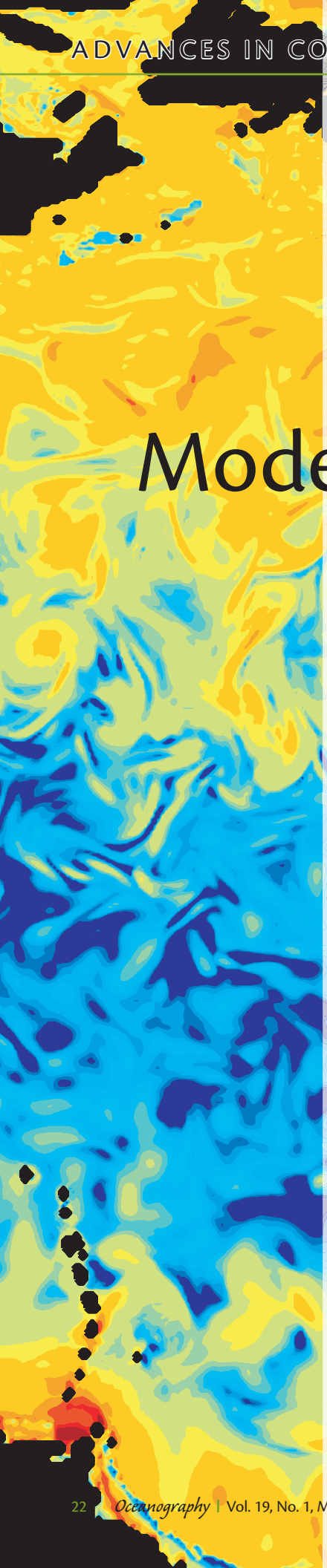

Modeling Ocean Ecosystems

THE PARADIGM PROGRAM

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THE ROLE OF THE OCEANS in Earth systems ecology, and the effects of climate variability on the ocean and its ecosystems, can be understood only by observing, describing, and ultimately predicting the state of the ocean as a physically forced ecological and biogeochemical system. This is a daunting but exciting challenge, because the ocean-atmosphere system is dynamically linked, and oceanic habitats are both diverse and complex, providing tremendous variety in environmental conditions and associated life forms. And paradoxically, as we learn more and more about ocean life, for example, through the genomics revolution (Doney et al., 2004), the number of unanswered questions increases.

Models, be they conceptual, statistical, or numerical simulations, are useful and necessary tools for studying the complex interactions that influence ecosystem structure and function. Originally, a primary function of marine ecosystem models was to help in the development of understanding; also, they were applied in fisheries models to predict the abundance of specific commercial fish stocks. Now, they are being asked to do much more. On local and regional scales, there is growing recognition that management of marine resources and assessment of human perturbations must encompass the whole ecosystem, not individual species. Extending further to basin and global scales, the potential impacts of global change present an immediate challenge, nationally and globally, to define and execute responsive strategies, based to a large extent on the predictions of interdisciplinary global models that must be validated by comparison with measurements. Consequently, the ultimate objective of any comprehensive marine ecosystem modeling program must be the development and implementation of reliable forecast systems, guided by and validated with systematic observations of the sea.

Rapid development of capabilities in marine modeling, supported by increased computer power and technical innovation in ocean observations, has set the stage for development of reliable interdisciplinary ocean forecast systems —but the goal is ambitious and the challenges are great. Faithful and quantitative description and prediction of real ocean ecosystems requires an interdisciplinary, coupled, and data-assimilative observation and modeling system. In other words, we must develop a holistic modeling approach that describes environmental complexity with interacting physical, ecological, biogeochemical, and optical component models that directly incorporate observations from a wide range of measurement systems. Each component of this systematic approach has its own stand-alone issues that are being addressed by specialists exploiting the latest research in their disciplines. Rapid and effective development of ocean ecosystem models will depend on integration of this leading-edge research through communication and coordination among a broad range of ocean scientists.

The PARtnership for ADvancing Interdisciplinary Global Modeling (PARADIGM), a National Ocean Partnership Program (NOPP) funded entity, was established in response to this need. It is a coordinated, multidisciplinary team of scientists that is developing the modeling infrastructure to go beyond present approaches in pursuit of interdisciplinary, predictive models of ocean ecosystems that are guided by and validated with observations of the ocean over a broad range of scales. Toward this end, our immediate scientific objective is *to improve our understanding of the mean state, seasonal cycle, and natural interannual-to-decadal variability of global and basin-scale biogeographical patterns.* This goal focuses our efforts on fundamentally important questions: What factors combine to establish the makeup of the marine ecosystem in a given location? What combination of physical forcing and biological responses drives the observed long-term variability and apparent ecosystem regime shifts? How will ecosystems respond to future climatic and anthropogenic perturbations? The questions are addressed with a range of approaches; the synergies are achieved when results are considered together and applied to the development of the next generation of marine ecosystem models. Here, we describe some of our efforts and our vision of how they might be applied in the future.

The role of the oceans in Earth systems ecology, and the effects of climate variability on the ocean and its ecosystems, can be understood only by observing, describing, and ultimately predicting the state of the ocean as a physically forced ecological and biogeochemical system.

Much of our research concerns fundamental problems confronting contemporary approaches to modeling marine ecosystems. At the forefront is the problem of complexity, driven by the growing recognition of (1) the varied and distinct ecological and biogeochemical functions of groups of marine microbes, and (2) details of planktonic behavior (e.g., grazing by different species of zooplankton) that defy simple representations. Models can account for ecological complexity by incorporating more and more biological components—functional groups—with distinct ecological roles, and by developing complicated mathematical descriptions of plankton behavior. However, these solutions conflict directly with another primary problem in contemporary ecosystem modeling—the evaluation of models by direct comparison with observations. As described below, complicated models have too many "knobs to turn" to be constrained with available observations, so that only the simplest simulations with only a few variables can be rigorously tested with comparisons to real-world measurements, and ultimately used in data-assimilation applications. Further, it is impractical to implement complicated models in global simulations because the computational demands are too high. Fortunately, we are often not required to describe the specific details of ecological interactions

(e.g., feeding history of an individual zooplankter) but rather the overall impact at a larger scale (e.g., total grazing by zooplankton). The solution, then, is to find robust, manageable rules to describe (i.e., parameterize) the integrated behavior of complex systems. Addressing the tension between the recognition of ecological complexity and the need for testable models is a major stimulus in the PARADIGM program.

The intrinsic scales of ocean ecology present another challenge to interdisciplinary ocean modeling. They are set by the growth and removal of the primary producers (phytoplankton) with time scales of one to a few days, and by the broad spatial-temporal spectrum of physical processes that influence pelagic ecosystems (all together defined as a "multi-scale" problem). Our project scope, therefore, is inherently multi-scale and encompasses the range of coupled dynamics of ocean ecology, biogeochemistry, and physics on time scales from hours to decades and horizontal scales from kilometers to global. Because of that, we employ a carefully constructed hierarchy of regional, basin-scale, and global modeling efforts.

The goal of model-data fusion in integrated ocean observation and prediction systems is a driver of PARADIGM. So, real data are important. The program includes a strong component of retrospective analysis for model development and evaluation, complemented with explicit efforts to exploit data from existing and planned ocean observation systems in model evaluation and for designing advanced data assimilation systems. Our models are designed to take advantage of global ocean color products (chlorophyll *a*, primary production, water clarity indices, and others), sea surface temperature, surface winds, and surface height data (currents and eddies) that are routinely produced and distributed. New products, such as ocean surface salinity (presently scheduled for 2009), are anxiously awaited.

As we address the challenges of ecological complexity, scales of variability, and model-data fusion, we collaborate on the development of novel approaches to ocean modeling, designed to exploit new information (e.g., from genomics), ideas (e.g., computer-generated natural selection) and technologies (e.g., interdisciplinary ocean observation systems). Our perspectives on future directions are presented here in the hope that they will contribute to the development of a truly revolutionary capability in oceanography—reliable, data-driven predictions of climate and marine ecosystems.

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CONTEMPORARY APPROACHES TO MODELING MARINE ECOSYSTEMS

Marine ecological modeling has undergone an exciting renaissance during the last decade (Doney, 1999). Concurrently, our understanding of marine ecosystems has been continually challenged by knowledge gained through the application of new tools to probe the ocean depths. In little more than a decade, a new group of microbial organisms, *Archaea*, has been found to inhabit much of the global ocean, a previously unknown group of microbes has been discovered that converts atmospheric nitrogen into the chemical forms that support ocean food webs and biogeochemical cycling, and new molecular and genomic techniques are rendering obsolete many of our strongly held views of the form and function of marine ecosystems, such as our concept of a species (e.g., Venter et al., 2004; Doney et al., 2004; DeLong and Karl, 2005; Giovannoni and Stingl, 2005).

As scientists developing and applying numerical models, we are confronted with this explosion of new knowledge and at the same time we are struggling to include "essential" complexity that we already know cannot be properly constrained with existing observations (e.g., Denman, 2003). If we are to incorporate realistic models of marine ecosystems into complex simulations of ocean circulation and biogeochemistry in order to forecast the future state and behavior of our oceans, then we must overcome three daunting challenges. First, we must introduce sufficient complexity to reproduce observed patterns of ocean physics, chemistry, and biology with some degree of confidence. Second, we must learn how to capture the essentials of marine ecosystems in a sufficiently parsimonious manner so that these models can be constrained and evaluated with observations. That is, models must be simple enough that a sufficient number of simulations can be performed to document the sensitivity of verifiable results to input data and parameterizations, so that multi-member ensembles can be generated to provide confidence intervals on our forecasts, nowcasts, and hindcasts. Finally, for long-term climate projections, we must include the basic set of mechanisms that we think are relevant on these longer time scales—even if they are not significant on seasonal to interannual scales—and construct a system with enough adaptability to reproduce ecosystem shifts in a changing climate. All along, we must be mindful of biological reality: the wonderful complexity of ocean ecosystems will never be fully described with numerical models of the global ocean.

Specifying "Functional Groups"

The earliest models of marine ecosystems (e.g., Riley, 1946) explored the fundamental drivers of food-web dynamics using an idealized system comprising three components: nutrients, phytoplankton, and zooplankton (NPZ). Now, the preferred approach to modeling marine ecosystems has been to include a distinct compartment for each "functional group," loosely defined as a group of organisms or species that performs a particular role within the ecosystem, with respect to the problem being addressed (Hood et al., accepted). For ecosystem-based models of ocean biogeochemistry, it has been necessary, but not necessarily sufficient, to include *a priori* the following four groups, because of their distinct but important roles, both in food-web interactions and biogeochemical cycling (Figure 1).

1. *Small phytoplankton* (<10 μm) that grow and are consumed by small grazers in the surface layer, tying up nutrients and energy in a microbial food web, described below. We usually consider these to be the "background" community of phytoplankton in the open ocean, contributing significantly to primary production but little to new production (including fisheries) or export of organic matter to the deep sea (Peinert et al., 1989). In nutrient-poor subtropical gyres, the phytoplankton assemblage is often dominated by the tiny (<2 μm) cyanobacteria *Prochlorococcus* and *Synechococcus*.
2. *Nitrogen-fixing bacteria and archaea* (diazotrophs), which convert atmospheric nitrogen gas to an organic form that ultimately increases the ocean inventory of nitrogen nutrients. Some diazotrophs fix both CO_2 and N_2 and can therefore have a major impact on ecosystem productivity, leading to a decoupling of nitrogen and phosphorus cycles. That is, if sufficient phosphorus is present, the new N delivered by N_2 fixation processes can lead to a net export of organic carbon from the surface layer over and above what might be supported by nitrate that is mixed from below, accompanied by dissolved inorganic carbon (Hood et al., 2004). Diazotrophs have a large requirement for iron, leading to important biogeochemical feedbacks between atmospheric dust deposition and the car-

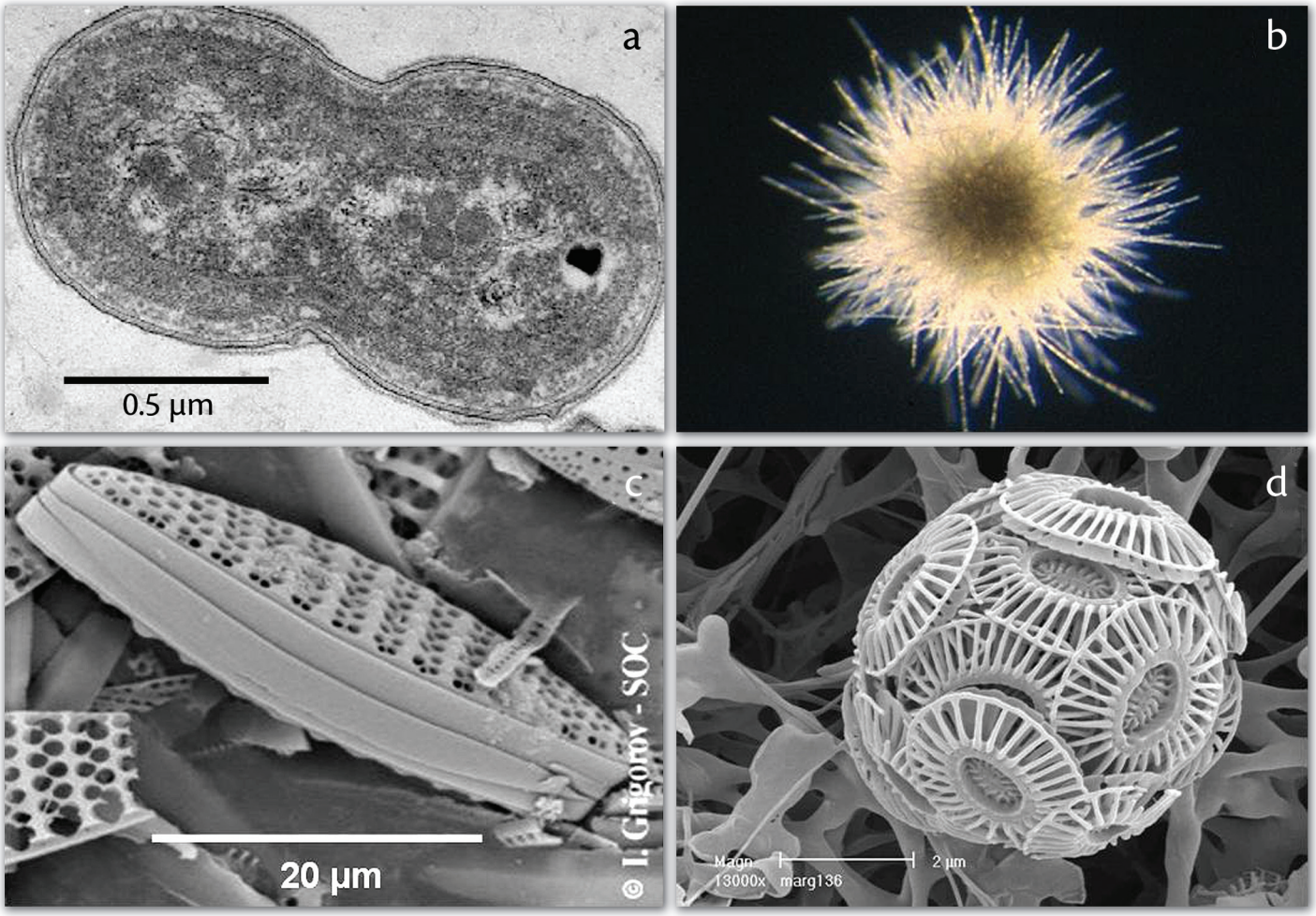


Figure 1. Oceanic photosynthetic microorganisms: (a) the prokaryotic *Synechococcus*, a key oceanic picoplankton species, especially in nutrient poor subtropical gyres, and one of the most abundant organisms on the planet; (b) colony of the cyanobacterium *Trichodesmium* (scale of image ~4 mm), a nitrogen fixing species common in warm, well-stratified tropical and subtropical environments; (c) the diatom *Fragilariopsis kerguelensis*, which has a thick, strong siliceous frustule that can protect it from being crushed and eaten by small crustacean zooplankton (Hamm et al., 2003)—it dominates the silica ooze accumulating under the Antarctic Circumpolar Current; (d) the coccolithophorid *Emiliania huxleyi*, which forms intricate calcium carbonate plates (liths), changing alkalinity and surface pCO_2. Top two photos courtesy of E. Webb and J. Waterbury, Woods Hole Oceanographic Institution, USA. Bottom two photos courtesy of National Centre for Oceanography, Southampton, UK.

bon and nitrogen cycles.

3. *Larger eukaryotic phytoplankton* (>10 µm), which are responsible for most sinking of organic carbon particles, either through direct sedimentation or incorporation into fecal pellets of larger zooplankton. Often, the large phytoplankton are dominated by diatoms, microalgae encased in beautiful siliceous frustules, that, if thick enough, can protect them from being crushed and eaten. Diatoms in iron-poor waters tend to be heavily silicified, suggesting that protection from being eaten compensates for low growth rates (Smetacek et al., 2004); in turn, diatoms in iron-rich waters require less Si relative to N to grow. The interactions among iron supply, nutrient cycling, food-web structure, and the vertical flux of carbon are thus complex and delightfully challenging to model.
4. *Coccolithophorids* are generally smaller phytoplankton, which produce $CaCO_3$ in addition to organic carbon. By removing Ca^{2+} ions they reduce surface

alkalinity, increasing surface pCO_2 and potentially reducing the ability of the oceans to take up atmospheric carbon. The sensitivities of coccolithophores to decreased pH in a high-CO_2 future could have major consequences on the ocean's capacity to sequester atmospheric CO_2 (Feely et al., 2004).

