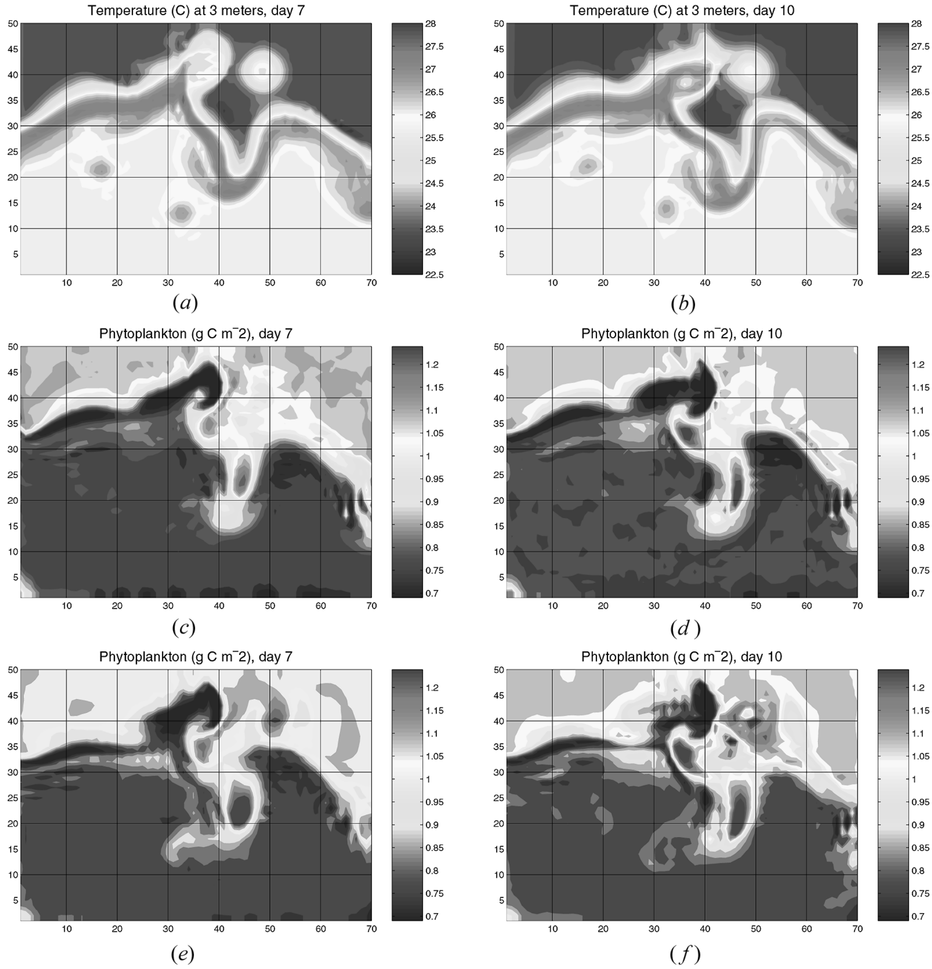


Fig. 12.18. Comparison of model simulation using assimilation of physical and biological fields versus assimilation of physical fields only: (*a*) temperature at day 7, physics and biology; (*b*) temperature at day 10, physics and biology; (*c*) phytoplankton at day 7; physics and biology; (*d*) phytoplankton at day 10, physics and biology; (*e*) phytoplankton at day 7, physics only; (*f*) phytoplankton at day 10, physics only.

3.8. Real-Time Biophysical Forecasting and Dynamics in Coastal Regions

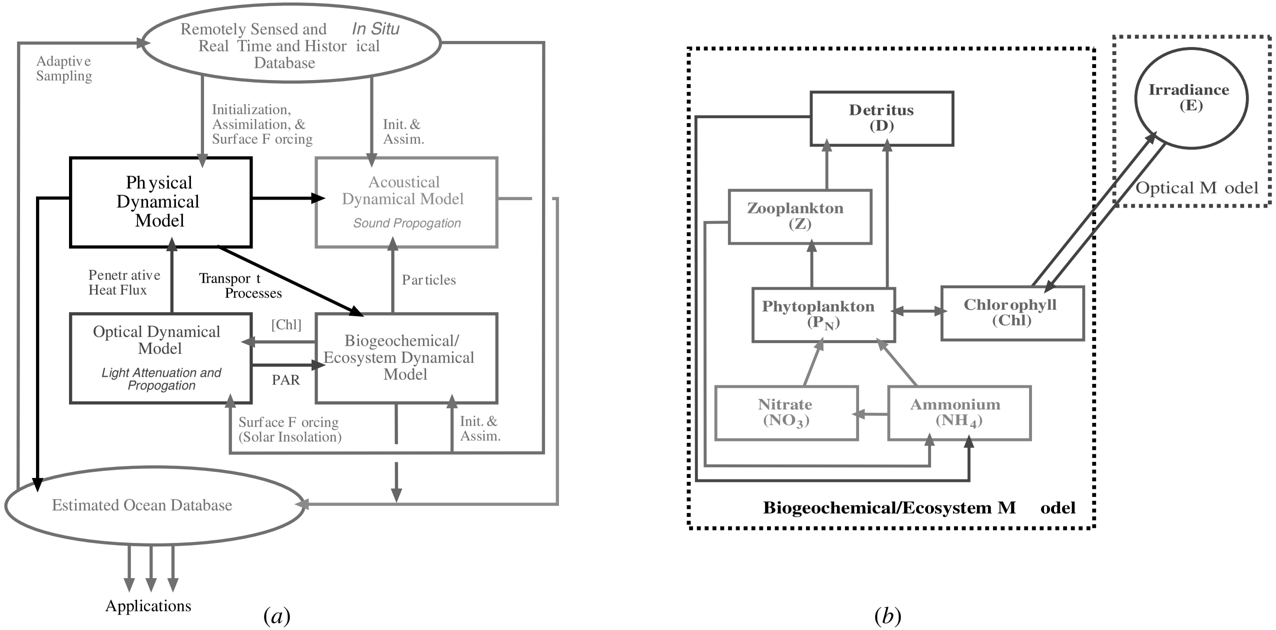
State estimation was first illustrated in this chapter (Fig. 12.2) by a real-time operational forecast for the Gulf of Cadiz region carried out with the Harvard Ocean Prediction System (HOPS; Robinson, 1999b). Recent real-time biophysical forecasts have been carried out with HOPS for regions of the western North Atlantic shelf and slope seas (Robinson and the LOOPS Group, 1999; Rothschild et al., 1999, 2000; Robinson et al., 2001). Issues involved relate to data and model compatibilities, the efficient mix of platforms and sensors, together with adaptive sampling and multiple two-way nested domains in the development of robust and accurate interdisciplinary forecast capabilities.