These four functional groups of phytoplankton, incorporated into a model with multiple nutrients (N, P, Si, Fe), can describe many features of marine biogeochemical cycling (e.g., Moore et al., 2002a). However, the set is by no means unique or universally applicable, because the problem being addressed should strongly influence the structure of the model that is being developed. The parsimonious approach to model building could lead to simpler models for more limited questions, whereas more or different functional groups might be needed to describe complex food webs or species succession.

The Microbial Food Web—Microzooplankton and Bacteria

Defining and/or generating functional groups of phytoplankton with their distinct biogeochemical functions and environmental sensitivities is only one step in the process of modeling the biological components of marine ecosystems. Ecological processes must be described by modeling the fate of materials produced by each functional group. There are two basic pathways of material flow from the phytoplankton in a functional or biogeochemical view of the marine ecosystem. The first is the export pathway by which biogenic particles and dissolved organic matter are transferred from the surface ocean to the ocean interior below. The second, and usually the larger, is the recycling pathway within the upper ocean, whereby respiration remineralizes organic matter into inorganic nutrients and CO_2; unicellular heterotrophic microbes (protozoans) and microzooplankton dominate this nutrient recycling. As a consequence of dominance of primary production and recycling by microbes, the ocean ecosystem has in essence a background recycling web of microbes and an episodic export food web of larger organisms (diatoms and copepods) (Figure 2). A major challenge is to represent the functions of export and recycling, and their control and variability in space and time, without expanding model complexity beyond tractable limits.

The challenge is compounded by the realization that a wide range of physiological and trophic capabilities exists besides the traditional autotroph and heterotroph modes—photoheterotrophy, for example (Doney et al., 2004). Current models now lag considerably behind new observations as far as incorporating recent genomic and ecological discoveries of the diverse and complicated food webs in the open sea (Karl, 2002). Despite the exploding genomic information on microbial organisms, our understanding of their role in regulating elemental cycles is still insufficient to produce more than a crude "black box approach" to incorporating microbial processes in models. One tactic is to apply the "background state hypothesis," whereby the microbial food web is a relatively stable presence in surface waters, through which nutrients escape to fuel larger cells, higher trophic levels, and vertical flux only when physical and biogeochemical perturbations supply nutrients to the surface layer in excess of the microbes' ability to absorb them (reviewed by Cullen et al., 2002). This hypothesis is being tested within PARADIGM by analysis of field data, along with complementary modeling of food-web responses to varying nutrient supply, including purposeful fertilization with iron (Denman et al., in press).

Model Closure and Mesozooplankton—Emergent Behavior

Biogeochemical models typically include rather rudimentary representations of zooplankton dynamics, parameterizing the ensemble of all grazing processes with simple mathematical formulae. Moreover, zooplankton are typically the highest explicitly represented trophic level; thus they also act to "close" the set of model equations. Model results are known to be highly sensitive to the form of this closure (Fasham et al., 1990; Steele and Henderson, 1992). Critical questions that PARADIGM scientists are investigating include: Can we continue to develop biogeochemical models with little or no evaluation of predicted zooplankton dynamics or parameterizations? Can we represent mesozooplankton meaningfully without any life history development? If not, can we represent the essence of life history development in a compact form? Such an alternative approach is now being attempted with behaviorally explicit numerical models that explore how zooplankton feeding strategies and morphological differences contribute to the efficiency of consumption and recycling of particulate organic material in pelagic ecosystems.

Spurred by the need to simplify the

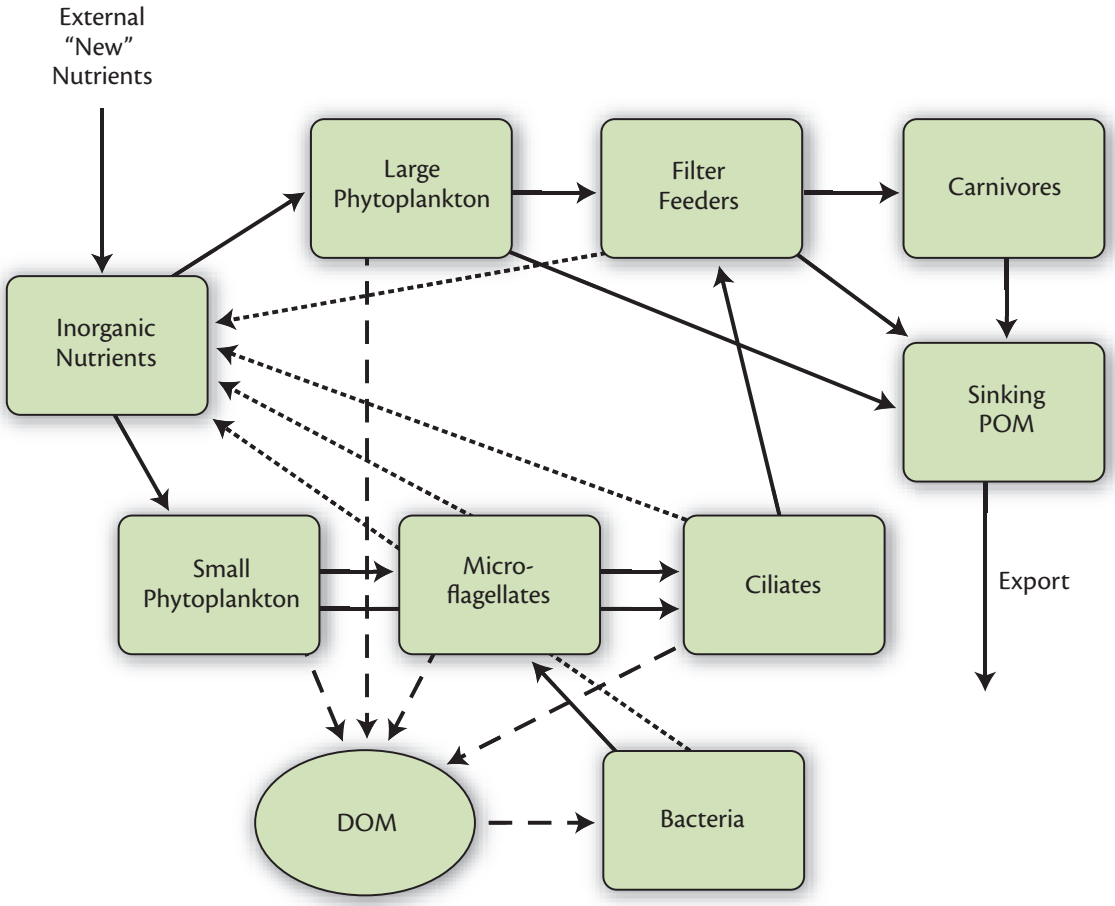
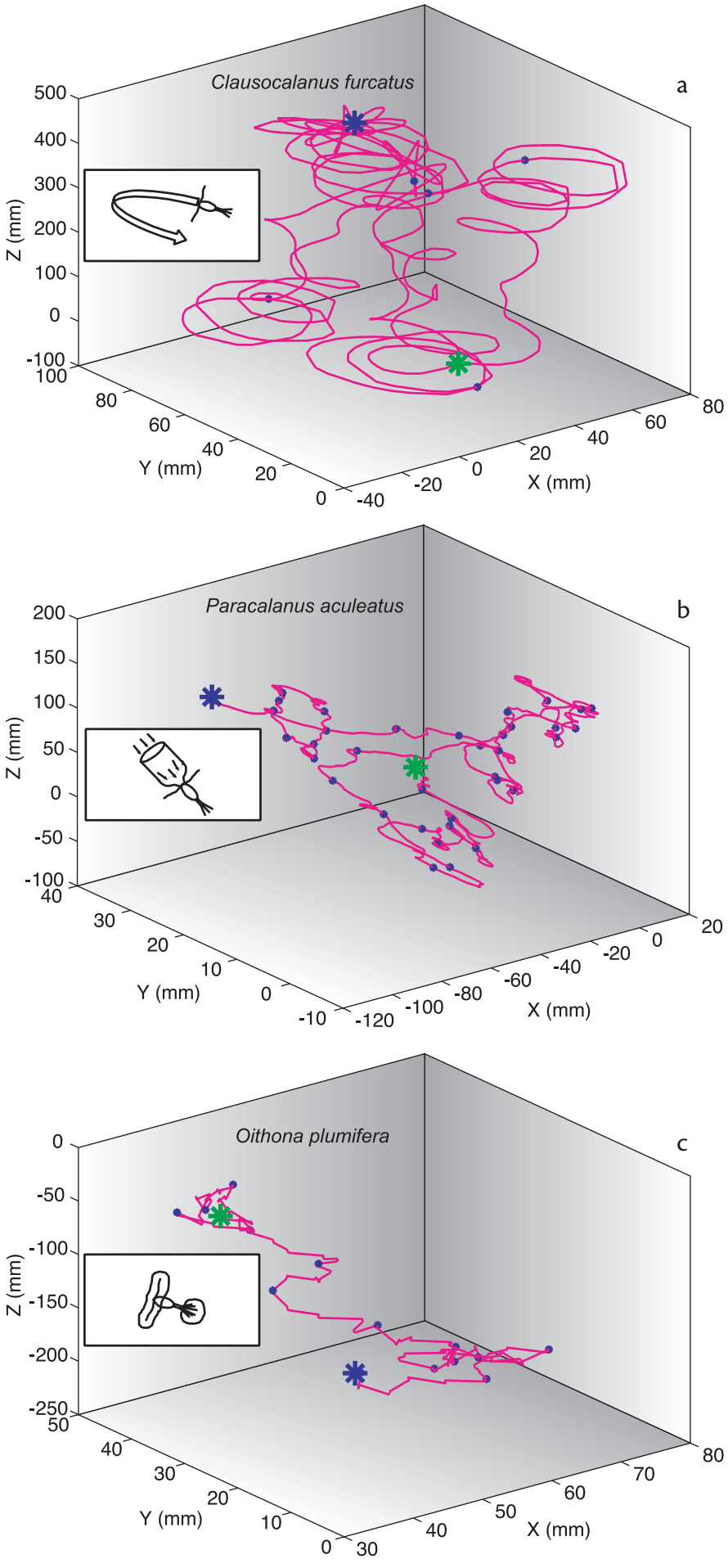


Figure 2. Oceanic plankton food web, after Laws et al. (2000). The upper pathway initiated by large phytoplankton contributes primarily to export from the upper ocean. The lower pathway starting with small phytoplankton results mainly in the recycling of nutrients. Solid arrows: flows of organisms and particulate matter (detritus and fecal pellets). Dashed arrows: flows of dissolved organic matter (DOM). Dotted arrows: flows of regenerated inorganic nutrients. Note that all organisms leak DOM but not all flows are depicted for clarity. All consumers release inorganic nutrients but not all arrows are shown.

modeling of ecological interactions, a goal of the PARADIGM program is to capture *emergent behavior* (i.e., the development of complex patterns from simple rules) that can manifest over the full range of spatial and temporal scales included in our model systems. For the modeling of grazing by zooplankton, our approach consists of realizing complex species and trophic interactions through the implementation of a computationally efficient set of rules that govern the behavior and feeding of the individual copepod species. This first step toward formulating these rules consists of developing simulations that explicitly track the distinct feeding methods of individual organisms representing three prominent tropical copepod species: *Clausocalanus furcatus*, *Paracalanus aculeatus*, and *Oithona plumifera*. Three components of copepod foraging are specified in this individual-based model—sampling ambit, area(s) of perception (sensory regions), and prey perception (size preference). The first two components utilize characteristics ascertained through careful behavioral studies (Figure 3) while the preference of grazers for larger prey is represented as increasingly reduced capture efficiency when prey diameter ranges below 15 µm. Accurate simulation of copepod foraging also requires a realistic prey field—one that is based on observed size spectra (Paffenhöfer et al., 2003). With these components in place, species-specific, size-partitioned grazing rates from the individual-based model results compared well with the observational data (see Figure 4 in Wiggert et al., 2005).

The simulation results indicate that adult copepod populations in an oligotrophic environment are limited by prey concentration and/or predation but not by resource competition—though this question must remain open until the full range of larval and juvenile growth stages is included (Wiggert et al., 2005). Additionally, the simulations demonstrate that their various foraging behaviors allow each species to access distinct sub-domains of the prey spectrum; yet all three have the same prey concentration threshold above which their metabolic needs can be attained. This implies that behaviorally induced prey size preferences contribute to the coexistence of these copepod species in the dilute prey environment that they inhabit.



How Much Complexity is Enough?

Functional groups, generalized representations of the microbial loop, and efficient representations of grazing relationships are all simplifications (i.e., parameterizations) of ecological complexity that are needed to construct models that can describe regional to global variability in ecological processes. Recognizing the complexity of marine food webs and biogeochemical cycles, one could easily define many more functional groups, food-web links, and grazing modes. However, each will require one or more new compartments in a model, and these must exchange material with many other compartments. Complexity rapidly becomes a problem: the number of parameters that must be specified and constrained to regulate one-way fluxes between X compartments increases basically as $X^2/2$ (Denman, 2003), assuming as well that only a single parameter is required to specify each flux.

Experience suggests that decisions to increase or decrease complexity depend

Figure 3. Individual-based modeling of grazing by copepods. *Clausocalanus furcatus* (a) is a fast continuous swimmer (Mazzocchi and Paffenhöfer, 1999). *Paracalanus aculeatus* (b) is a slow continuous swimmer that employs chemoreception and generates a feeding current (Paffenhöfer, 1998). *Oithona plumifera* (c) is an ambush predator that uses long feathered setae to sense for hydrodynamic signals emitted by its prey (Paffenhöfer and Mazzocchi, 2002; Svensen and Kiørboe, 2000). Representative simulated sampling ambits are shown for each copepod species, with the corresponding sampling method illustrated in the inset diagram. The start (large green star) and end (large blue star) points of each ambit are shown, along with intermediate steps (small black stars) at 50 second intervals. The individual trajectories represent 5, 30, and 12 minutes respectively, with corresponding travel distances of 4.2, 1.3, and 0.6 meters. Redrawn from Figure 3 in Wiggert et al. (2005), with permission from Oxford University Press.

essentially upon the specific context. Fundamentally, we are trying to model both the behavior of living organisms *and* the processes that trigger changes in that behavior. In many ecosystem models, phytoplankton or zooplankton are treated not as individual cells or organisms but as an aggregated biomass concentration (e.g., mol phytoplankton carbon per cubic meter). A question to ask is whether there are alternative approaches to this so-called compartment or continuum method that might better capture changes both in ecosystem structure and in the behavior of individuals or groups of organisms, in response to changes in the ocean environment.

So how can we proceed? Borrowing from the experience of other scientific communities studying complex systems (e.g., climate dynamics), we need to address the problem from two distinct but complementary directions. First, using targeted observations and laboratory and field experiments, we need to continue to test and improve the functional forms and parameter values used to simulate specific processes. Second, we need to develop a comprehensive approach for evaluating the overall system behavior that results from coupling together the individual components (including physics). Because of the strong interaction among model components, individual parameterizations cannot be studied solely in isolation. Changes to one parameterization may require adjustments or "tuning" of other model parameters, many of which are not specifically well constrained from the available data. The data assimilation and parameter optimization methods discussed below are invaluable in this regard because they provide an automated, objective method for judging the improved skill of a new parameterization in the context of the entire coupled system.

We should aim to add complexity only where there are appropriate observations by which it can be constrained or evaluated (see Figure 4). As ocean observation systems develop and relevant data become more available, direct evaluation of model results during incremental development of models will become an increasingly important tool.

Ecosystem model development is problem-driven, and it is thus not surprising that application of these principles has followed two streams: one for biogeochemical or carbon cycle models, and one for fisheries-food web models. In PARADIGM, we are exploring and developing general principles of ocean ecosystem modeling that can be applied to both applications. Forging linkages between these two disciplines is especially timely given recent trends toward ecosystem-based approaches to fisheries management (NMFS, 1999).

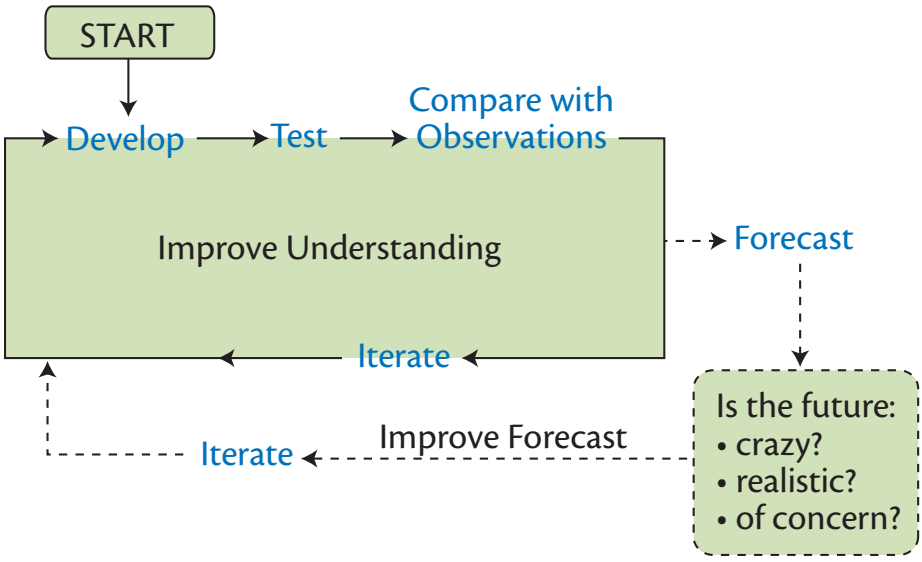


Figure 4. Top-down approach to developing coupled ocean biogeochemical plus general circulation models: Start with a model aimed at improving our understanding, depicted by the solid line with arrows. "Iterate" denotes many repetitions through this loop of developing, testing, and comparing with observations in a "hindcast" or retrospective mode. Eventually, modelers will step into the loop with the dashed line, where the objective is to simulate the future. Again, "iterate" indicates traveling around this loop many times, evaluating where the forecasts fail, identifying the weakness(es) in the model, then stepping back into the first loop to add complexity to address the weakness(es) that have been identified. Ultimately, data-assimilation modeling will be used as an integral component of the forecast itself.

A HIERARCHY OF COUPLED MODELS SPANNING MULTIPLE SCALES

Given the recognition that physically and chemically influenced ecological interactions in the plankton occur on small scales, but that they are intimately linked with processes on larger scales extending to the global scale, a central PARADIGM challenge is to implement new and evolv-

ing ecological concepts within a hierarchy of coupled physical-biological numerical models representing a range of spatial and temporal scales. Due to both computational constraints and limitations in our mechanistic understanding, no single modeling framework can capture the full range of relevant scales, which extend from millimeters to thousands of kilometers in space, and from seconds to millennia in time (Dickey, 2003). Global climate models resolve oceanic spatial scales from a few hundred kilometers to global, and temporal scales from a few days to many centuries. These models thus include distinct marine biogeographical regimes as well as the dominant modes of climate variability (e.g., the El Niño–Southern Oscillation, the North Atlantic Oscillation). Higher-resolution eddy-resolving regional models are being used on domains ranging from coastal- to basin-scales to explore the impact of specific physical and biogeochemical dynamics including the role of mesoscale eddies, continental-shelf processes, and coastal-open ocean exchange. For any given framework, the sub-grid-scale processes (smaller or more frequent than that which can be explicitly resolved), and in some cases super-grid scale processes, must be parameterized, with often critical but poorly understood impacts on overall system behavior (Doney, 1999). PARADIGM uses models of several scales to explore these consequences.

Global BEC Community Model

An example of a model in the global climate-scale class is the PARADIGM coupled Biogeochemistry-Ecosystem-Circulation (BEC) "community" model. The BEC is a "community model" in the sense that the model code and solutions will be fully accessible by scientists within *and* outside of PARADIGM, and the model will evolve with time—and hopefully improve—based upon community input. (Model results are available at the web address http://usjgofs.whoi.edu/mzweb/smppi/doney3.html.) This model addresses a major objective of the project, namely to assess our ability to construct an ecosystem model that contains the minimum ecological functions and state variables required to credibly represent major biomes from oligotrophic subtropical gyres to the iron-limited Southern Ocean, using a single set of model functions and parameters. The global BEC simulation embeds a generalized multi-element, multi-functional group ecosystem module (Moore et al., 2004) and a marine biogeochemistry code (Doney et al., 2001, 2004) into the global three-dimensional physics of the Parallel Ocean Program (POP). It partitions primary production among small pico/nano-phytoplankton, siliceous diatoms, and nitrogen-fixing diazotrophs. Iron limitation is included in an explicitly modeled iron cycle. Calcification rates are incorporated to mimic the observed distribution and production of coccolithophorids and depend on temperature and the growth rate and biomass of the model pico/nano-phytoplankton compartment.

The resulting coupled simulations reproduce known basin-scale patterns of primary and export production, air-sea CO_2 and O_2 fluxes, biogenic silica production, calcification, nitrogen fixation, and the concentrations of chlorophyll, macronutrients, and dissolved iron (Moore et al., 2004). The model solutions also capture the observed high nitrate, low chlorophyll (HNLC) conditions in the Southern Ocean, subarctic, and equatorial Pacific. These HNLC conditions are generated in the simulation by low atmospheric dust deposition, low surface iron concentrations, and iron limitation of phytoplankton growth, particularly for the functional group of large diatoms that contribute the majority of the particle export flux (Figure 5).

Significant biases, in particular excessively broad HNLC conditions, arise in the Equatorial Pacific in the coarse-resolution simulations (3.6° longitude and 0.9°–2.0° latitude); the errors are likely due to problems with the physical upwelling patterns and model-derived vertical fields of nutrients along the equator. To more fully understand these biases, we performed an additional high-resolution (4/10° grid) simulation, configured the same way as one of the low-resolution experiments, and compared the results of both to satellite-based estimates of chlorophyll (Figure 6). Clearly, increased spatial resolution of the model led to better fidelity with observations in the tropics. Other comparisons are being conducted to discern which characteristics of the solutions (e.g., errors) depend more on the formulation of the biological model than on the spatial resolution of the simulation.

The BEC model is a baseline for assessing against field observations and remote-sensing data our current capabilities in simulating coupled physical-biological dynamics across a range of different biogeographical regimes. In addition, it is a laboratory within PARADIGM, also intended for use by the external scientific community, for applying and testing the lessons learned from more sophisticated

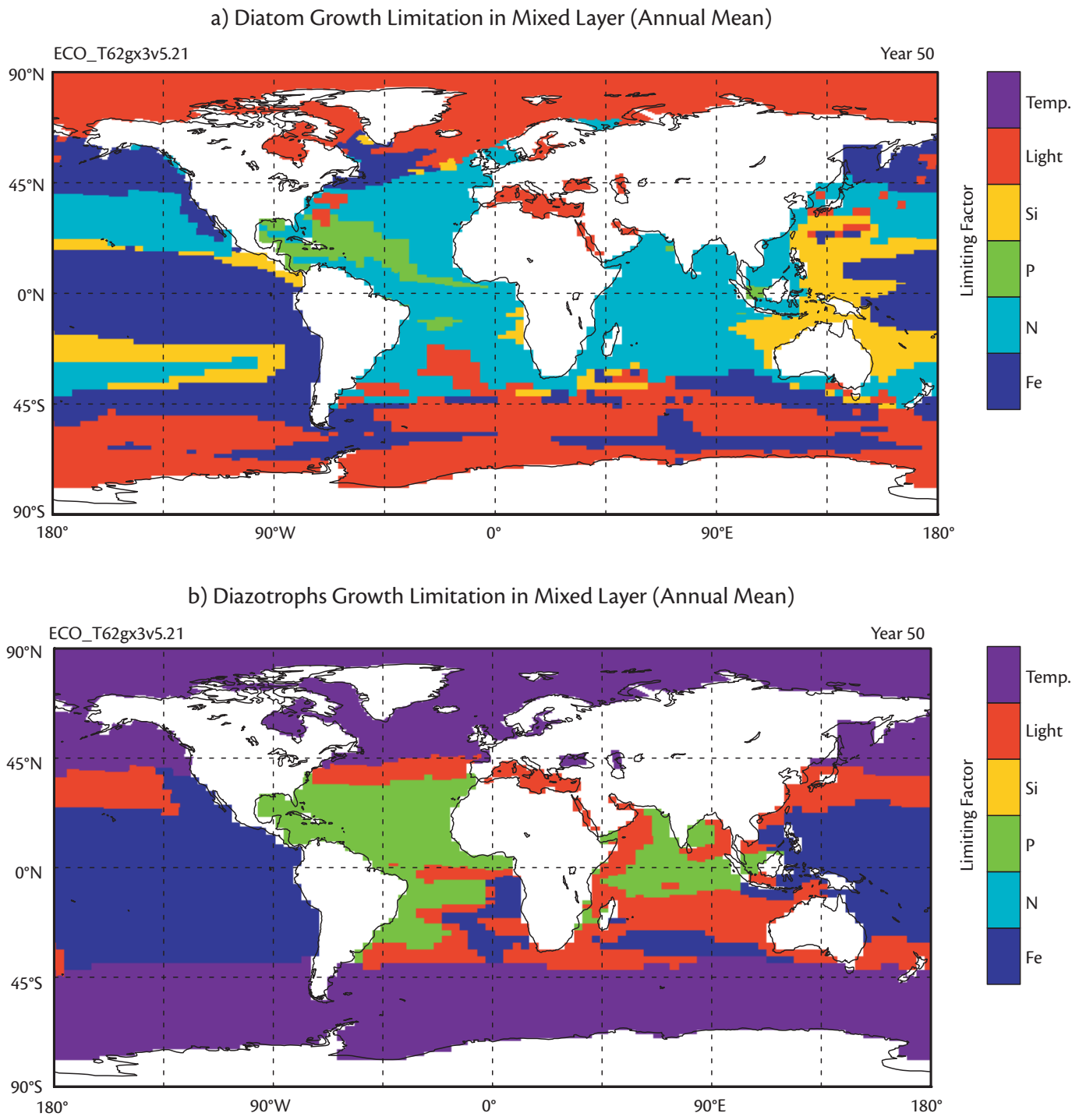


Figure 5. Spatial maps of the dominant factor limiting phytoplankton growth over the annual mean for (a) diatoms and (b) diazotrophs (nitrogen fixers) from the PARADIGM global Biogeochemistry-Ecology-Circulation (BEC) simulations. Diazotrophs generate less than 1 percent of the total global primary production directly but indirectly support more than 10 percent of the global production through the creation and release of new bioavailable nitrogen into the nutrient-poor subtropical gyres. The diazotrophs are predicted to be iron limited over much of the Indo-Pacific.

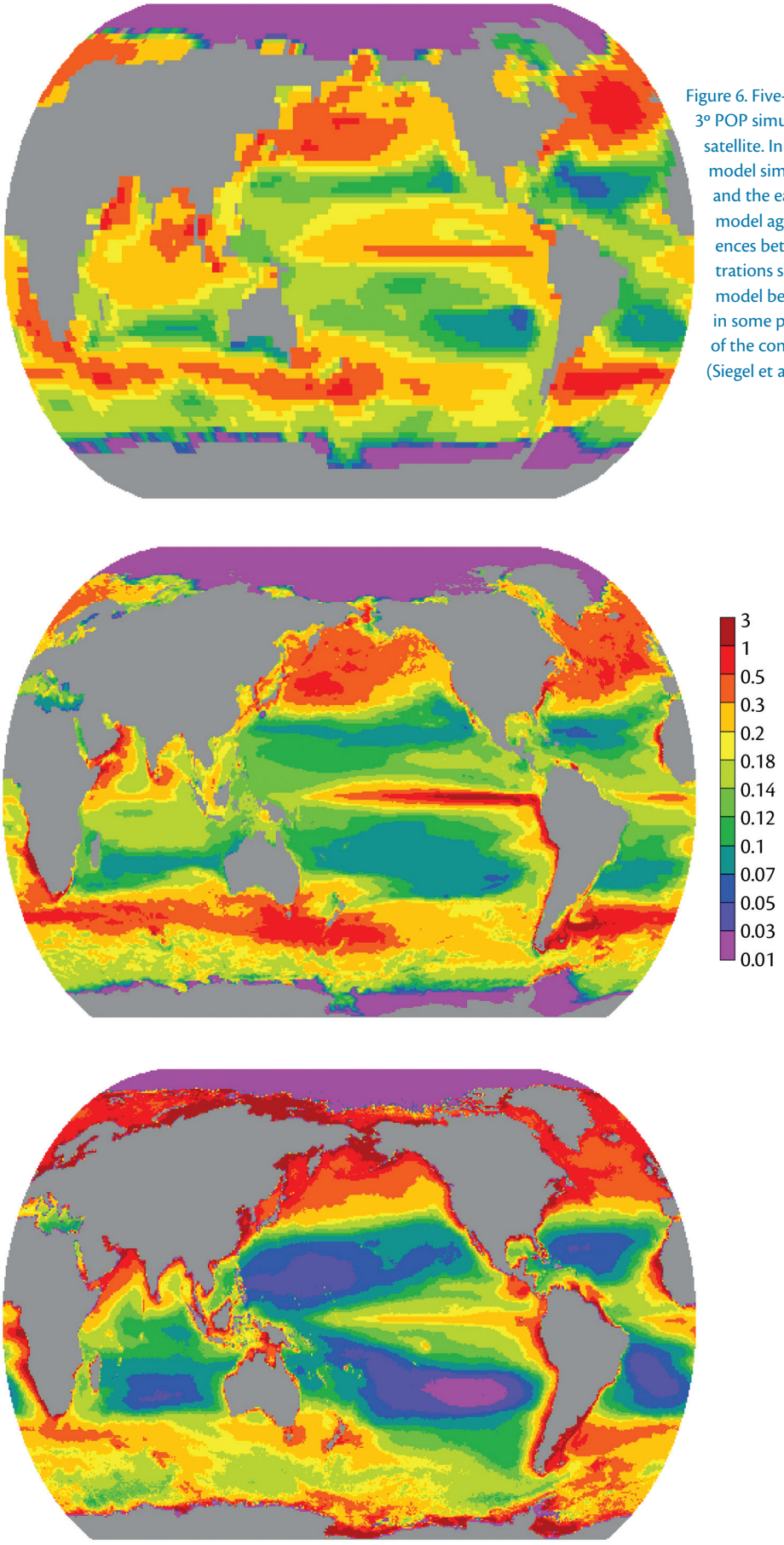


Figure 6. Five-year averages of surface chlorophyll (mg/m^3) from the 3° POP simulation, the 4/10° POP simulation, and the SeaWiFS satellite. In all cases where there are significant differences in the model simulations, such as the width of the equatorial regions and the eastern basin upwelling zones, the higher-resolution model agrees more closely with the data. Note that the differences between the model and SeaWiFS chlorophyll concentrations should not necessarily be taken as problems with the model because the remote-sensing algorithms may be too high in some places, for example, northern high latitudes, because of the confounding effects of colored dissolved organic matter (Siegel et al., 2005).

ecological simulations, emergent behavior, data assimilation experiments, and targeted regional simulations.

Basin-Scale Regional Simulations

As indicated in the comparison of results for models with differing spatial resolution (Figure 6), explicit description of processes on the scale of ten to a few hundred kilometers (the mesoscale) can greatly improve model performance. PARADIGM investigators are exploring the role of mesoscale processes in basin-scale biogeochemical cycling (McGillicuddy et al., 2003). This research was originally motivated by the question of what processes supply the nutrients required to sustain levels of new production implied by oxygen budgets in the main subtropical gyres (Shulenberger and Reid, 1981; Jenkins and Goldman, 1985). Regional studies suggested that eddy-driven upwelling could supply the "missing" nutrients (McGillicuddy et al., 1998). To test this hypothesis, a nitrate-based model of new production has been incorporated into eddy-resolving (0.1°) POP simulations (Figure 7). The biological model includes light- and nutrient-limited production within the euphotic zone, and relaxation of the nitrate field to

climatology below. Model skill was quantitatively evaluated with observations using an objective error metric; simulated new production falls within the range of observed values at several sites throughout the basin. Detailed diagnosis of the "best fit" model indicates that eddy-driven vertical advection of nutrients is sufficient to overcome the mean wind-driven downwelling in the subtropical gyre. These simulations are thus consistent with the hypothesis that mesoscale dynamics fuel a significant fraction of the annual new production in that area.