HOPS (Fig. 12.19*a*) is a flexible, portable, and generic system that can be deployed rapidly to any region of the world ocean. Physical and acoustical, real time at sea forecasts have been carried out at numerous coastal and deep-sea sites (Robinson, 1999b) and biological forecasts were initiated in 1997 (Srokosz, 1997). Currently, a primitive equation physical dynamical model incorporates effects of tidal mixing and tidal advection of scalar fields computed from an external tidal model. Multiple sigma vertical coordinates have been calibrated for accurate modeling of steep topography. Data assimilation methods include optimal interpolation and a quasioptimal scheme, error subspace statistical estimation (ESSE; Lermusiaux, 1999a,b; Lermusiaux and Robinson, 1999). The latter method determines the nonlinear evolution of the oceanic state and its uncertainties by minimizing the most energetic errors under the constraints of the dynamical and measurement models and their errors. Real-time efficiency is achieved by reducing the error covariance to its dominant eigendecomposition.

The biogeochemical–ecosystem model is modular to accommodate critical state variables for regions and problems of interest. The model used for the western North Atlantic has six state variables (nitrate, ammonium, phytoplankton biomass, phytoplankton chlorophyll, zooplankton, and detritus), as schematized in Fig. 12.19*b*. Phytoplankton productivity is modeled using a simple two-parameter phytosynthesis–irradiance model with a chlorophyll-dependent exponential attenuation coefficient. All ecosystem variables are nitrogen-based except chlorophyll, and photoacclimation kinetics can be incorporated into the model framework.

The nested domains that have been used for forecasts and simulations to be discussed here (Fig. 12.20) include the western North Atlantic Gulf Stream meander and ring region, Gulf of Maine, Georges Bank, and Massachusetts Bay. In addition to atmospheric and riverine fluxes and tides, the coastal ocean is driven by a buoyancy current that flows in from the Scotian shelf and flows out along the shelf break of the Middle Atlantic Bight and by Gulf Stream warm-core rings impinging across the shelf break. The buoyancy flow penetrates Massachusetts Bay and usually encircles Georges Bank. Information from the coarser-resolution domain is interpolated around the boundaries of the finer-resolution domain, and in two-way nesting, averaged information from the finer-resolution domain is fed to the coarser domain.

A demonstration of the real-time interdisciplinary forecast concept took place in Massachusetts Bay from August 17 to October 5, 1998 (Robinson and the LOOPS Group, 1999). The scientific focus was phytoplankton and zooplankton patchiness: in particular, the spatial variability of zooplankton and its relationship to physical and phytoplankton variabilities. Simultaneous synoptic physical and biological data sets were obtained over a range of scales, and platforms included ships, satellites, and autonomous underwater vehicles (AUVs). The multiscale sampling strategies were based on (1) ocean field forecasts (regions of most active or interesting dynamics) and (2) forecasts of error variances and of dominant eigendecompositions of error covariances (Lermusiaux, 2001), assimilating yesterday's data today for tomorrow's forecast and sampling. There resulted a combined and compatible physical, biological, and chemical multiscale data set applicable to interactive process studies and OSSEs. Dynamically, much more variability than described previously was found in the circulation structures (Fig. 12.21*a*). Strong-wind events can control the qualitative structures of the buoyancy flow. The Gulf of Maine current can have three branches: (1) the Massachusetts Bay coastal current, (2) one that enters the bay (but not Cape



(*a*) (*b*)

Fig. 12.19. (*a*) Harvard Ocean Prediction System (HOPS) schematic; (*b*) schematic of the biogeochemical/ecosystem model component of HOPS.

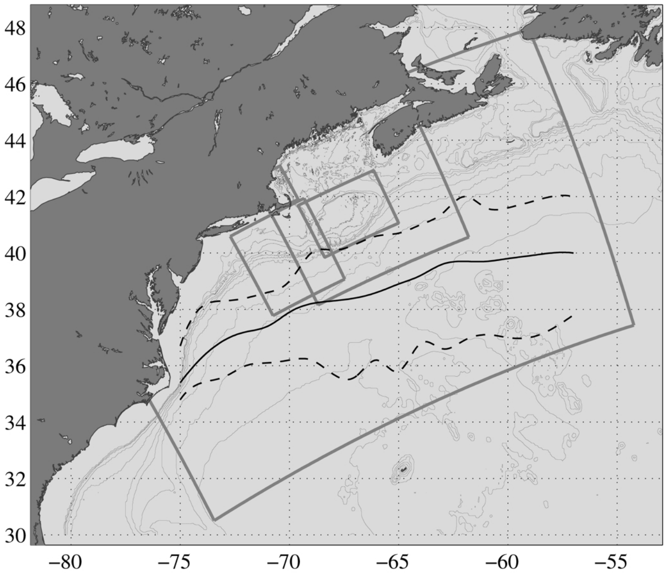
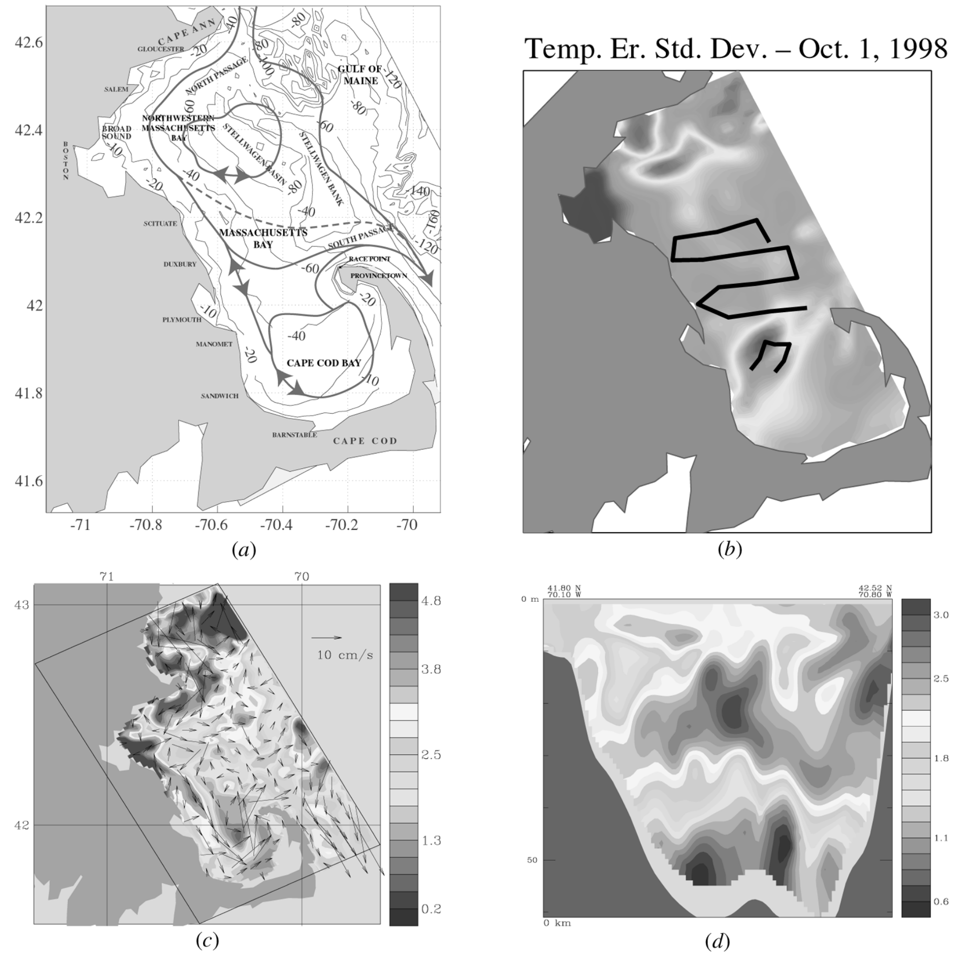