This model also revealed another aspect that was particularly surprising: eddies constitute a net *sink* of nutrients in the subpolar gyre (Figure 8). Diagnosis of the solutions indicates that the downward nutrient flux results from mesoscale processes associated with restratification following deep convection. In essence, a portion of the nutrients supplied to the surface layer by convective mixing is downwelled before it is utilized by the biota. The magnitude of the sink appears to be consistent with that estimated from Marshall's (1997) kinematic model of eddy-driven transport applied to deep convection in the North Atlantic. In some ways this eddy-driven sink of nutrients is related to the mechanism described by Levy et al. (1998, 1999), in which mesoscale restratification increases productivity following convection by releasing phytoplankton from light limitation. What we have described here is the counterpart to that process deeper in the water column: the same mesoscale dynamics that restratify the near-surface region also pump nutrients downward through the base of the euphotic zone. This flux occurs at a time when the ambient nutri-

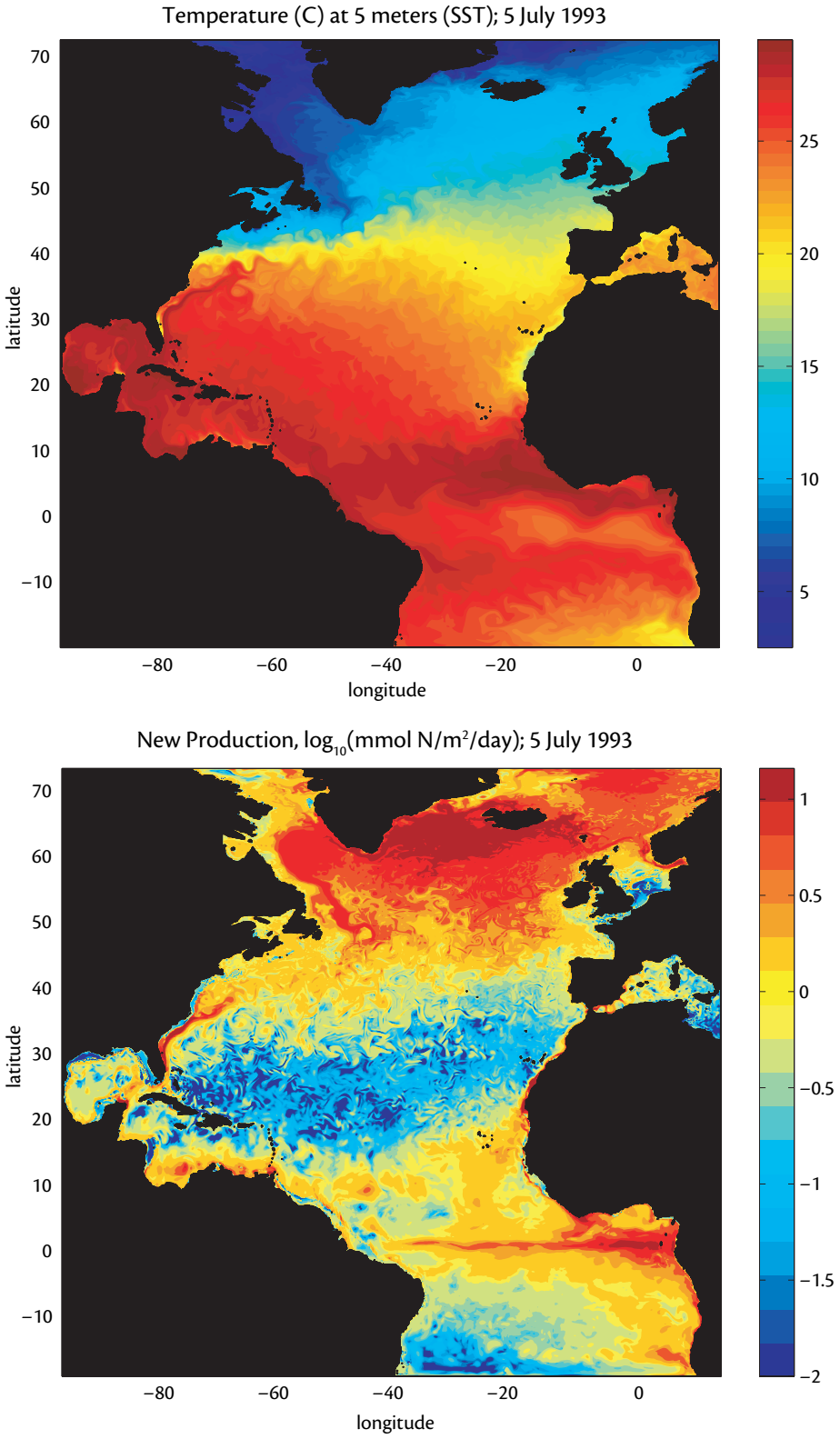


Figure 7. Snapshots of temperature (top) and new production (bottom) in a 0.1° resolution simulation of the North Atlantic. The temperature field reveals active mesoscale processes throughout the basin; biological uptake of nutrients is replete with mesoscale structure in nearly all areas except for the subpolar region, where production is still light limited in early July. Eddies play an important role in determining the mean.

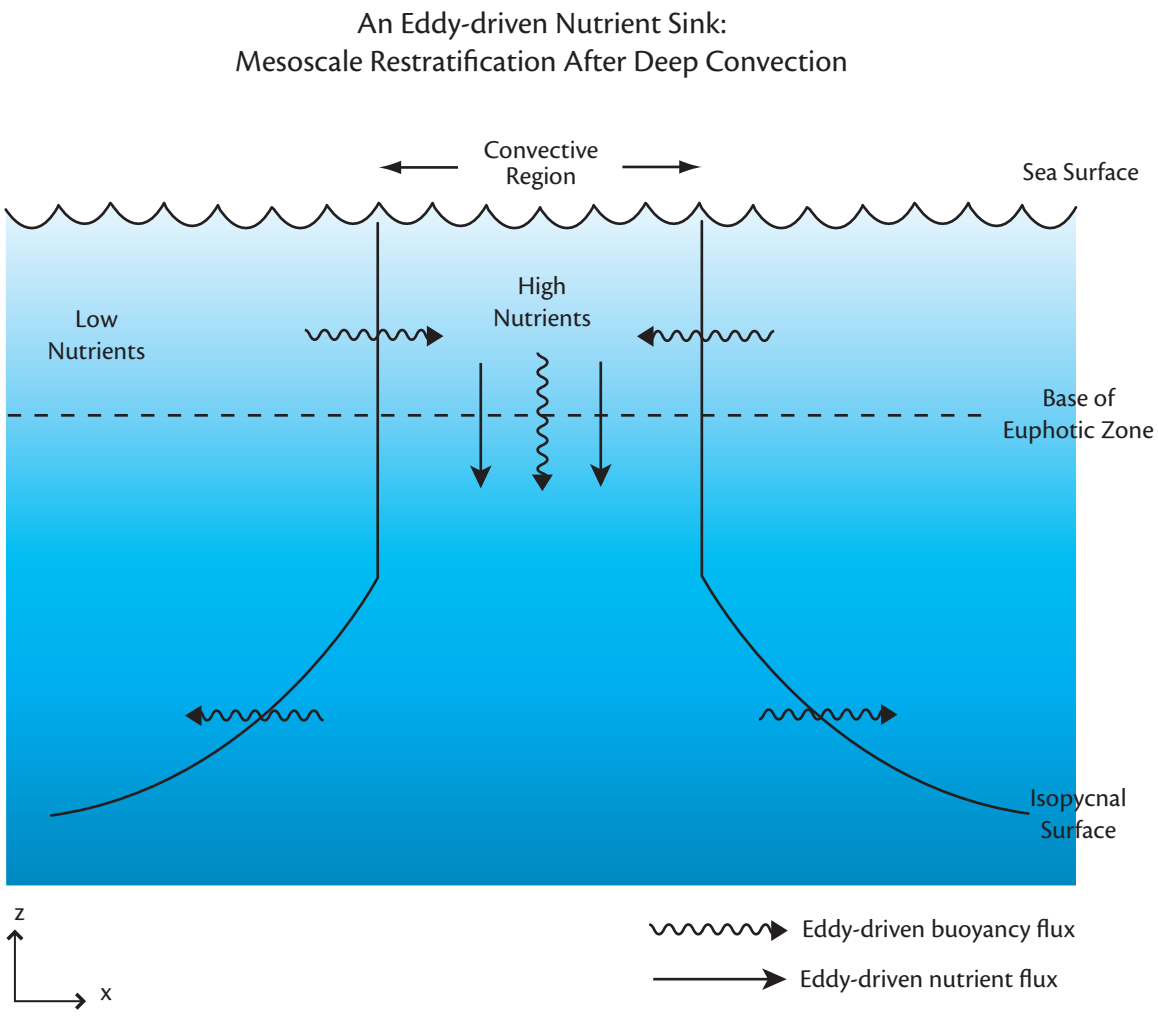


Figure 8. Schematic of the eddy-driven processes that tend to restratify an area of deep convection in the open ocean. Inward flux near the surface and outward flux at depth imply a downward eddy-driven transport that removes nutrients from the euphotic zone. Note that the convective area does not represent an individual chimney but the larger region over which mesoscale and submesoscale convective events take place.

ents are well in excess of limiting concentrations, so the influence on productivity is not felt immediately. However, the impact on the nutrient budgets is significant and does lead to decreased productivity on seasonal time scales. Surprisingly, the magnitude of this sink is sufficient to counterbalance the mean wind-driven upwelling of nutrients over much of the subpolar gyre. Based on these simulations, it appears that the oceanic mesoscale has major impacts on nutrient supply to, and removal from, the euphotic zone (McGillicuddy et al., 2003). An important next step is to develop mechanistic parameterizations of these processes to facilitate their representation in coarse-resolution climate models.

Coastal-Open Ocean Exchange

PARADIGM is concerned with assessing the role of coastal and continental shelf processes, which are known to be key components in the biogeochemical cycling of nitrogen and carbon, but which have historically been poorly resolved in basin-wide and global models. Challenges in modeling these systems arise from the high spatial and temporal resolution that is required to capture the inherent physical and biogeochemical variability, from the tight benthic-pelagic coupling that must be quantitatively described, and from the problem of accounting for input of material from the terrestrial biosphere through river and groundwater inflow and atmospheric deposition. Coupled models are now becoming available that are capable of addressing multi-scale variability by employing multiple nested spatial domains of variable resolution (see Box 1 on Advanced

BOX 1: ADVANCED NUMERICAL TECHNIQUES: ADAPTIVE AND NESTED GRIDS

Coupled modeling of the ocean and its biogeochemical cycles is inherently a multi-scale activity, with the interplay between spatial approximation and numerical resolution taking central stage. The natural scales of variability for biogeochemical interactions are often much finer than those characterizing the physical system itself and, furthermore, the regional distribution of biogeochemical interactions is heterogeneous ("hot spots" of activity are often highly localized spatially, for example, on the narrow continental shelves of the world's oceans). Several specialized approaches are being developed within PARADIGM to broaden the window of spatial and temporal scales that can be simulated, without the computational requirements of resolving all the scales. The first of these technologies, and by far the most widely practiced today, is spatial nesting or embedding of multiple fixed grids. Nesting has long been used in mesoscale atmospheric modeling for fine-scale, limited-area forecasting. In common with their atmospheric counterparts, the majority of regional-, basin-, and global-scale ocean models use traditional approximation methods characterized by structured horizontal and vertical meshes. The nesting of finer-resolution, sub-regional grids within a larger-scale "parent," with an appropriate exchange of information between the two, is therefore an attractive multi-scale alternative to more traditional "telescoping" (i.e., increasing resolution towards boundaries) grid techniques, which are limited to increasing resolution towards real (coastal) and dynamical (equatorial) boundaries only. The nested grid approach has been employed to obtain results presented elsewhere in this article (see the *Coastal-Open Ocean Exchange* section).

Despite the overall simplicity of spatially structured grids, the inherent advantages of regionally enhanced resolution, and ultimately the adaptivity of that resolution as the simulation progresses, continue to spur the development and exploration of alternate spatial approximations. One such future alternative is the use of heterogeneous, unstructured spatial grids (see Chen et al., this issue). Such grids, based upon either triangular or quadrilateral decomposition, may be generated to place maximum resolution in perhaps changing regions of interest (as the simulation progresses), while preserving global coverage at reduced grid spacing. Prototype unstructured-grid ocean models are now in the early stages of deployment. Finally, these fixed-grid spatial representations may be extended using time adaptivity to more faithfully follow the time evolution of fine-scale features, again with feedback from the evolving simulation.

Numerical Techniques). Examples include the PARADIGM regional models for both the U.S. East Coast continental shelf and the U.S. West Coast.

The East Coast regional model is comprised of a high-resolution (~10 km in the horizontal direction) ocean circulation model (ROMS v.2) implemented for the North Atlantic shelf and adjacent deep ocean and coupled with a nutrient-phytoplankton-zooplankton-detritus (NPZD) biogeochemical model. The shelf domain is nested within a larger-scale circulation model for the North Atlantic basin that allows us a high spatial and temporal resolution for the shelf region while retaining large-scale variability and remotely forced deep-ocean/shelf exchange processes. Spatial and temporal patterns in chlorophyll dynamics and primary productivity on the shelves are captured, for example, increasing chlorophyll concentrations and higher levels of primary productivity on the inner shelf, spring and autumn blooms, and a phytoplankton maximum near the pycnocline in summer.

The West Coast regional model consists of an NPZD ecosystem model embedded in HYCOM (Hybrid Coordinate Ocean Model) configured with 1/12° resolution, to be enhanced to 1/24° resolution in 2006. The regional model extends from 30°N to 50°N and from 115°W to 135°W and is nested within the 1/12° Pacific Basin HYCOM. The model is being used to examine coastal-open ocean exchanges as well as to help evaluate the ability of the coarser-resolution global PARADIGM model to represent mesoscale processes near the coastal boundaries.

Annual mean nitrogen budgets have been derived for the east coast Middle Atlantic Bight (MAB) and the West Coast California Current System (CCS) by diagnosing model-simulated fluxes of particulate and dissolved nitrogen (Figures 9 and 10). Nitrogen enters the MAB from the north (in currents across Nantucket Shoals and around Georges Bank), mostly in the form of nitrate (Figure 9). The nitrogen load of the along-shore southwest mean current is then modified by river and estuarine inputs, by sediment denitrification, and by an exchange across the shelf-break front that is mostly due to mesoscale processes. The majority of total nitrogen entering the MAB shelf is removed by sediment denitrification (~90 percent) while the remainder is exported across the shelf break in the form of particulate organic nitrogen (PON). There is significant exchange across the shelf break with a net on-welling of inorganic nitrogen and net export of particulate nitrogen. Denitrification removes 90 percent of all the nitrogen entering the MAB, sig-

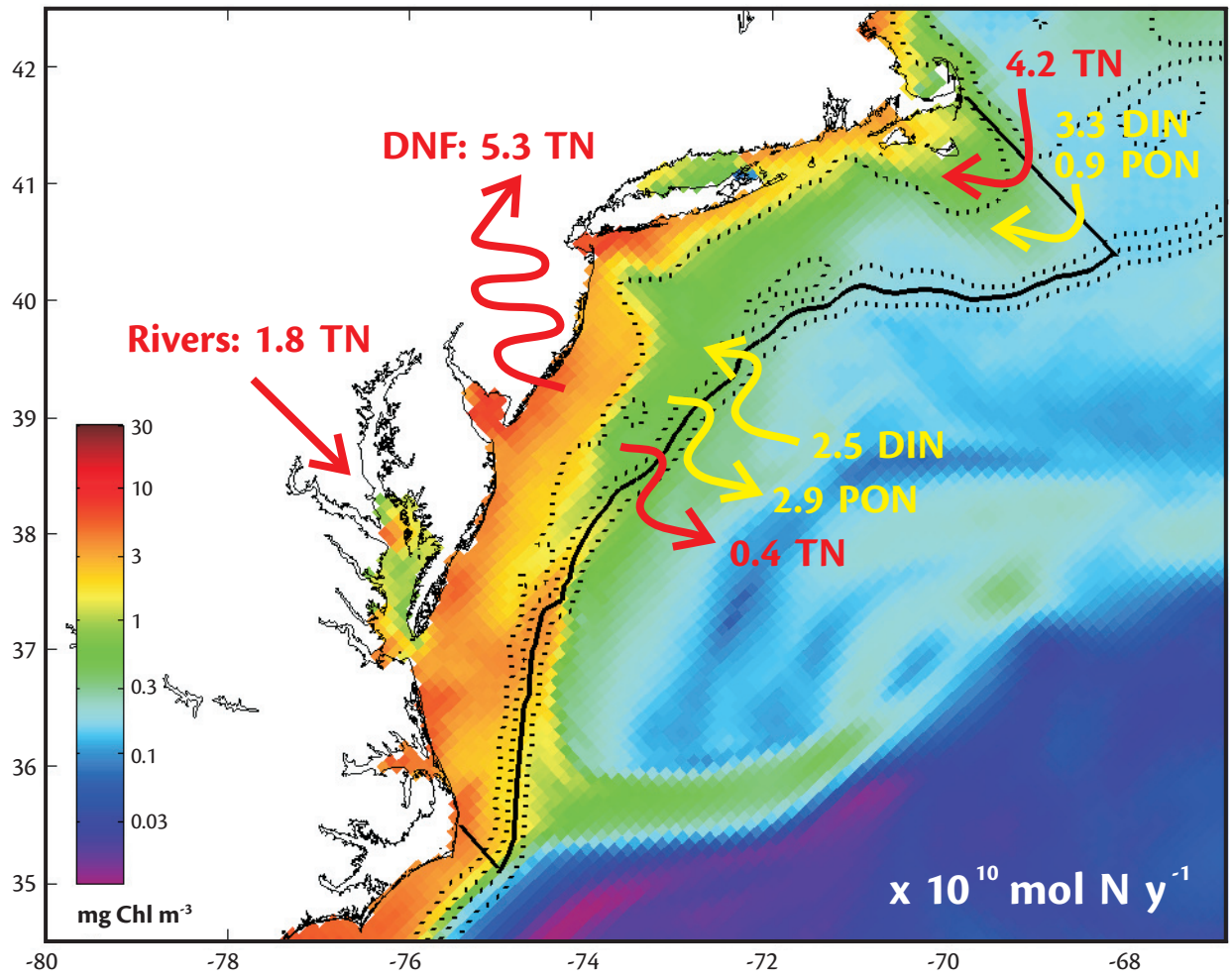


Figure 9. Model-predicted mean surface chlorophyll for July 1994 in the Middle Atlantic Bight (MAB) overlain by a model-derived nitrogen budget for the MAB shelf region. The annual mean nitrogen budget for the MAB shelf region (indicated by the solid black lines) was derived by diagnosing the fluxes of total nitrogen (TN, red numbers and arrows), dissolved inorganic nitrogen (DIN, yellow) and particulate organic nitrogen (PON, yellow) across two cross-shelf transects at Cape Cod and Cape Hatteras and across the 200 m isobath (the 40, 100, 200, and 500 m isobaths are indicated by dotted black lines) in addition to the annual river input and the denitrification (DNF) loss.

nificantly more than enters from rivers and estuaries, thus making the shelf of the MAB a net sink of bio-available fixed nitrogen. Extrapolation of the sediment denitrification flux to the whole North Atlantic shelf area results in a sink that exceeds the most recent estimate of North Atlantic N_2 fixation (by Hansell et al., 2004) by an order of magnitude (Fennel et al., accepted). The existence of such a significant nitrogen sink on the continental shelf is consistent with observational-based estimates (Seitzinger and Giblin, 1996).