Fig. 12.20. Locations of various one- and two-way nested forecast domains.

Code Bay) and then exits at Race Point, and (3) one that flows along Stellwagen Bank without entering Massachusetts Bay. A Cape Code Bay gyre can be cyclonic, anticyclonic, or absent. For several days following a wind event, the structure of the buoyancy current is maintained by a combination of inertia, topography, coastal geometry, and internal dynamics. Submesoscale vortices form between branches and filaments of the buoyancy currents and/or mesoscale gyres. Figure 12.21*b* shows ship sampling patterns superimposed on forecast surface temperature error standard deviation. The shorter track represents objective adaptive sampling designed to reduce the error maximum upon which it is superimposed.

During real-time modeling, physical data were assimilated while the coupled biological model was initialized and run forward. Figure 12.21*c* shows the chlorophyll-*a* concentration at 10 m; Fig. 12.21*d* is a cross-section of zooplankton concentration. Multiscale patchiness is clearly visible. Higher concentrations occur: northeast of Cape Ann and near Boston Harbor because of advected nutrients, over Stellwagen Bank in part due to tidal mixing, and along the coastline due to wind-driven upwelling and episodic wind mixing. Modeled subsurface chlorophyll agreed relatively well with observations. The coupled dynamics were much more vigorous and diverse than previously thought to be the case in the fall.

A real-time demonstration of concept for forecasting physics, biology, and fish stock abundance for fisheries management applications was carried out in Georges Bank from April 17 to May 15, 2000 (Rothschild and the AFMIS Group, 1999; Robinson et al., 2001). The Georges Bank forecasts and associated preliminary OSSEs in the nested Gulf of Maine and western North Atlantic domains utilized primarily (1) satellite data (sea surface: temperature, SST; color, SSC; and height, SSH), (2) feature models, and (3) historical quasisynoptic surveys adjusted to year 2000 conditions by atmospheric fluxes. The SeaWiFS SSC measurement model (Sec-



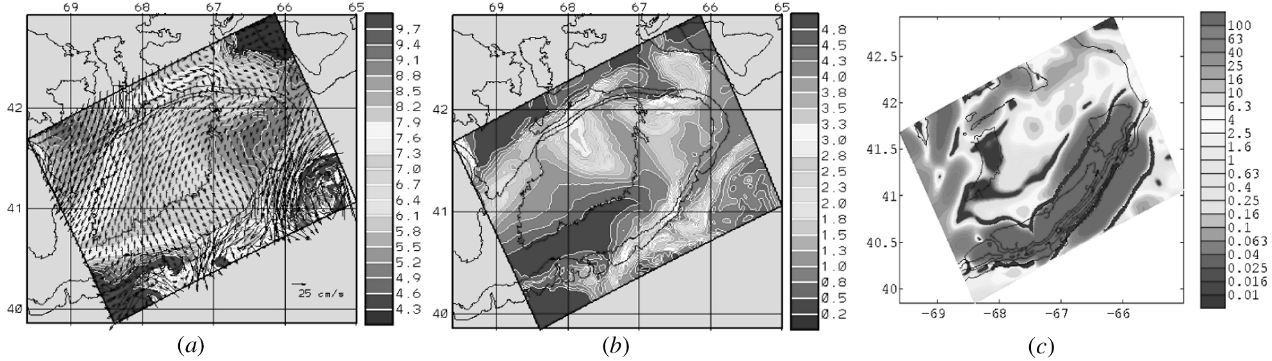
(*a*) (*b*)

(*c*) (*d*)

Fig. 12.21. See color insert. Massachusetts Bay. (*a*) Schematic of circulation features and dominant variabilities. The lines with divergent arrowheads indicate that the direction of circulations is variable. Dashed lines indicate that the location of features varies. (*b*) Forecast of the standard error deviation for the surface temperature, with tracks for adaptive sampling. (*c*) Chlorophyll *a* at 10 m, with overlying velocity vectors. (*d*) Vertical section of zooplankton along the entrance of Massachusetts Bay.

tion 2.5) involved the scaling and filtering of the SSC to surface chlorophyll and an extension in the vertical based on a feature model (Section 2.4). The highly idealized fish dynamics model represented cod swimming behavior as an attraction to a preferred bottom temperature together with a dispersive tendency. The model was regarded as exemplary rather than realistic. Nowcasts and forecasts of one or two days' duration were issued twice a week. The products included daily maps of surface temperature with superimposed vectors of subtidal velocity, chlorophyll at a depth of 15 m, bottom temperature with superimposed vectors of subtidal velocity, and idealized cod abundance at the bottom. Sample products are displayed in Fig. 12.22.