In the CCS region, more than half of the (mostly) inorganic nitrogen gained via upwelling is found to be transported offshore as PON. The computed carbon flux offshore is roughly 1260 g C m^{-2} y^{-1} of the western boundary of the box model (Figure 10). Similar values were obtained by Moisan et al. (1996), who estimated that the California Current filaments can carry between 158–1890 g C m^{-2} y^{-1} offshore.

So far our results emphasize the importance of proper representation of coastal upwelling regions and continental-shelf processes in biogeochemical models and suggest that spatial nesting of regional and larger-scale models is a feasible approach. Different processes regulate nutrient supply, primary production, and export on the relatively narrow upwelling shelves of the U.S. West Coast versus the wider passive margin shelves of the East Coast. The large-scale biogeochemical impact of these two coastal domains is also fundamentally different. The East Coast shelves appear to remove bio-available fixed nitrogen, thus acting as a nutrient sink, while the West Coast region supports upwelling-fuelled production and export of organic matter—with qualitatively and quantitatively different consequences for carbon export.

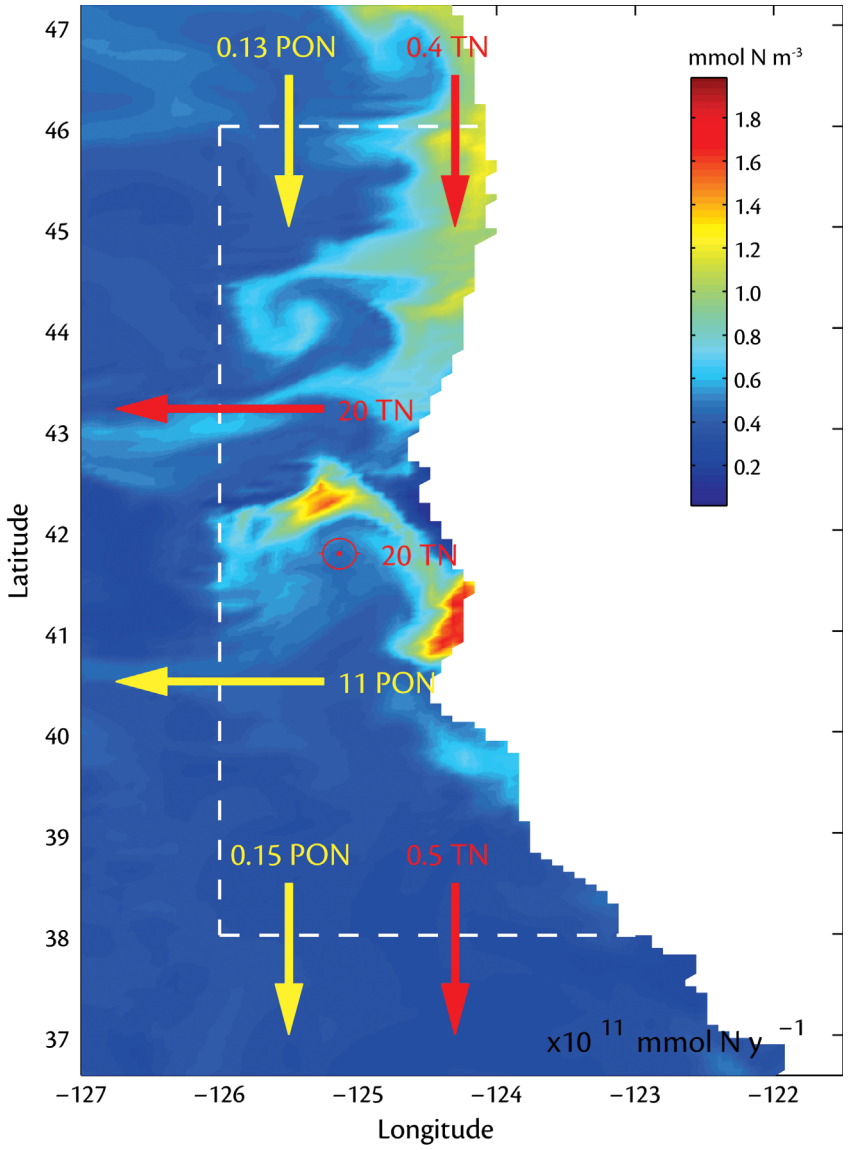


Figure 10. Model-predicted mean surface phytoplankton concentration for July in the California Current System overlain by a model-derived annual mean nitrogen budget within a near-surface box delimited from below by the σ_{25} isopycnal and horizontally as indicated by the white dashed lines. Shown in the figure are transports of total nitrogen (TN) and particulate organic nitrogen (PON). Note that more than a half of the upwelled inorganic nitrogen (as indicated by the up-arrow symbol) is exported offshore as PON, manly via filaments of the California Current.

DATA ASSIMILATION AND MODEL-DATA FUSION

The development of predictive models must be guided by quantitative comparison of the predictions with observations. Ideally, we should validate not only the variables predicted by the model (e.g., biomass of functional groups, concentrations of nutrients), but also the fluxes and rates that determine their variability, and the parameters that define model functions, by direct comparison with measurements. This is not easy. Many model variables can be measured by generally agreed-upon protocols; the accuracy and precision of methods have been defined, if not always realized (Knap, et al., 1994). Some other processes of interest (e.g., N_2 fixation, bactivory [feeding by ingesting bacteria]) can be measured, but seldom at the frequency and resolution needed for oceanographic understanding. Important physiological parameters can be determined either *in situ* or in controlled laboratory experiments (e.g., half saturation coefficients, phytoplankton maximum growth rates, grazing rates), and others can be estimated from satellite-based remote sensing (e.g., the upwelled visible light in a few wavelength bands from the upper optical depth can be used to estimate the amount of chlorophyll, and more recently, carbon biomass and physiological status of phytoplankton [Behrenfeld et al., 2005]). But many other parameters (e.g., specific mortality coefficients, remineralization and detritus sinking rates, bioavailability of iron) are difficult, if not impossible, to measure and are traditionally adjusted subjectively in the model until the "best" agreement between the simulation and the observations is reached. Further, as biogeochemical/ecosystem models become more complex, they require the specification of an increasing number of parameters, many of which are poorly known, much less directly observed. Validation and guidance of models with data are clearly difficult tasks. All of this combines with the equally daunting issues of measurement capability and resolution that further complicate model evaluation.

Model-data fusion is thus confronted with two major issues, largely related to the realities of dealing with sparse and inaccurate data: (1) finding ways to make the best use of observations to minimize discrepancies between predicted and observed variables and (2) using observations to constrain parameters of the models so they better predict variability in nature. These issues have been addressed using techniques of data assimilation and inverse modeling (Fasham and Evans, 1995; Matear, 1995; Harmon and Challenor, 1996; Spitz et al., 2001). Although traditional data assimilation led to improvement of model simulated biomass and fluxes at specific research sites, there has been no study to our knowledge that has focused on the quantification of the coupled circulation/ecosystem model errors, or the basin-wide errors in the observations and forcing (e.g., wind stress, solar and non-solar radiation) (see Box 2: Representation Error). In addition, one should recognize the changing landscape of direct ocean observables, with ocean optics playing a more central role, and then begin to adjust traditional approaches to data assimilation to directly account for these valuable data sets. Ultimately, data assimilation will be used in real time to incorporate information from ocean-observing systems directly into models of ocean circulation, ecology, and biogeochemistry—this is our vision of model-data fusion. Toward this end, the rigorous evaluation of the performance of a coupled BEC model needs careful attention. PARADIGM researchers are taking the following approaches to model evaluation and data assimilation.

Models, be they conceptual, statistical, or numerical simulations, are useful and necessary tools for studying the complex interactions that influence ecosystem structure and function.

Parameter Optimization

The U.S. Joint Global Ocean Flux Study (JGOFS) long-term time series (e.g., the Hawaii Ocean Time-series [HOT] and the Bermuda Atlantic Time-series Study [BATS]) and process-oriented studies (e.g., EqPac, Arabian Sea, and Southern Ocean) have allowed the development

BOX 2: REPRESENTATION ERROR

Our current capabilities in using models for simulating coupled physical-biological dynamics across various temporal and spatial scales must be assessed against the limitations of not only the *in situ* and remotely sensed observations, but also against the errors inherent in the model itself. An estimate of the "representation error" of model simulations includes not only that part of the signal that cannot be represented by the model itself, but also the errors due to observational sampling variability and instrument error. In recent years, data assimilative techniques have been developed to estimate the error of representation. Because estimating the error of representation in coupled circulation/biogeochemistry models shares many of the same issues with the problem of assimilating remotely sensed sea surface temperature (e.g., sampling issues, atmospheric forcing, and the ambiguity of representation of the observed quantity in terms of the model state), the Reduced State Space Kalman Filter (first devised and implemented for assimilating remotely sensed sea surface temperature [SST] data [Richman et al., 2005] into a circulation model of the North Pacific basin) is a good choice for estimating representation error. This technique is based on the computation of model-data misfit using the principal components of the model. For example, using statistical tests on the principal components of multidecadal circulation model simulations and the misfits between model simulations and remotely sensed data (SST), it was found that the model and data have a small number of independent degrees of freedom (approximately 30–40), which is much less than the dimension of the model or data.

This approach for estimating the error of representation can be further applied to objectively evaluate both the performance of the coupled BEC model and the associated explicit error bounds to the model outputs. In addition, this analysis will identify regions where observations will be most valuable and will identify those types of observations that have the greatest impact on the assessment of coupled BEC models and the understanding of coupled physical-biological processes.

of data assimilative ecosystem modeling using techniques such as the variational adjoint method (Lawson et al., 1995). This method consists of minimizing the misfit between the model solution and the available observations by systematically modifying the values assigned to ecosystem parameters, such as growth and mortality rates. Once a specified misfit tolerance has been achieved, an objectively determined set of optimized ecosystem parameters is recovered. For example, using data from BATS, and applying this method to an eleven-component nitrogen-based ecosystem model for the upper-ocean mixed layer, Spitz et al. (2001) found that the microbial loop as defined in Fasham et al. (1990) was not adequate to simulate the behavior of the ecosystem at BATS. Further, the assimilation of data from both BATS and HOT (Figure 11) revealed that the parameters determined through the optimization process were slightly different from one site to the other, which is consistent with the dominance of *Synecococcus* at BATS and *Prochlorococcus* at HOT. In addition, it was found necessary to include N_2 fixation to simulate the annual nitrogen cycle in the upper mixed layer at HOT. Nitrogen fixation was modeled as its end result—a source of ammonium and dissolved organic nitrogen in the system; the annual mean modeled N_2 fixation rate (Figure 12) over the climatological mixed layer (25.81 ± 15.32 mmol N m^{-2} yr^{-1}) compared well with the estimated rates from the abundance of *Trichodesmium* trichomes (21.90 ± 10.95 mmol N m^{-2} yr^{-1}). This assimilative modeling approach is a powerful tool to determine missing model pathways, improve model parameterization, estimate optimal parameters of the model (values of the parameters that lead to a minimum of the data-model output misfit) and increase our understanding of the biological system under study. PARADIGM is using this approach to refine the ecosystem model and to address the issue of model complexity.

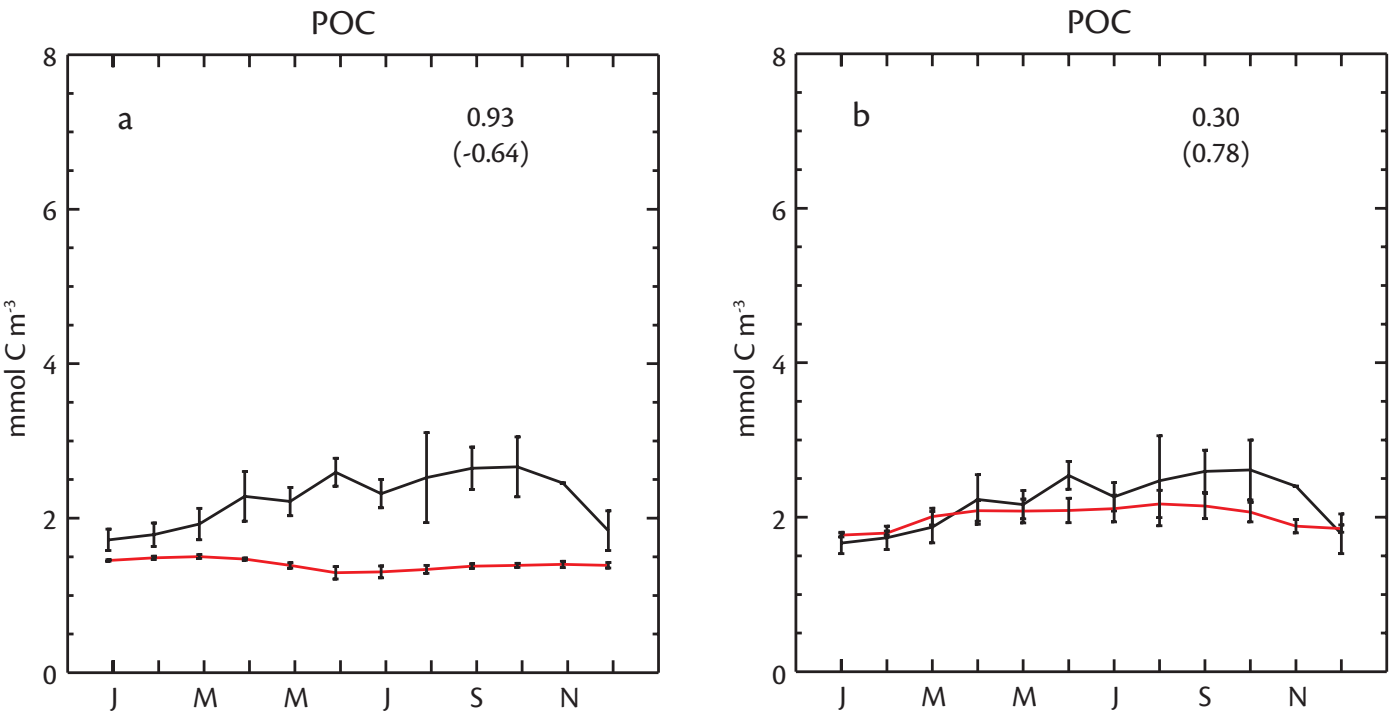


Figure 11. Modeled (black line) and observed (red line) particulate organic carbon (POC) for the climatological upper mixed layer at the Hawaii Ocean Time-series station (HOT). The upper number in the right corner of the figure represents the RMS error while the lower number represents the correlation coefficient. In (a), model parameters were derived from assimilation of observations at the Bermuda Atlantic Time-series Study (BATS) as in Spitz et al. (2001), which led to a poor agreement with the observations at HOT. (b) corresponds to the assimilation of the HOT observations, which led to a different set of parameters than the first assimilation and to a better fit with the observations. In both cases, N_2 fixation was included in the model. This figure indicates that while the HOT and BATS stations are both in an oligotrophic environment (North Pacific and North Atlantic subtropical gyres), they are dominated by physiologically different plankton species. This approach of parameter optimization will guide us in the development of an ecosystem model that can be applied to the global ocean.

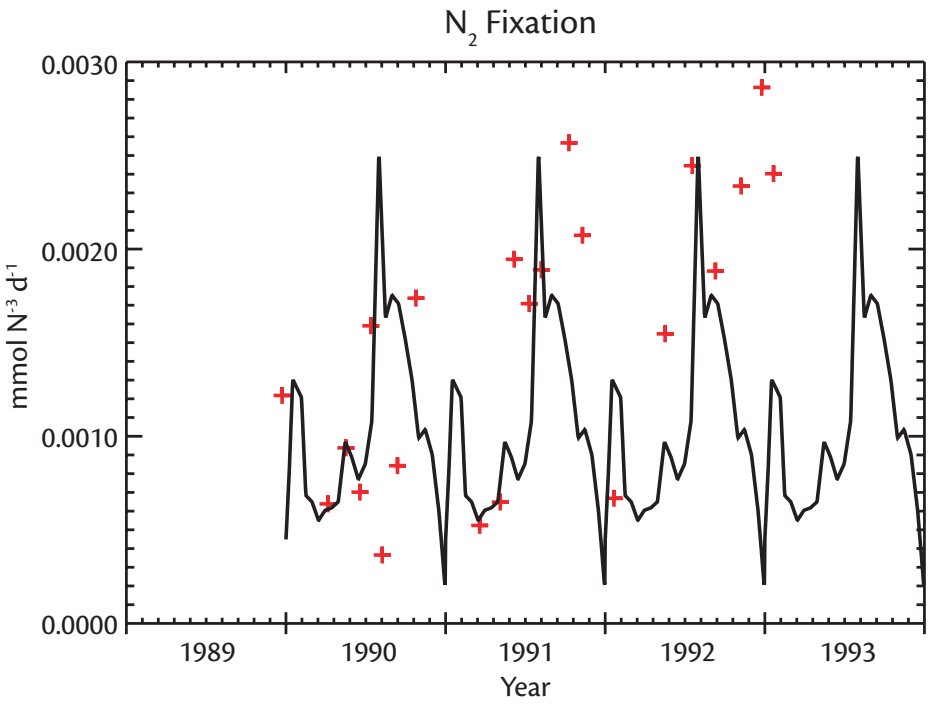


Figure 12. Nitrogen fixation rate in the upper 45 m as estimated from data assimilation of the HOT observations (black line) and from *in situ* measurements of trichome biomass (Letelier and Karl, 1996; Karl et al., 1997) (red crosses). In the model, the nitrogen-fixation rate was obtained by estimating via data assimilation (variational adjoint method) the external sources of ammonium and dissolved inorganic nitrogen (end result of N_2 fixation) every five days. The external source as defined in the model is indeed representative of nitrogen fixation because the time evolution shows the observed trend of high rates in the late summer early fall and a low rate in the winter. A similar approach could be used to estimate missing model pathways when little information is available and a comprehensive parameterization of the pathway might not be possible.

More recently, the variational adjoint method has been used to assimilate JGOFS Arabian Sea Process Study data into three ecosystem models of varying complexity in order to objectively assess which model structure best represents the fundamental underlying biogeochemical processes (Friedrichs et al., accepted). The systematic identification and optimization of an uncorrelated subset of model parameters led to ecosystem models that exhibit greater predictive skill. Subsequent quantitative comparisons of the optimized models indicated that at a single location additional model complexity did not provide an advantage. However, when data are assimilated simultaneously from multiple sites with distinct environments, the more complex models do demonstrate greater portability (Friedrichs et al., accepted). PARADIGM is using parameter optimization approaches such as these to refine the ecosystem models we employ and to address the issue of model complexity.

Inverse Analysis

Inverse modeling of ecosystems is an effective and objective method to attain new understanding of ocean ecosystem structure and trophic interactions by melding observations with models. This approach consists of a family of analytical techniques that are used to infer properties of a system when insufficient data are available for attaining a full characterization (Parker, 1977; Wunsch, 1978). The practical application of this technique consists of defining mass-balance equations that describe each system component, and the equations that constrain the individual exchanges between each component. The resulting set of equations is then solved.

For a marine application, system components may include, for example, size classes of phytoplankton and grazers, bacteria, and nutrient and detrital pools, while the constraint equations define such quantities as the assimilation and production efficiencies of different groups of organisms. Vézina and Platt (1988) were the first to apply an inverse model to solve a marine food web of the Celtic Sea. For the Ross Sea system depicted in Figure 13, a total of 12 balance equations (one per component)

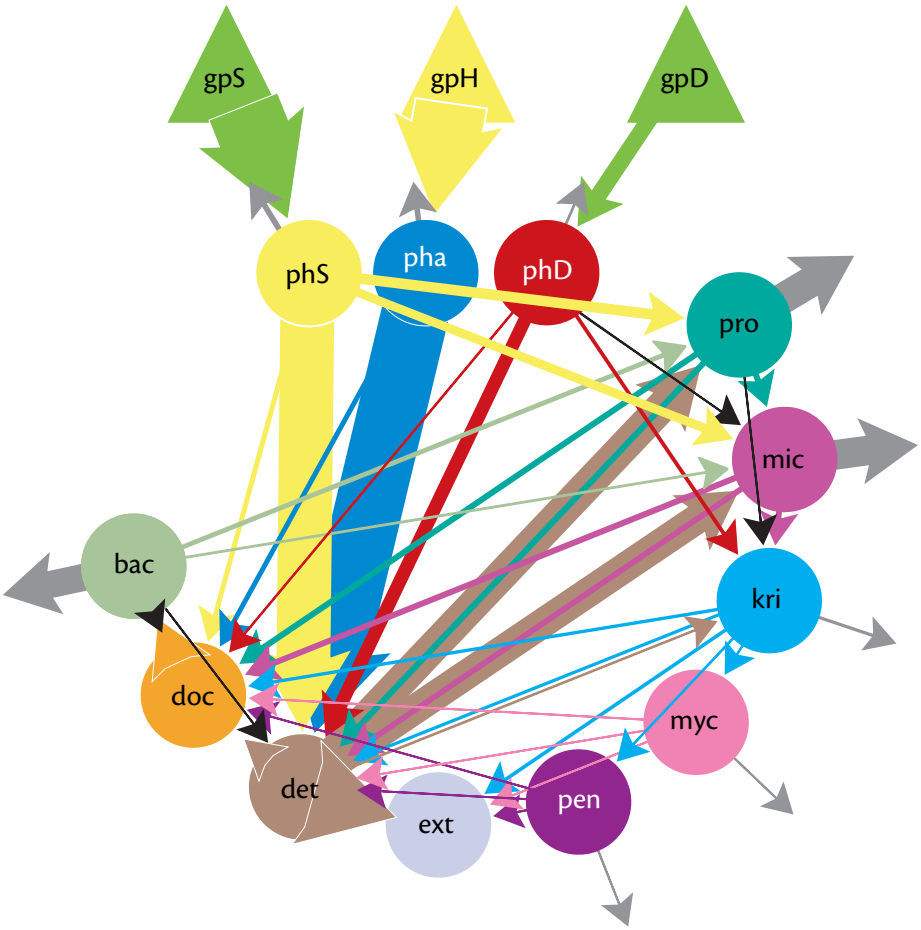


Figure 13. Flow diagram of carbon exchanges for the Ross Sea, Antarctica, obtained by an inverse technique. The living compartments include three size classes of phytoplankton: small flagellates, phS; *Phaeocystis*, pha; and diatoms, phD; and three classes of grazers: protozoans, pro; microzooplankton, mic; and krill, kri. Other compartments are mycotophid fish, penguins, and bacteria (myc, pen, and bac respectively). The nonliving compartments are detritus and dissolved organic carbon. Exports from the system pass through the external (ext) compartment. The radial grey arrows are respiration. Flow magnitudes are proportional to the width of the arrows. Thin black arrows are flows permitted in the model that had a value of zero in the solution. No flows exist or were allowed where no arrow exists (e.g., krill do not ingest *Phaeocystis*). Note the lack of grazing and preponderance of flow to detritus (mortality) in this model.

and 30 constraint equations were solved to define the flow structure. Solutions are required to respect the observations and other constraints within some specified tolerance. In these approaches and subsequent studies, information such as trophic pathways and physiological parameters were used along with observed flows to constrain a complete system of material exchanges among components of a marine or lake ecosystem (e.g., Figure 13; Ducklow et al., 1989; Jackson and Eldridge, 1992; Niquil et al., 1998; Richardson et al., 2004).

The complete ecosystem descriptions provided by inverse solutions offer a significant enhancement over observation-based descriptions for a variety of purposes. Data on rates of processes provide powerful validation tools for simulation models, preferable to the much more commonly used time series of standing stock observations (Fasham, 1984). Once a complete solution is in hand, a battery of network-based analyses (Leontief, 1966; Ulanowicz, 1986; Ducklow et al., 1989) can be applied to reveal higher-level structure and properties of the system, and different systems can be compared (Moloney and Field, 1991; Legendre and Rassoulzedegan, 1996; Daniels et al., accepted). For example, Daniels et al. (accepted) showed that spring phytoplankton blooms in the North Atlantic and Antarctic that differed greatly in size composition of phytoplankton and grazers were both dominated by microbial food-web processes and detritus utilization. These comparisons were not evident from observations alone. In PARADIGM we are synthesizing abundant measurements from JGOFS, Global Ocean Ecosystem Dynamics (GLOBEC), Long-Term Ecological Research (LTER), and other observational programs using inverse analysis to provide a uniform and consistent family of flow networks. The information these analyses provide will be invaluable for subsequent modeling-oriented ecosystem studies.

A Light/Energy Data Assimilation Framework: Bio-Optics

As we have described above, regional and global ecological and biogeochemical models have increased in their relevance to processes in the real ocean by incorporating greatly enhanced spatial resolution and more sophisticated representations of functional groups. Still, most simulations of pelagic ecosystems retain basic structures that trace back to the earliest models (Riley, 1946; Ryther and Yentsch, 1957) that, in turn, were strongly constrained by the observational capabilities of the day. In particular, phytoplankton is represented as chlorophyll (Chl), photosynthesis is calculated from relationships between photosynthesis per unit chlorophyll and irradiance (P^B vs. E), the chemical composition of phytoplankton (C:N:P:Fe:Chl) is either assumed or modeled as a function of nutrition and light, and results are compared to fields of Chl, often from remote sensing of ocean color.

As we contemplate oceanography's near future in which data from ocean-observing systems will be assimilated directly into highly resolved models of pelagic ecosystems, it is time to reconsider the conventional approach. Phytoplankton biomass is no longer assessed globally by direct measurements of chlorophyll pigment—it is estimated from measurements of ocean color, which are fundamentally influenced by the absorption of light by phytoplankton. Likewise, photosynthesis is directly related to this same absorption of light: we can calculate photosynthesis as the product of irradiance (E), absorption by phytoplankton (a_p), and its quantum efficiency (ϕ_p). So, if one is to compare models to measurements (and assimilate measurements into models), why not model the absorption of light by phytoplankton as a state variable, represent photosynthesis using functions of ϕ_p vs. E (cf. Bidigare et al., 1987; Lee et al., 1996) and compare results directly to estimates of phytoplankton absorption from ocean color or other optical-observing technologies? Conversion of phytoplankton absorption to other measures of biomass, such as carbon or nitrogen, is no more complicated than calculating phytoplankton C or N from chlorophyll, and the potential exists to infer more about the taxonomic and physiological status of phytoplankton from optical measurements (Sosik, in press). The stage is set for development of a new generation of bio-optical models.

Already, models have been developed that predict the optical properties of phytoplankton as functions of taxonomic and physiological status (Bissett et al., 2001), and optical measurements from space are being used to specify the chemical composition of phytoplankton, thereby constraining physiological rates (Behrenfeld et al., 2005). In Figure 14 we outline how the philosophy of modeling what is measured might be employed in an interdisciplinary modeling system guided by advanced ocean observations, not only observations of phytoplankton (absorption) but also of zooplankton (acoustical backscatter).

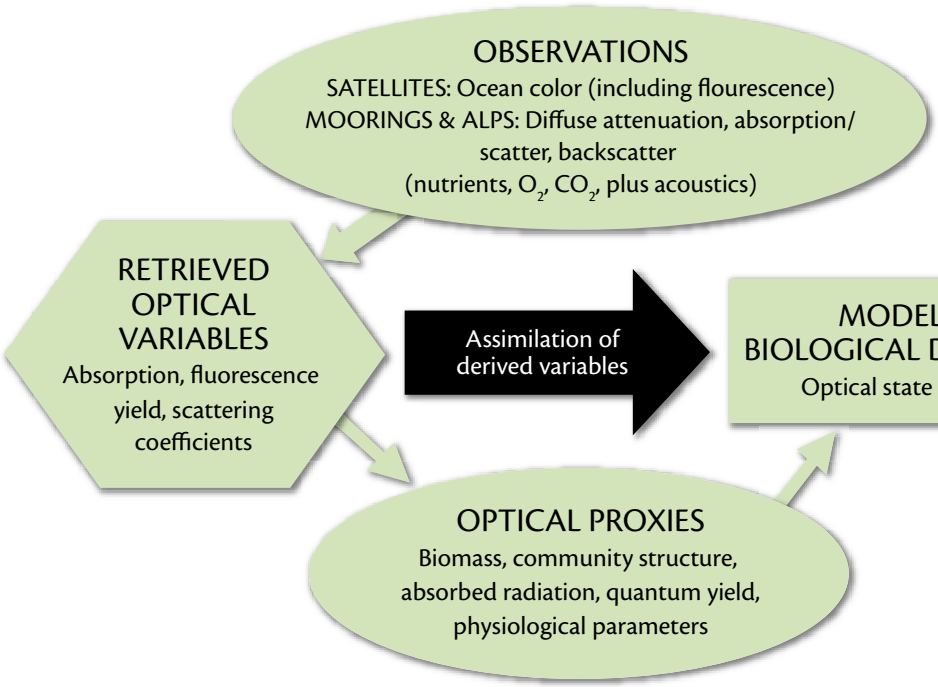


Figure 14. Schematic view of an advanced data assimilation model of marine ecosystems. Data would be provided by interdisciplinary ocean observation systems, including satellites, moorings, and Autonomous and Lagrangian Platform and Sensor Systems (ALPS) (e.g., gliders and autonomous ocean profilers). Optical observations will be incorporated as directly as possible into models that use optical properties as state variables (e.g., photosynthetic absorption as a proximate measure of phytoplankton). Optical proxies of biological properties will be derived from the observed variables to serve as additional variables (phytoplankton carbon from scattering coefficients, cf., Behrenfeld et al., 2005) or predictors of model parameters—such as patterns of fluorescence yield predicting the quantum yield of photosynthesis (cf., Letelier et al., 1997). With the addition of chemical and acoustic sensors to the observing system, models would also predict and assimilate chemical variables and higher trophic levels (e.g., zooplankton from acoustics). No such model exists, but it is a logical outcome of the development of interdisciplinary ocean observing systems.

Using BEC Model Results for Designing Oceanographic Observatories

The vision of an integrated, interdisciplinary global ocean observation and prediction system depends on coordinated design of models and ocean observatories, because the guidance that observations provide to models depends on detection of variability at appropriate scales and locations. In turn, the value of the models for forecasts depends strongly on how well they correspond to measurements.

One current application of models is to help design effective ocean-observing systems for research and operations. In particular, choosing the locations for sustained ocean observations is a critical step towards developing an effective global network. In practice, the locations for sustained ocean observations are based on many criteria, some of which are not science-based. Once observing sites are established, however, ocean scientists still need to determine, for example, which sites need more extensive instrumentation, more frequent observations, or targeted process studies. PARADIGM model results are being compared with *in situ* and remote-sensing measurements to help provide a scientific basis for making such choices. First results show that the models and data are yielding similar answers for objectively grouped stations showing common mean seasonal hydrographic and biogeochemical characteristics. The ocean is still very under-sampled, however, and comprehensive ocean measurements are sparse. Thus, one of the important outcomes of these particular analyses is to determine if the model results are useful for choosing observing locations in the global ocean that capture not only mean patterns but, more importantly, the significant sources of ocean variability at seasonal to interannual time scales. Contributing to the effective design of a global ocean observing system for research and operations could be an important heritage of PARADIGM models.

FUTURE DIRECTIONS

PARADIGM was designed as a very interdisciplinary program with the express intention of developing new approaches through cross-fertilization. And, indeed, there are a number of exciting new ecosystem modeling directions that PARADIGM research is highlighting, built upon our foundation of contemporary model development, model-data

fusion techniques, and our hierarchal approach to modeling. The broad interdisciplinary nature of the new directions described below emphasizes the importance of programmatic encouragement of cross-cutting activities through the formation of interdisciplinary research groups such as PARADIGM.