The real-time research-operational forecasts discussed here may be regarded as



(*a*) (*b*) (*c*)

Fig. 12.22. See color insert. Example Real-Time Demonstration of Concept (RTDOC-98) products for April 28, 2000; (*a*) 15 m temperature; (*b*) 15 m chlorophyll *a*; (*c*) idealized bottom cod and abundance forecast, based on an exemplary rather than realistic model.

precursors to new powerful interdisciplinary ocean observing prediction systems anticipated to become operative over the next decades for management of and operations in multiuse coastal oceans. Their development will involve many of the data assimilation issues introduced in Section 2.

4. Progress and Prospectus: Overall Review

Having discussed case studies in detail, our intent in this section is to present an overview of progress in, and prospects for, biological data assimilation. We have compiled an extensive bibliography by searching libraries and the World Wide Web, by direct inquiry to researchers, and from GLOBEC (2000). The discussion here is topically arranged by general methodological concepts and issues rather than by processes or oceanic regions. Comprehensive presentations of general progress in parameter estimation and state estimation are followed by an overall review of issues related to models, data, and errors. The detailed reports of work accomplished in these latter three areas complement the conceptual discussions in the corresponding subsections of Section 3.

4.1. Research Progress in Parameter Estimation

There is a large body of research in parameter estimation for engineering systems as described in the books by Young (1984), Tarantola (1987), and Stortelder (1998), some of which is closely related to oceanic ecosystems, as in freshwater ecology reviewed by Beck (1987). Parameter estimations in biophysical oceanography to date are mainly for zero- and one-dimensional models. The discussion here is presented in terms of (1) network fluxes, (2) ecosystem parameters, (3) methods, and (4) observability.

Network Fluxes

Inverse methods have been applied in several regions to estimate fluxes of, for example, nitrogen and/or carbon between compartments of primarily steady-state ecosystem models. Many of the models used are zero-dimensional linear balance equations involving one to several vertical layers and linear data relationships, with or without parameter constraints. Solutions are often computed by direct singular-value decomposition. In the future, dynamic flux inversions and inversions involving error weights for the data and dynamical model should be considered, as in physical inversions. Vézina and Platt (1988) utilize data at two surface sites off the English coast in late summer when planktonic food webs can be close to a steady state and confirm common flux patterns for those coastal euphotic zones. Using data from the warm-core rings program in the Atlantic, Ducklow et al. (1989) obtain large algal fluxes to detritus. Using cruise data for a planktonic system off southern California, Jackson and Eldridge (1992) find that most of the algal production is consumed about equally by protozoa and microzoa, and that zooplankton is important to transport organic matter from the euphotic zone to deeper regions. Fluxes for benthic systems in the California coastal basin (Eldridge and Jackson, 1993) and in the Bay of Saint-Brieuc on the French Atlantic coast (Chardy et al., 1993), as well as fluxes for tropical and lake ecosystems (e.g., Carpenter et al., 1994), have been estimated and studied. Niquil et al. (1998) assess food web fluxes in the tropical lagoon of Takapoto Atoll (French

Polynesia), combining a seven-variable planktonic model with data collected as part of pearl oyster farming studies. Vézina and Pace (1994) reconstruct ecosystem carbon fluxes for three lakes, two of which had their fish community altered experimentally. Other examples are given in Vézina (1989) and Eldridge and Jackson (1993). Biological inversions coupled to physical constraints have been carried out to study water qualities and mass balances of nutrients in bays and larger coastal seas (Legovic et al., 1989, 1990, 1995).

Ecosystem Parameters

Identical twin experiments are useful to evaluate estimation schemes. Lawson et al. (1996) utilize this approach based on simulated data to investigate the ability to recover parameters as a function of the data types and distributions available. A five-variable model is chosen and an adjoint method used to estimate the rates, initial conditions, and amplitudes of episodic events in the mixed layer. Harmon and Challenor (1997) employ a similar approach, but with a more advanced Bayesian estimation, combining Markov chain, Monte Carlo, and simulated annealing methods. Rothschild et al. (1997) estimate growth and mortality rates based on simulated data from a linear stage-structured model (e.g., larval fish model). Gunson et al. (1999) use an adjoint method to fit a one-dimensional, four-variable (NPZD) model to simulated ocean color data. The biological model is implemented as a Lagrangian ADR equation without horizontal diffusion such that biological parcels follow the flow field of a three-dimensional general circulation model of the North Atlantic forced by climatological atmospheric data. Ten numerical floats are seeded in various locations and followed over six months, assimilating the local simulated surface color. The authors argue that about five of their parameters can be estimated from satellite color data and that the importance of parameters varies spatially. Other examples are given in Marsili-Libelli, 1992; Crispi and Mosetti, 1993; Ishizaka, 1993; Lawson et al., 1995; and Section 3.1 of Spitz et al., 1998.

Real ocean data have been used for model calibration, validation, and process studies. Rates in larval fish and zooplankton models have been estimated from concentration data (e.g., Banks et al., 1991; Somerton and Kobayashi, 1992; Aksnes et al., 1997; Rothschild et al., 1997; Ackleh, 1999). For coupled problems, Prunet et al. (1996a,b) calibrate a class of surface biophysical models for various combinations of the data at Station Papa in the northern Pacific. A Newton-type algorithm and singular-value decomposition directly minimize an error-weighted least squares cost function. Using only surface chlorophyll data with a comprehensive model, half of the parameters are estimated consistently. With a simplified model and all of the surface chlorophyll, temperature, and nitrate data, most parameters are obtained. This shows that for a robust inversion, the complexities of the models and data should be compatible. Using data from two sites in the North Atlantic, Hurtt and Armstrong (1996, 1999) assess a class of seasonal models similar to that of Fasham et al. (1990). Parameters are estimated by simulated annealing based on a likelihood cost metric. The authors identify dynamical features that are either essential or unnecessary. Fasham and Evans (1995) and Evans (1999) fit an analogous class of models, but to shipboard data collected during the JGOFS North Atlantic Bloom Experiment. A main objective is to exemplify how local models and local data can be useful for regional studies. Parameters are estimated based on a conjugate-gradient algorithm, and the fits of models and constraining power of data are discussed. Other examples with real data are given in Legovic, 1987; Marcos and Payre, 1988; Section 3.2 of Matear, 1995; Section 3.1 of Spitz et al., 1998; Section 3.3 of Vallino, 2000; and Section 3.4 of Friedrichs and Hofmann, 2001.