A Natural Selection Approach to Modeling Ocean Ecosystems

New observational approaches, including molecular and genetic probes, show even greater levels of diversity in the marine ecosystem, beyond the functional groups of species described above. Several genetically distinct functional types (ecotypes) have been discovered within closely related members of the same genus (i.e., *Synechococcus* and *Prochlorococcus*), and these have been found to populate distinct physical domains (Ferris and Palenik, 1998; Johnson et al., in press). Efforts to relate the genetic differences among strains to environmental factors are accelerating (Moore et al., 2002b). We therefore seek to adopt modeling strategies that can interface with, and help interpret, the new genetic view of ocean ecology. In one PARADIGM study, we are exploring an approach to marine ecosystem modeling that explicitly brings to bear natural selection (Follows et al., in preparation). Instead of imposing the community structure by specifying a small number of functional groups with static or even adaptive prescribed behavior (e.g., switching behavior that simulates species succession in response to specific types of growth limitation), we construct a model with many tens or hundreds of functional groups of phytoplankton, each of which has characteristics (initially, growth responses to light and ambient phosphate concentration) that are determined, in part by chance, from within realistic bounds. Then, we simulate natural selection by letting the interaction of physical forcing and food-web processes determine which functional forms of phytoplankton survive and structure the ecosystem. Embedded initially in a one-dimensional, oceanic physical framework, plausible and robust community structures emerge in ensemble integrations of this model (Figure 15) (Follows et al., in preparation), molded by the physical environment and nutrient availability (Tilman, 1977; Tozzi et al., 2004; Johnson et al., submitted). Although, on the surface, this approach introduces complexity to the model, the explicit application of the principle of natural selection provides a simplifying principle. Potentially, it will do two things: (1) identify a subset of possible functional groups that is adequate to represent the major features of ecosystem function and (2) indicate the possible existence of functional groups that we have not previously identified and that are important for structuring the ecosystem. Ongoing explorations of this system in a more realistic, three-dimensional, multi-nutrient setting suggest this approach may be fruitful.

Genomics: Where Ocean Ecosystem Modeling May Need to Go

Genomics is the study of whole genomes of organisms. The ability to determine a portion, or the entire genome sequence, of natural microbial assemblages and pure cultures of selected isolates (e.g., Venter et al., 2004; Giovannoni et al., 2005a) has revolutionized ocean ecology (Doney et al., 2004; DeLong and Karl, 2005). The importance of genomic discoveries for ocean modeling is that these revolutionary approaches are telling us about new aspects of previously modeled processes or organisms (e.g., the ecotypes discussed previously) and also about previously unknown organisms and processes that need to be simulated. Two examples illustrate the challenges that genomics research is presenting to oceanographers and ecosystem modelers.

Genome-based probes were used to enumerate planktonic archaea in the mesopelagic water column in the North Central Pacific Gyre and off the West Antarctic Peninsula (Karner et al., 2001; Church et al., 2003). Archaea are structurally similar to bacteria (they are both prokaryotes) but are genetically and, perhaps, physiologically distinct. With *Bacteria* and *Eukarya*, the *Archaea* form the three fundamental domains of life. They may be numerically dominant in a large part of all ocean waters, but we are still not certain of what they do: current evidence suggests they are chemoautotrophs, possibly nitrifiers (Francis et al., 2005; Könneke et al., 2005). Models of nitrogen cycling and material fluxes in mesopelagic systems need to address the existence of these organisms; they must be guided by the latest information on biogeochemical capabilities and distributions of archaea, obtained through genomic analyses. This calls for enhanced integration of genomics research with oceanography and the modeling of Earth systems ecology—an alliance of approaches that is sure to pay off.

Another example concerns N_2 fixation, the ultimate process supplying fixed nitrogen to the ocean over long

time scales. The principal N_2-fixing organism in the central gyres has been assumed to be the large filamentous cyanobacterium *Trichodesmium* (Capone et al., 1997; Karl et al., 1997). This organism exists as large bundles of filaments a few millimeters long, is favored in warm calm seas, lives mostly at the surface where irradiance is greatest, and is resistant to grazing. *Trichodesmium* is now represented in several models (e.g., Figures 10 and 11). For this sea-surface-dwelling organism, the main challenges for modelers are high light tolerance and mechanisms for acquiring iron and phosphorus in nutrient-depleted waters (Fennel et al., 2002; Hood et al., 2004). Recently, genomic probing for the gene that expresses the N_2-fixing nitrogenase enzyme has revealed that there are also abundant, small unicellular N_2 fixers (Zehr et al., 2001), and that these are sufficiently abundant to be a significant source of fixed nitrogen (Montoya et al., 2004). Indeed, Montoya et al. (2004) concluded that they may fix as much or more nitrogen than *Trichodesmium* in the North Pacific gyre. Because these unicellular N_2-fixers are small, they are probably vulnerable to microzooplankton grazers. It follows from these observations that the environmental influences on net growth rates, and thus the distributions and population dynamics, of the unicellular N_2-fixers may be quite distinct from those for *Trichodesmium*. Future models of oceanic N dynamics must address the diversity of N_2-fixing organisms and their dynamics in order to represent the N_2-fixation process correctly (Arrigo, 2005). Furthermore, inclusion of both classes of N_2-fixers is probably also critical if we are to predict the response of the ocean nitrogen fixation system to regime shifts and climate change. The need for examining this detail once again puts pressure on the complexity-simplicity battle in ocean ecosystem modeling.

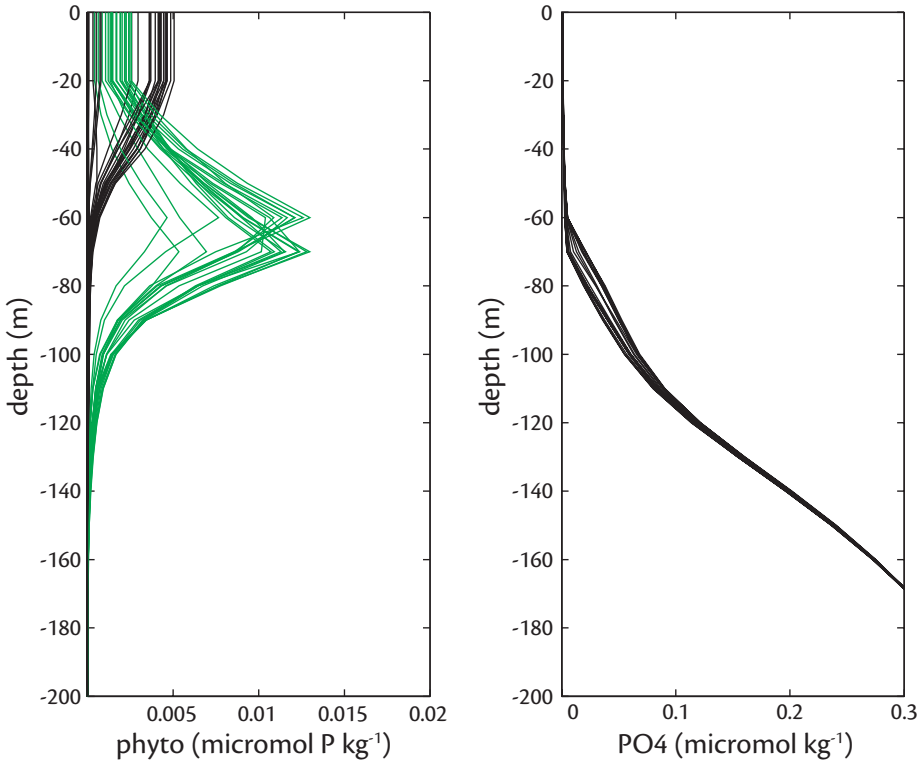


Figure 15. (a) Modeled annual mean phytoplankton phosphorus concentration (μmol P kg^{-1}) and (b) annual mean phosphate concentration (μmol kg^{-1}) as a function of depth from an ensemble of twenty integrations with a one-dimensional ecosystem model (Follows et al., in preparation). The idealized model represents the annual cycle by imposing sinusoidal cycles of sea-surface temperature, which drive wintertime convection and insolation. Winter mixed layers reach 120-m depths, shoaling to 25 m in the summer. Thirty-six functional groups of phytoplankton are initialized in each integration, differing in light sensitivity and phosphate half saturation coefficient, assigned randomly within realistic ranges. The figure shows the annual mean phytoplankton and phosphate profiles from the tenth year of integration of each of the twenty simulations. The simple environment with only two resources, light and phosphate, supports limited diversity, selecting for a surface-oriented, "high-light, low-nutrient" functional group (black lines) and a "low-light, high-nutrient" functional group (green lines) that forms a deep chlorophyll maximum in each integration. Of a possible 720 functional groups (the total from all ensemble members) only about 40 are viable (left panel) after a decade of competition. The nature of the viable functional groups is qualitatively consistent and robust between ensemble members, a consequence of the control of the resource environment (Tilman, 1977). The annual mean phosphate profiles of the ensemble members are dependent on ecosystem structure but closely consistent (right panel).

A New Model Currency—Energy

Another consequence of technological advances, including the genomics revolution, has been a serious challenge to our view of the role of microorganisms in controlling the fluxes of carbon and

energy. New taxonomic groups, including the two most abundant photoautotrophs, *Synechococcus* and *Prochlorococcus*, were not known and, therefore, were not considered in early models of marine ecosystems. We now have the full genome sequences of these and several other key microorganisms available to us, which provide the beginning of what will become the blueprint for life in the sea. Furthermore, the broad genotypic and phenotypic diversity that is emerging within selected groups of otherwise "identical" marine microorganisms (like *Prochlorococcus* ecotypes) may require a formal redefinition of the species concept and the development of new ecological theory—in fact, it may not be premature to state that for marine microbes, the species concept is "road kill" on the genomics highway.

Models based on carbon or nitrogen may soon need to shift their currency to energy, now that we have evidence that many chemoheterotrophic marine bacteria may also have the ability to harvest light energy without coupled fixation of carbon dioxide. This process of proteorhodopsin-based phototrophy, if found to be quantitatively important, will challenge our well-established view of the relationship between carbon and energy flux, and it may require a wholesale revision of our conceptual models of marine ecosystems (Karl, 2002). For now, however, the process is shrouded in mystery, because initial experimentation has failed to show any influence of light on growth of the microbe expressing proteorhodopsin in a laboratory-reared strain originally isolated from the Oregon coast (Giovannoni et al., 2005b). Integration of bio-optical modeling with physiological information on proteorhodopsin may provide answers. Sorting out the species concept and the quantitative roles of alternate trophic strategies are but a few of the future grand challenges in microbial oceanography (DeLong and Karl, 2005).

> ...the ultimate objective of any comprehensive marine ecosystem modeling program must be the development and implementation of reliable forecast systems, guided by and validated with systematic observations of the sea.

Marine Ecosystems and Near-Term Climate Change—Elemental Decoupling

Another important application of our evolving ecological models will be to depict the role of the marine ecosystem in regulating the exchange of CO_2 with the atmosphere on near-term climate-change times scales. On millennial time scales, this is usually considered to be controlled by the phosphorus cycle (except see Falkowski, 1997). If, however, we are interested in how the marine ecosystem participates in climate change on scales of centuries or less, then other elements exert more control, primarily nitrogen, iron, and silica. Most existing biogeochemical models including marine ecosystems use nitrogen as the base "currency." A valuable principle that has served biological oceanography well states that the cycles of N, P, and C are connected through fixed elemental stochiometry (so called "Redfield ratios" after, for example, Redfield et al., 1963), even though it is very well known among biologists that at any one place or time, Redfield stoichiometry is likely to be violated due to imbalances in the supplies of light, N, and P to phytoplankton (Klausmeier et al., 2004). On the global scale, the N cycle decouples from the C and P cycles through the processes of nitrification, denitrification, and dust deposition. Iron, which limits the uptake of carbon and hence the photosynthetic fixation of carbon into organic forms, is required in trace amounts. Yet iron seems to regulate carbon fixation in about one quarter of the world ocean, and it influences N:Si stoichiometry in phytoplankton. Our models must explicitly include these "control points," where the fluxes of the different elements decouple. Furthermore, the representation of these controls in our models must be sufficiently detailed and flexible so as to allow changes in their functioning (i.e., "adaptive" control points) in response to a changing climate.

Prospects for Operational Forecast Systems

We are keenly aware that, although the tools of PARADIGM have great value for

increasing our understanding of marine ecosystems, our models must ultimately be held to the strictest of all tests: as the major component of a reliable system for quantitative predictions of marine ecosystems. For that, their value will be determined solely by the quality of forecasts. What we forecast and on what time and space scales depends, of course, upon the problems we are given; a good example would be the deployment of a seasonal forecast system (i.e., an integrated observational network and forecast model) in support of an ecosystem-based management program, whether regional, basin-scale, or global. The modeling elements for accomplishing that are firmly in place in PARADIGM, revealing a pathway to developing reliable interdisciplinary regional to global models that will assimilate data from ocean-observing systems in an *operational* forecast mode. The hurdles for achieving this in the not-too-distant future are admittedly still great and are directly linked to our fundamental scientific knowledge. Some of those challenges are outlined in this article. The dual roles of models as tools for both understanding and prediction are inseparable and PARADIGM has approached its objectives with that realization firmly in mind.

CONCLUDING REMARKS

Contemporary modeling approaches are pointing towards ever more complexity in ecosystem models, with specific applications ultimately determining just how much complexity is enough. But the complexity of nature does not necessarily demand simply adding more compartments and/or processes; there are important new fundamental developments (e.g., incorporating evolutionary rules, genome-based model structuring, and models that represent emergent behavior) that we have highlighted above that hold significant promise. Extending our contemporary models in these directions will be increasingly guided by new approaches to developing model-data fusion systems (e.g., the direct merging of optical data), with all of this pointing towards the ultimate goal of implementing reliable marine ecological forecast systems that, for certain time scales, will be run in operational mode. These efforts are significant and will clearly require a community effort, with PARADIGM and other groups needing to designate their data and model codes as "open-source" resources.

Modeling challenges drive PARADIGM. However, we conclude by highlighting a major challenge that has been with our community from the beginning of our science—we are and likely always will be "data challenged." With vital societal issues at play, such as the role of the marine ecosystem in regulating the exchange of CO_2 with the atmosphere on multiple temporal and spatial scales, we need now, more than ever, to bring significant resources to bear for designing an *interdisciplinary* observational network (e.g., Doney and Hood, 2002) that is up to the task of providing dependable data directly to the models for this and other "grand challenge" type issues. As well, models have an important role to play *a priori* in helping to define the essential locations and scales of ecosystem variability, and thus are a central tool for designing the observational network. The ever-closer synergy between observations and models is the future.

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REFERENCES

Arrigo, K.R. 2005. Marine microorganisms and global nutrient cycles. *Nature (London)* 437:349–355.

Behrenfeld, M.J., E. Boss, D.A. Siegel, and D.M. Shea. 2005. Carbon-based ocean productivity and phytoplankton physiology from space. *Global Biogeochemical Cycles* 19(1):B1006+ doi: 10.1029/2004GB002299.

Bidigare, R.R., R.C. Smith, K.S. Baker, and J. Marra. 1987. Oceanic primary production estimates from measurements of spectral irradiance and pigment concentrations. *Global Biogeochemical Cycles* 1:171–186.

Bissett, W.P., O. Schofield, S. Glenn, J.J. Cullen, W.L. Miller, A.J. Plueddemann, and C.D. Mobley. 2001. Resolving the impacts and feedback of ocean optics on upper ocean ecology. *Oceanography* 14:30–53.

Capone D.G., J. Zehr, H. Paerl, B. Bergman, and E.J. Carpenter. 1997. Trichodesmium: A globally significant marine cyanobacterium. *Science* 276:1,221–1,229.

Church, M.J., E.F. DeLong, H.W. Ducklow, M.B. Karner, C.M. Preston, and D.M. Karl. 2003. Abundance and distribution of planktonic Archaea and Bacteria in the waters west of the Antarctic Peninsula. *Limnology and Oceanography* 48:1,893–1,902.

Cullen, J.J., P.J.S. Franks, D.M. Karl, and A. Longhurst. 2002. Physical influences on marine ecosystem dynamics. In: *The Sea: Biological-Physical Interactions in the Ocean*, A.R. Robinson, J.J. McCarthy and B.J. Rothschild, eds. John Wiley and Sons, Hoboken, NJ, 297–335.

Daniels, R.M., H.W. Ducklow, and T.L. Richardson. Accepted. Food web structure and biogeochemical processes during oceanic phytoplankton blooms: An inverse model analysis. *Deep-Sea Research II*.

DeLong, E.F. and D.M. Karl. 2005. Genomic perspectives in microbial oceanography. *Nature* 437(7057):336–342.

Denman, K.L. 2003. Modelling planktonic ecosystems: Parameterizing complexity. *Progress in Oceanography* 57:429–452.

Denman, K.L., C. Voelker, M.A. Peña, and R. Rivkin. In press. Modelling the ecosystem response to iron fertilization in the subarctic NE Pacific: The influence of grazing, and Si and N cycling on CO_2 drawdown. *Deep-Sea Research II*.

Dickey, T. 2003. Emerging ocean observations for interdisciplinary data assimilation. *Journal of Maine Syst*ems 40–41:5–48.

Doney, S.C. 1999. Major challenges confronting marine biogeochemical modeling. *Global Biogeochemical Cycles* 13:705–714.

Doney, S.C., I. Lima, K. Lindsay, J.K. Moore, S. Dutkiewicz, M.A.M. Friedrichs, and R.J. Matear. 2001. Marine biogeochemical modeling. *Oceanography* 14(4):93–107.

Doney, S.C. and M. Hood. 2002. A Global Ocean Carbon Observation System, A Background Report, Global Ocean Observing System Report No. 118, UNESCO Intergovernmental Oceanographic Commission IOC/INF-1173, 55pp.

Doney, S.C., M.R. Abbott, J.J. Cullen, D.M. Karl, and L. Rothstein. 2004. From genes to ecosystems: The ocean's new frontier. *Frontiers In Ecology And The Environment* 2(9):457–466.