Parameter Estimation Methods

Both local (e.g., steepest descent) and global (e.g., simulated annealing) direct minimization schemes have been successful. With descent methods, knowledge of the gradient of the cost function often accelerates the rate of convergence. It is usually computed using the adjoint equations, but sensitivity approaches or finite differences are also employed. Conjugate gradient methods are useful but are usually modified to allow nonlocal searches. Due to the scarcity of data and nonlinearities, global schemes such as simulated annealing and Bayesian estimation are found among the best for parameter estimation in zero-dimensional models. When biogeochemical models are embedded in three- or four-dimensional physical models, these methods can be expensive and schemes based on conjugate gradient, Newton and adjoint methods, and error subspace methods can be more efficient. It is worth mentioning that when standard multipurpose optimization routines are used, algorithmic parameters have to be chosen, which can be challenging for ecosystem applications, and results should thus be analyzed with care.

Quality of Fits, Constraints, and Observability

The fit of ecosystem models to ocean data using parameter estimation often leads to large a posteriori data residuals (Section 2.5) or dynamical behaviors that appear unrealistic. The reasons for unsuccessful fits are often multiple and of various types. They include nonobservable parameters, inappropriate cost functions, multiple local optima, inefficient optimization schemes, limited ocean data, improper dynamical model structures, and inadequate error models for the dynamics or measurements.

Prior to data assimilation, parameters generally should be scaled or normalized. To accelerate the convergence and avoid unrealistic or unstable models, parameters can also be bounded by strong a priori constraints (Box, 1966; Fasham and Evans, 1995; Section 3.3 of Vallino, 2000). Another option consists of imposing weak parameter constraints, (e.g., penalty weighting the difference between the final and of a priori parameter values) (Vézina and Platt, 1988; Section 3.2 of Matear, 1995; Prunet et al., 1996a,b; Evans, 1999; Gunson et al., 1999). Parameters that deviate far from their a priori estimated values are then permitted, but heavily discounted in the cost function. Since biological data are often limited, both parameter bounds and weak parameter constraints can be utilized to avoid solutions that are unrealistic or at the wrong scales. Cases with more rather than fewer constraints are often most successful (Vézina and Pace, 1994; Section 3.2 of Matear, 1995; Prunet et al., 1996b; Section 3.3 of Vallino, 2000).

Care should be taken to ensure that the parameters to be estimated are independent. Combinations of parameters (sums, ratios, products) in the original equations should first be eliminated by grouping or other manipulations (e.g., Carpenter et al., 1994; Section 3.1 of Spitz et al., 1998). The observability or identifiability of the remaining parameters can be estimated, at least locally from the error covariance, Hessian, or resolution matrices at an optimum (e.g., Tziperman and Thacker, 1989; Wunsch, 1996). In particular, the diagonal terms of the resolution matrix identify the extent to which each parameter is resolved, and the off-diagonal terms identify the linear dependencies among parameters. The a posteriori parameter error covariance and cross-validation or bootstrap techniques (Wahba and Wendelberger, 1980; Efron and Tibshirani, 1993) give parameter uncertainties and local shape of the cost function. To eliminate unrealistic solutions and reduce the number of local optima (e.g., fast and slow data fits with similar final costs), indetermination due to parameters that are not completely observable (e.g., Jazwinski, 1970; Wunsch, 1996) may be removed. This can be done either by sampling new data, imposing stronger constraints on the parameters (e.g., fixing their values), or simplifying the models. Such observability and dependency studies have been carried out for marine parameters (e.g., Marsili-Libelli, 1992; Section 3.2 of Matear, 1995; Prunet et al., 1996a,b; Evans, 1999; Section 3.3 of Vallino, 2000) and flux estimates (e.g. Vézina and Platt, 1988; Jackson and Eldridge, 1992). Questions of controllability, observability, and predictability, and the corresponding data requirements, are linked and important, both in theory and practice. Further research in these areas would probably be useful.

4.2. *Research Progress in Field Estimation*

Early Approaches

Preliminary work toward coupled data assimilation for biophysical field estimation can involve the assimilation of physical data to predict flow fields used for adaptive biological sampling (Robinson et al., 1993; Bowen et al., 1995; Lozano et al., 1996; Robinson, 1996). A subsequent step consists of data assimilation via initialization (i.e., initializing coupled biophysical predictive models based on data) with or without physical data assimilation. Extensive research has been carried out using this approach and numerous results have been obtained in many regions of the world ocean. The published applications cannot all be cited here. For example, recent studies for the Mediterranean sea include (Crise et al., 1998, 1999; Crispi et al., 1998, 1999; Napolitano et al., 2000), for the Black sea (Oguz et al., 1996, 1998, 1999), for the Gulf of Maine and Georges Bank (Section 3.5 of Lynch et al., 1998; Lynch 1999; Rothschild and the AFMIS Group, 1999) and for Massachusetts Bay (Besiktepe et al., 1998; Section 3.8 of Robinson and the LOOPS Group, 1999).

The simplest forward method for data assimilation is data insertion. When new data become available, the model field forecast at data points is simply replaced by the data. It was first applied for biology during a multidisciplinary study of the southeastern U.S. continental shelf (Atkinson et al., 1985). The supplies of nutrients on the shelf, induced by Gulf Stream upwellings, were measured and inserted into ecosystem models, aiming to investigate the shelf dynamics of nutrients and organic carbon production. Continuing this research, Ishizaka (1990, 1993) objectively analyzed velocity and temperature data to provide physical forcings to a four-variable biological model. However, the resulting coupled simulations did not reproduce the observed biological variabilities. To improve the short-term predictive capability, Ishizaka (1990) directly inserted a one-month time series of Coastal Zone Color Scanner (CZCS) images into the modeled phytoplankton, updating the other state variables based on a constant nitrogen ratio.

Steady Biophysical Interactions

Nihoul et al. (1994) use a two-dimensional variational inverse method to fit a three-dimensional physical primitive equation model and a five-variable ecosystem model to physical and biological data collected in the summer for five years in the northern Bering Sea. The two-dimensional variational method for a steady-state inversion is applied at selected depths, with the physical and biological models imposed as weak constraints. To examine the steady-state cycling of phosphorus in the North Pacific, Matear and Holloway (1995) use an adjoint method, combining a three-dimensional phosphate ADR equation, historical three-dimensional gridded phosphate data, steady three-dimensional flow data from a general circulation model, and geostrophic constraints. Due to the biological sensitivities to small changes in the circulation, the authors found that physical constraints need to be weak. McGillicuddy et al. (1998, Section 3.6) use an adjoint method to compute the biological dynamics itself.

Seasonal Cycles

Nudging zero- to one-dimensional biological models embedded in three-dimensional steady-state circulation models has been employed by Najjar et al. (1992) to study vertical transports of organic matter based on phosphate data. The role of remineralization of organic matter at depth in the global cycling of carbon by oceanic organisms is studied by Anderson and Sarmiento (1995), also via nudging to phosphate data, and evaluated based on apparent oxygen utilization data. Misfits in the phosphate simulations were attributed mainly to errors in the coarse-resolution, world ocean general circulation model employed, especially in the thermocline dynamics. To monitor the seasonal evolution of the three-dimensional net primary productivity and other ecological quantities in the Atlantic, Armstrong et al. (1995) nudge satellite color data in two types of zero-dimensional seasonal ecosystem models embedded in a three-dimensional ocean general circulation model. The first ecosystem model, using a single phytoplankton and single zooplankton, cannot be forced to the monthly surface data without producing too-high ammonium distributions; the modeled phytoplankton is limited by zooplankton grazing to a maximum steady-state value. However, a food-chain ecosystem model based on multiple phytoplankton and zooplankton size classes prevents too-high ammonium by distributing the surface chlorophyll forcing to the chain of size classes.

Mesoscale Variabilities and Bloom Events

Fields and parameters can be estimated jointly. For example, to study a coastal spring bloom in the Gulf of Gdansk (Baltic sea), Semovski et al. (1994) use a hybrid assimilation scheme consisting of (1) a blending method to estimate the NPZ field evolution, combining chlorophyll profiles from three coastal stations with a one-dimensional biophysical–optical model, and (2) a variational method to subsequently optimize the model parameters. For the spring of 1993, Semovski et al. (1996) couple the same one-dimensional model with a data-assimilative barotropic model of the wind-driven currents in the gulf. Even though the fit to chlorophyll data are improved, the authors show the need for modeling three-dimensional physical effects (e.g., mesoscale features, rivers). Semovski et al. (1999) consider such effects in coastal regions of the Baltic Sea, combining satellite and in situ observations of various types but without carrying out the coupled four-dimensional assimilation. To analyze the annual phytoplankton cycle at a site in the North Atlantic (Semovski et al., 1995) and over the three-dimensional North Atlantic and Baltic Sea (Semovski and Wozniak, 1995), satellite color data (CZCS; Section 2.4) are assimilated, again for both field and parameter estimates. Ecosystem fields are estimated in the North Atlantic via an optimal-interpolation-based blending method. Parameters are estimated for the Baltic Sea by direct minimization. The optimized simulations are discussed and the primary production variability studied by empirical orthogonal function decomposition. Anderson et al. (2000, Section 3.7), Robinson and the LOOPS Group (1999, Section 3.8), and Rothschild and the AFMIS Group (1999, Section 3.8) assimilate biophysical data in coupled four-dimensional models by optimal interpolation for forecasting and process studies.

Toward Real Ocean, Multivariate, Verified Fields

Important issues in field estimation relate to the coupled adjustment of the biophysical fields (Section 3.7 of Anderson et al., 2000) and the establishment of real-time predictive capabilities, verification procedures, and efficient acquisition of data based on forecasts and adaptive sampling (Robinson and the LOOPS Group, 1999, Section 3.8). Obtaining realistic biophysical simulations and real-time forecasts is especially challenging (e.g., McGillicuddy et al., 2001), both for scientific investigations and coastal operations (e.g., naval) and for management (e.g., fisheries). The validation of predictions via efficient skill metrics is also important (Section 4.5). Forecasts of the error fields and variability fields for each state variable, and the associated statistics, are likely to become increasingly necessary (Rothschild and the AFMIS Group, 1999; Lermusiaux, 2001).

Several field estimation methods remain to be tested and nonlinear, coupled four-dimensional advances are now possible. To date, significant results are based either on nudging, adjoint, or optimal interpolation schemes. Physical oceanography and meteorology have made substantial progress in multivariate, four-dimensional, and nonlinear data assimilation schemes (Daley, 1991; Bennett, 1992; Malanotte-Rizzoli, 1996; Wunsch, 1996; Ehrendorfer, 1997; Lermusiaux, 1999a,b; Lermusiaux and Robinson, 1999; Miller et al., 1999). Many of these schemes could be useful for idealized, realistic, or operational research, and important biophysical results can be expected from their applications.

4.3. Research Progress and Issues: Models

In Section 2.3, basic concepts and issues related to dynamical models were discussed which we summarize in this paragraph. Fundamental models exist for physical dynamics but not for biological dynamics, which is generally governed by a set of advection–diffusion–reaction equations in which the representation of biological processes is challenging. Model structures should be consistent with dominant scales and processes of interest, and appropriate aggregations and linkages of state variables should be chosen (e.g., Iwasa et al., 1989; Rothschild and Ault, 1992). Reasonable parameterizations of larger- and smaller-scale processes are necessary for the physics and biology and their interactions. The spatial dimensionalities required to represent the biological processes should be guided by both theoretical considerations and data assimilation constraints. Models and data compatibilities are essential. Here, we survey research results and directions.

To identify model structures from data, some guidance can be obtained from applied mathematical biology (e.g., Banks and Fitzpatrick, 1990, 1991; Fitzpatrick, 1991, 1995) and from freshwater resources and ecology (Gardner et al., 1982; Beck, 1985, 1986, 1987, 1990; Carpenter et al., 1994). Dominant time and space scales can be challenging to identify. In some regions, the biological effects of horizontal advection and diffusion can be small (e.g., Frost, 1991), in others the vertical advection and mixing can be usefully simplified (e.g., biology confined to a homogeneous mixed layer and biomass in the pycnocline neglected). When such hypotheses lead to oversimplifications, they have been altered in the course of the study (e.g., Anderson et al., 1977; Section 3.2 of Matear, 1995). To be most useful in data assimilation, low-dimensionality simplification can be combined with adequate error models. Increased biophysical modeling in four physical dimensions is also anticipated.

Models can be quantitatively improved by data assimilation feedbacks. Armstrong et al. (1995) indicate that parameterizing the effects of mulitple size classes may be necessary in simple aggregated models to prevent too-high ammonium when such models assimilate satellite color data. Using data collected at BATS during 1988–1991 [as in Spitz et al. (1998, Section 3.1) but less data], Hurtt and Armstrong (1996) estimate that the zooplankton variable in the model of Fasham et al. (1990) is unnecessary at that site. However, several improvements of the model are found useful. They include a nitrate pool varying linearly with depth, a biodiversity effect on phytoplankton (algal and detrital size classes becoming larger as phytoplankton and detritus biomasses increase), and a physiological effect for the phytoplankton (chlorophyll/nitrogen ratio function of light intensity and nutrient concentrations). Fitting an extension of their 1996 model to data from two sites in the North Atlantic simultaneously (BATS and Ocean Weather Ship Station I), Hurtt and Armstrong (1999) indicate the need for more research on community structures and on spatiotemporal variability of the model parameters and state variables. To model the steady seasonal cycle during the JGOFS North Atlantic Bloom Experiment, Evans (1999) finds that quadratic zooplankton mortality (Steele and Henderson, 1992) is not a refinement of the model of Fasham et al. (1990) that is necessary. However, the author shows that the detrital production in the model requires improvements and that the passage from a zero- to a one-dimensional model may be necessary (e.g., see also Gunson et al., 1999). Friedrichs and Hofmann (2001, Section 3.4) found that in the presence of a tropical instability wave, the species composition needed to be modified.

4.4. Research Progress and Issues: Data

In Section 2.4, basic concepts and issues related to data were discussed which we summarize in this paragraph. Compatibilities are essential between both biophysical models and data sets, and also among interdisciplinary observations. Missing data can be generated from simulations, correlations, and feature models. An efficient mix of sensors and platforms for specific-purpose data sets should be chosen. Synergies among in situ, mesocosm, and laboratory experiments can be helpful. New biophysical data sets dedicated to assimilation studies are greatly needed. Data impact and sensitivity studies, OSSEs, and oceanic test beds can contribute much now. Rapidly evolving new sensors, especially remotely mounted on platforms both in space and in situ, are powerful resources. Here, we survey research results and research needs.

There should be enough data to estimate parameters when models are complex and models should be simple enough when limited data are available (Section 3.2 of Matear, 1995; Hurtt and Armstrong, 1996, 1999; Prunet et al., 1996a,b). The assimilation of data obtained by averaging higher-frequency data over several years (e.g., Nihoul et al., 1994; Section 3.2 of Matear, 1995) or by integrating depth-dependent data over climatologically varying mixed-layer depth (e.g., Section 3.1 of Spitz et al., 1998; Evans, 1999; Hurtt and Armstrong, 1996, 1999) can misrepresent some of the dynamics. Physical climatological fields are estimated using complex procedures, objective analyses, and filtering (e.g., averages along potential density surfaces). Similar efforts are probably required in biology. Another direction for future research is based on coupled models, nested in time, space, and varied levels of aggregation, where all data are assimilated at the proper frequency, resolution, and aggregation level.

Data assimilation can help in assessing data impact and determining the most useful data. To increase the impact of satellite color data, in situ profiles of productivity, nutrients, phytoplankton classes, and chlorophyll have been essential (Armstrong et al., 1995; Semovski et al., 1999; Rothschild and the AFMIS Group, 1999). For the estimation of new production. Evans (1999) shows that bacterial data are perhaps not as useful as phytoplankton or nutrient data. Another research issue involves the relative priorities in the allocation of limited resources to low-dimensional versus four-dimensional data acquisition. It must be borne in mind that, at certain scales, the physical forcing of the biology is not only in the advection–diffusion terms but also in the qualitative form of the biological dynamics: i.e., B_i in equation (1), then depends at least implicitly on the physical scales and processes. Most assimilation studies indicate the need for new observations [e.g., ammonium data (Hurtt and Armstrong, 1996), zooplankton data (Section 3.2 of Matear, 1995), and mesocosm data (Section 3.3 of Vallino, 2000)]. Data requirements may be attainable only with new sensors and platforms (Dickey, et al., 1998). As the capabilities of biophysical models improve, the role of adaptive sampling research (Robinson and Glenn, 1999; Section 3.8 of Rothschild and the AFMIS Group, 1999; Lermusiaux, 2001) should also increase.

Biological measurement models (equation 2c) should be compatible with dynamical models and their errors estimated (e.g., Fuller, 1987). Their deterministic component can increase the impact of limited data and their error component eliminate the scales that are not of interest (e.g., data ramping, surface-to-depth extension). They are relatively easy to obtain when data consist of linear combinations of state variables (e.g., particulate organic carbon or nitrogen) but less so when data consist of a portion of a state variable (e.g., biomass of a species of an aggregated state variable). To employ all the data, even if scarce, feature model constraints and weak data constraints can be applied (e.g., Section 3.2 of Matear, 1995; Hurtt and Armstrong, 1996, 1999) and statistical models computed from data [e.g., multivariate decorrelation scales (Abbott and Letelier, 1998) and covariances (Lermusiaux et al., 2000)]. To convert state variables that are nitrogen- or carbon-based to data variables of different nature or units, models with nonstatic factors or ratios should be developed (e.g., Armstrong et al., 1995; Semovski and Wozniak, 1995; Lawson et al., 1996; Prunet et al., 1996b; Hurtt and Armstrong, 1996, 1999; Section 3.1 of Spitz et al., 1998; Evans, 1999; Section 3.3 of Vallino, 2000). In some cases, the spatiotemporal variability due to such ratio variations can dominate the variability due to actual conversions of biomass. The derivation of models for linking the three-dimensional biological state variables to the surface satellite color data are important today since satellite observations are emerging as the main source of wide coverage data for verification of nutrient-based models (e.g., Balch, et al., 1992; Armstrong et al., 1995; Semovski and Wozniak, 1995; Semovski et al., 1995; Gunson et al., 1999).

4.5. Research Progress and Issues: Errors and System Evaluation

In Section 2.6, basic concepts and issues related to errors were discussed which we summarize in this paragraph. The attribution, representation, and propagation of errors require error models, including a variety of quantitative metrics for the evaluation of results and for relative weights of data and dynamics. This is a most important area of current data assimilation research. Errors arise from approximate dynamical and measurement models and from limited and imprecise observations. In general, both the deterministic and stochastic components of data assimilation systems must be validated, calibrated, and verified. Regional predictability limits for biophysical forecast must be established. Here, we survey results to date and research directions.

Field and parameter estimates are enhanced if accompanied by error estimates. A priori and a posteriori errors should be compared, and for most cost functions and constraints, the a posteriori residuals should on average be smaller than the a priori ones (e.g., Jazwinski, 1970). If this is not the case, either there are not enough data, the assimilation schemes are not converging, or the a priori models and errors are inadequate. Both physical and biological uncertainties can be important. Biological examples have been discussed, but misfits that are probably due to physical shortcomings also occur (e.g., Najjar et al., 1992; Anderson and Sarmiento, 1995). Measurement error models are essential since they often weight data residuals in cost functions. Their statistics can be obtained via several means, including replicate observations, sensor calibrations, or environmental noise data (e.g., higher-frequency data).

Determining efficient biological cost functions is important. Absolute, relative, square-root, quadratic, and likelihood cost measures have already been utilized with real biological data as well as Bayesian estimation with Gaussian priors in twin experiments. To evaluate the validity of models and sufficiency of data, simple cost functions can now be useful, but guidance from nonlinear estimation and control will be valuable. Cost functions should be in accord with prior information and statistics. Many biophysical processes are multivariate and have multiscales, with strong correlations between variables and parameters (Bennett and Denman, 1985; Denman and Abbott, 1988, 1994; Harris, 1996; Abbott and Letelier, 1998). There is thus a need to investigate multivariate error covariances, by combination of data and dynamics (GLOBEC, 2000; Lermusiaux et al., 2000). Adjoint methods consider the dynamical model as a strong constraint and were originally derived for linear models. With real oceanic data, they have been reported to perform well (e.g., Section 3.6 of McGillicuddy et al., 1998b; Section 3.4 of Friedrichs and Hofmann, 2001) or not so well when compared to less restrictive schemes (e.g., Section 3.3 of Vallino, 2000). When model structures are known to be approximate, weak dynamical constraints should be investigated. Methodologies such as generalized inverse or Bayesian schemes (Jazwinski, 1970; Bennett, 1992; Miller et al., 1994, 1999; Harmon and Challenor, 1997; Lermusiaux, 1997, 1999b; Lermusiaux and Robinson, 1999) are useful in this regard.

System evaluations include the validation, calibration, and verification of the data and models, based on efficient skill metrics (e.g., Lynch and Davies, 1995). To do so, ecosystem manipulations are helpful. For example, to discriminate between alternative zero-dimensional models for phytoplankton–zooplankton interactions, Carpenter et al. (1994) fit these models to time series data from a reference lake and manipulated lake (addition and removal of bass and minnows). This facilitates the discrimination of models and yields model formulations capable of predicting wider ranges of conditions. The equivalent in oceanography are large enclosure experiments. To assess the potentials of data assimilation, twin experiments are also helpful. If the assimilation with real data fails but the twin experiment is successful, the data and assimilation algorithm usually do not require improvements, but the constraints, the models, and their error estimates (equations 2a to 2c) do. Several studies attempt to validate pelagic models by comparisons with data collected at fixed stations (Section 3.2 of Matear, 1995; Hurtt and Armstrong, 1996, 1999; Prunet et al., 1996a,b; Section 3.1 of Spitz et al., 1998) along a few cruise tracks (Fasham and Evans, 1995; Evans, 1999), or at the surface (Armstrong et al., 1995). Some of the four-dimensional effects of ocean dynamics are then neglected (e.g., horizontal advections) (Robinson, 1997), and temporal and spatial changes can be confounded. The reasons for failure or success of the modeling effort can then be ambiguous (data, model, or assimilation scheme). There are several remedies to these issues. Mesocosm data assimilations can be carried out to reduce dimensions from four to one and thus justify one-dimensional models. Error models can be established for the largest differences between four- and one-dimensional biological dynamics, and one-dimensional models then used as weak constraints. Finally, physical and biological four-dimensional models can be coupled (e.g., Section 3.7 of Anderson et al., 2000; Section 3.8 of Robinson and LOOPS Group, 1999). Useful feedbacks among these approaches are likely to occur.

5. Concluding Remarks

Oceanography is maturing into an essentially interdisciplinary science in which interactive biological–physical dynamics plays a central and critical role. Data assimilation has recently entered oceanography and is just now beginning to be applied to coupled biophysical processes. Data assimilation methods for complex system science are generally evolving mathematically, computationally, and in scope and breadth of applicability. It must be anticipated that in coming years interdisciplinary ocean science will evolve with a systems science component linked to novel and advanced data assimilation techniques.

Since coupled biological–physical data assimilation is in its infancy, much can be accomplished now by the immediate application of existing methods as evinced in progress and prospectus. Since data assimilation intimately links dynamical models and observations, it can play a critical role in the important area of fundamental biological oceanographic dynamical model development and validation over a hierarchy of complexities. Since coupled assimilation for coupled processes is challenging and can be complicated, care must be exercised in understanding, modeling, and controlling errors and in performing sensitivity analyses to establish the robustness of results. Compatible interdisciplinary data sets are essential and data assimilation should iteratively define data impact and data requirements.

Data assimilation is powerfully applicable and must be expected to enable future marine technologies otherwise impossible or not feasible. Interdisciplinary predictability research, multiscale in both space and time, is required. State and parameter estimation via data assimilation is central to the successful establishment of advanced interdisciplinary ocean observing and prediction systems, which, functioning in real time, will contribute to novel and efficient capabilities to manage and to operate in our oceans.

Our conceptualization of nature is changing. Syntheses of sensor data provide our view of nature. The syntheses that now best represent objective reality fuse data and dynamics.

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