Ducklow, H.W., M.J.R. Fasham, and A.F. Vézina. 1989. Derivation and Analysis of flow networks for oceanic plankton systems. In: *Network Analysis in Marine Ecology*. F. Wulff, J.G. Field, and K.H. Mann, eds. Springer-Verlag, Berlin, 159–205.

Falkowski, P.G. 1997. Evolution of the nitrogen cycle and its influence on the biological sequestration of CO_2 in the ocean. *Nature* 387:272–275.

Fasham, M.J.R. 1984. Flows of Energy and Materials. In: *Marine Ecosystems: Theory And Practice.* Plenum Press, New York, 733pp.

Fasham, M.J.R., H.W. Ducklow, and S.M. McKelvie. 1990. A nitrogen-based model of plankton dynamics in the oceanic mixed layer. *Journal of Marine Research* 48:591–639.

Fasham, M.J.R., and G.T. Evans. 1995. The use of optimization techniques to model marine ecosystem dynamics at the JGOFS station at 470N 200W. *Transactions of the Royal Society of London, Ser. B,* 348:203–209.

Feely, R.A., C.L. Sabine, K. Lee, W. Berelson, J. Kleypas, V.J. Fabry, and F.J. Millero. 2004. Impact of anthropogenic CO_2 on the $CaCO_3$ system in the oceans. *Science* 305(5682):362–366.

Fennel, K., Y.H. Spitz, R.M. Letelier, M.R. Abbott, and D.M. Karl. 2002. A deterministic model for N_2 fixation at stn. ALOHA in the subtropical North Pacific Ocean. *Deep-Sea Research II* 49:149–174.

Fennel, K., J. Wilkin, J. Levin, J. Moisan, J. O'Reilly, and D. Haidvogel. Accepted. Nitrogen cycling in the Mid-Atlantic Bight and implications for the North Atlantic nitrogen budget: Results from a three-dimensional model. *Global Biogeochemical Cycles*.

Ferris, M.J., and B. Palenik. 1998. Niche adaptation in ocean cyanobacteria. *Nature* 396:26–228.

Follows, M.J., S. Grant, S. Dutkiewicz, and S.W. Chisholm. In preparation. Modeling the selection of *Prochlorococcus* ecotypes in the Atlantic.

Francis, C.A., K.J. Roberts, J.M. Beman, A.E. Santoro, and B.B. Oakley. 2005. Ubiquity and diversity of ammonia-oxidizing archaea in water columns and sediments of the ocean. *Proceedings of the National Academy of Sciences* 102:14,683–14,688.

Friedrichs, M.A.M., R.R. Hood, and J.D. Wiggert. Accepted. Ecosystem model comparison in the Arabian Sea: A prototype regional modeling testbed. *Deep-Sea Res. II*, 3rd Special Issue on the U.S. JGOFS Synthesis and Modeling Project.

Giovannoni, S.J. and U. Stingl. 2005. Molecular diversity and ecology of microbial plankton. *Nature* 437(7057):343.

Giovannoni, S.J., H.J. Tripp, S. Givan, M. Podar, K.L. Vergin, D. Baptista, L. Bibbs, J. Eads, T.H. Ricardson, M. Noordewier, M.S. Rappe, J.M. Short, J.C. Carrington, and E.J. Mathur. 2005a. Genome streamling in a cosmopolitan oceanic bacterium. *Science* 309:1,242–1,245.

Giovannoni, S.J., L. Bibbs, J.-C. Cho, M.D. Stapels, R. Desiderio, K.L. Vergin, M.S. Rappe, S. Laney, L.J. Wilhelm, H.J. Tripp, R.J. Mathur, and D.F. Barofsky. 2005b. Proteorhodopsin in the ubiquitous marine bacterium SAR11. *Nature* 438:82–85.

Hamm, C.E., R. Merkel, O. Springer, P. Jurkojc, C. Maier, K. Prechtel, and V. Smetacek. 2003. Architecture and material properties of diatom shells provide effective mechanical protection. *Nature* 421:841–843.

Hansell, D.A., N.R. Bates, and D.B. Olson. 2004. Excess nitrate and nitrogen fixation in the North Atlantic Ocean. *Marine Chemistry* 84:243–265.

Harmon, R. and P. Challenor. 1996. A Markov chain Monte Carlo method for estimation and assimilation into models. *Ecological Modelling* 101:41–59.

Hood, R.R., V.J. Coles, and D.G. Capone. 2004. Modeling the distribution of *Trichodesmium* and nitrogen fixation in the Atlantic Ocean. *Journal of Geophysical Research* 109:C06006, doi:10.1029/2002JC001753.

Hood, R.R., E.A. Laws, R. Armstrong, N. Bates, C.W. Brown, C. Carlson, F. Chai, S. Doney, P. Falkowski, R.A. Feely, M. Friedrichs, M. Landry, J.K. Moore, D. Nelson, T. Richardson, B. Salihoglu, M. Schartau, D. Toole, and J.D. Wiggert. Accepted. Functional group modeling: progress, challenges and prospects. *Deep-Sea Res. II*, 3rd Special Issue on the U.S. JGOFS Synthesis and Modeling Project.

Jackson, G.A. and P.M. Eldridge. 1992. Food web analysis of a planktonic system off Southern California. *Progress in Oceanography* 30:223–251.

Jenkins, W.J. and J.C. Goldman. 1985. Seasonal oxygen cycling and primary production in the Sargasso Sea. *Journal of Marine Research* 43:465–491.

Johnson, Z.I., E.R. Zinser, A. Coe, N.P. McNulty, E. Malcolm, S. Woodward and S.W. Chisholm. In press. Niche Partitioning among *Prochlorococcus* ecotypes along ocean-scale environmental gradients. *Science.*

Karl, D., R. Letelier, L. Tupas, J. Dore, J. Christian, and D. Hebel. 1997. The role of nitrogen fixation in biogeochemical cycling in the subtropical North Pacific Ocean. *Nature* 388:533–538.

Karl, D.M. 2002. Hidden in a sea of microbes. *Nature* 415:590–591.

Karner, M.B., E.F. DeLong, and D.M. Karl. 2001. Archaeal dominance in the mesopelagic zone of the Pacific Ocean. *Nature* 409:507–510.

Klausmeier, C.A., E. Litchman, T. Daufresne, and S.A. Levin. 2004. Optimal nitrogen-to-phosphorus stoichiometry of phytoplankton. *Nature* 429:171–174.

Knap, A., A. Michaels, A. Close, H. Ducklow, and A. Dickson. 1994. Protocols for the Joint Global Ocean Flux Study (JGOFS) Core Measurements. JGOFS Report No. 19, vi+170 pp. Reprint of the IOC Manuals and Guides No. 29. UNESCO, IOC, Paris.

Könneke, M., A.E. Bernhard, J.R. de la Torre, C.B. Walker, J.B.Waterbury, and D.A. Stahl. 2005. Isolation of an autotrophic ammonium-oxidizing marine archeon. *Nature* 437:543–546.

Laws, E.A., P.G. Falkowski, W.O. Smith, Jr., H. Ducklow, and J.J. McCarthy. 2000. Temperature effects on export production in the open ocean. *Global Biogeochemical Cycles* 14:1,231–1,246.

Lawson, L.M., Y.H. Spitz, E.E. Hofmann, and R.B. Long. 1995. A data assimilation technique applied to a predator-prey model. *Bulletin of Mathematical Biology* 57(4):593–617.

Lee, Z.P., K.L. Carder, J. Marra, R.G. Steward, and M.J. Perry. 1996. Estimating primary production at depth from remote sensing. *Applied Optics* 35(3):463–474.

Legendre, L. and F. Rassoulzadegan. 1996. Food-web mediated export of biogenic carbon in oceans: Hydrodynamic control. *Marine Ecology Progress Series* 145:179–193.

Leontief, W. 1966. *Input-Output Economics*. Oxford

University Press, New York, 257 pp.

Letelier, R.M. and D.M. Karl. 1996. Role of *Trichodesmium* spp. in the productivity of the subtropical North Pacific Ocean. *Marine Ecology Progress Series* 133(1–3):263–273.

Letelier, R.M., M.R. Abbott, and D.M. Karl. 1997. Chlorophyll natural fluorescence response to upwelling events in the Southern Ocean. *Geophysical Research Letters* 24:409–412.

Levy, M., L. Memery, and G. Madec. 1998. The onset of a bloom after deep winter convection in the northwestern Mediterranean Sea: Mesoscale process study with a primitive equation model. *Journal of Marine Systems* 16:7– 21.

Levy, M., L. Memery, and G. Madec. 1999. The onset of the spring bloom in the MEDOC area: Mesoscale spatial variability. *Deep Sea Research I* 46:1,137–1,160.

Marshall, D. 1997. Subduction of water masses in an eddying ocean. *Journal of Marine Research* 55:201– 222.

Matear, R.J. 1995. Parameter optimization and analysis of ecosystem models using simulated annealing: A case study at Station P. *Journal of Marine Research* 53:571– 607.

Mazzocchi, M.G. and G.A. Paffenhöfer. 1999. Swimming and feeding behaviour of the planktonic copepod *Clausocalanus furcatus*. *Journal of Plankton Research* 21(8):18.

McGillicuddy, D.J., A.R. Robinson, D.A. Siegel, H.W. Jannasch, R. Johnson, T.D. Dickey, J. McNeil, A.F. Michaels, and A.H. Knap. 1998. Influence of mesoscale eddies on new production in the Sargasso Sea. *Nature* 394:263–265.

McGillicuddy, D.J., L.A. Anderson, S.C. Doney, and M.E. Maltrud. 2003. Eddy-driven sources and sinks of nutrients in the upper ocean: Results from a 0.1 degree resolution model of the North Atlantic. *Global Biogeochemical Cycles* 17(2):1035, doi:10.1029/2002GB001987.

Moisan, J.R., E.E. Hofmann, and D.B. Haidvogel. 1996. Modeling nutrient and plankton processes in the California coastal transition zone 2 —A three-dimensional physical-bio-optical model. *Journal of Geophysical Research* 101:22,677–22,691.

Moloney, C.L. and J.G. Field. 1991. The size-based dynamics of plankton foodwebs. II. Simulations of three contrasting southern Benguela foodwebs. *Journal of Plankton Research* 13:1,039-1,092.

Montoya, J.P.C. M. Holl, J.P. Zehr, A. Hansen, T.A. Villareal, and D.G. Capone. 2004. High rates of N_2 fixation by unicellular diazotrophs in the oligotrophic Pacific Ocean. *Nature* 430:1027–1032.

Moore, L.R., A.F. Post, G. Rocap, and S.W. Chisholm. 2002a. Utilization of different nitrogen sources by the marine cyanobacteria *Prochlorococcus* and *Synechococcus*. *Limnology and Oceanography* 47(4):989–996.

Moore, J.K., S.C. Doney, J.C. Kleypas, D.M. Glover, and I.Y. Fung. 2002b. An intermediate complexity marine ecosystem model for the global domain *Deep-Sea Research II* 49:403–462.

Moore, J.K., S.C. Doney and K. Lindsay. 2004. Upper ocean ecosystem dynamics and iron cycling in a global 3-D model. *Global Biogeochemical Cycles* 18(4):GB4028, 10.1029/2004GB002220.

Niquil, N., G.A. Jackson, L. Legendre, and B. Delesalle. 1998. Inverse model analysis of the planktonic food web of Takapoto Atoll (French Polynesia). *Marine Ecology Progress Series* 165:17–29.

NMFS. 1999. Ecosystem-based fisheries management: A report to Congress by the Ecosystem Principles Advisory Panel. U.S. Department of Commerce, National Oceanic and Atmospheric Administration, National Marine Fisheries Service, Silver Spring, MD, 54 pp.

Paffenhöfer, G.A. 1998. On the relation of structure, perception and activity in marine planktonic copepods. *Journal of Marine Systems* 15(1–4):457–473.

Paffenhöfer, G.A. and M.G. Mazzocchi. 2002. On some aspects of the behaviour of *Oithona plumifera* (Copepoda: Cyclopoida). *Journal of Plankton Research* 24(2):7.

Paffenhöfer, G.A., M. Tzeng, R. Hristov, C.L. Smith, and M.G. Mazzocchi. 2003. Abundance and distribution of nanoplankton in the epipelagic subtropical/tropical open Atlantic Ocean. *Journal of Plankton Research* 25(12):1,535–1,549.

Parker, R.L. 1977. Understanding inverse theory. *Annual Review of Earth and Planetary Sciences* 5:35–64.

Peinert, R., B. v. Bodungen, and V.S. Smetacek. 1989. Food web structure and loss rate. In: *Productivity of the Ocean: Present and Past*, W.H. Berger, V.S. Smetacek, and G. Wefer, eds. John Wiley & Sons, Hoboken, NJ, 35–48.

Redfield, A.C., B.H. Ketchum, and F.A. Richards. 1963. The influence of organisms on the composition of sea-water. In: *The Seas*, 2, N.H. Hill, ed. Wiley-Interscience, New York, 26–77.

Richardson, T.L., G.A. Jackson, H.W. Ducklow and M.R. Roman. 2004. Carbon fluxes through food webs of the eastern equatorial Pacific: an inverse approach. *Deep-Sea Research I* 51:1,245–1,274.

Richman, J.G., R.N. Miller, and Y.H. Spitz. 2005. Error estimates for assimilation of satellite SST data in ocean climate models. *Geophysical Research Letters* 32(18), L1860810.1029/2005GL023591.

Riley, G.A. 1946. Factors controlling phytoplankton populations on Georges Bank. *Journal of Marine Research* 6:54–73.

Ryther, J.H. and C.S. Yentsch. 1957. The estimation of phytoplankton production in the ocean from chlorophyll and light data. *Limnology and Oceanography* 2:281–286.

Seitzinger, S.P. and A.E. Giblin. 1996. Estimating denitrification in North Atlantic continental shelf sediments. *Biogeochemistry* 35:235–260.

Shulenberger, E. and J.L. Reid. 1981. The Pacific shallow oxygen maximum, deep chlorophyll maximum, and primary productivity, reconsidered. *Deep-Sea Research* 28A:901–919.

Siegel, D.A., S. Maritorena, N.B. Nelson, M.J. Behrenfeld, and C.R. McClain. 2005. Color dissolved organic matter and its influence on satellite-based characterization of the ocean biosphere. *Geophysical Research Letters* 32(L20605), doi:10.1029/2005GL024310.

Smetacek, V., P. Assmy, and J. Henjes. 2004. The role of grazing in structuring Southern Ocean pelagic ecosystems and biogeochemical cycles. *Antarctic Science* 16(4):541–558.

Sosik, H.M. In press. Characterizing seawater constituents from optical properties. In: *Real-time Observation Systems for Ecosystem Dynamics and Harmful Algal Blooms*, M. Babin, C.S. Roesler and J.J. Cullen, eds. UNESCO, IOC, Paris.

Spitz, Y.H., J.R. Moisan, and M.R. Abbott. 2001. Configuring an ecosystem model using data from the Bermuda-Atlantic Time Series (BATS). *Deep-Sea Research II* 48:1,733–1,768.

Steele, J.H., and E.W. Henderson. 1992. The role of predation in plankton models. *Journal of Plankton Research* 14:157–172.

Svensen, C. and T. Kiørboe. 2000. Remote prey detection in Oithona similis: Hydromechanical versus chemical cues. *Journal of Plankton Research* 22(6):1,155–1,166.

Tilman, D. 1977. Resource competition between planktonic algae: An experimental and theoretical approach. *Ecology* 58:338–348.

Tozzi, S., O. Schofield, and P. Falkowski. 2004. Historical climate change and ocean turbulence as selective agents for two key phytoplankton functional groups. *Marine Ecology Progress Series* 274:123–132.

Ulanowicz, R.E. 1986. *Growth and Development: Ecosystems Phenomenology*. Springer-Verlag, New York.

Venter, J.C., K. Remington, J.F. Heidelberg, A.L. Halpern, D. Rusch, J.A. Eisen, D.Y. Wu, I. Paulsen, K.E. Nelson, W. Nelson, D.E. Fouts, S. Levy, A.H. Knap, M.W. Lomas, K. Nealson, O. White, J. Peterson, J. Hoffman, R. Parsons, H. Baden-Tillson, C. Pfannkoch, Y.H. Rogers, and H.O. Smith. 2004. Environmental genome shotgun sequencing of the Sargasso Sea. *Science* 304(5667):66–74.

Vézina, A.F. and T. Platt. 1988. Food web dynamics in the ocean: I. Best-estimates of flow networks using inverse methods. *Marine Ecology Progress Series* 42:269–287.

Wiggert, J.D., A.G.E. Haskell, G.-A. Paffenhöfer, E.E. Hofmann, and J.M. Klinck. 2005. The role of feeding behavior in sustaining copepod populations in the tropical ocean. *Journal of Plankton Research* 27:1,013–1,032.

Wunsch, C. 1978. The North Atlantic general circulation west of 50°W determined by inverse methods. *Reviews of Geophysics and Space Physics* 16:583–620.

Zehr, J.P., J.B. Waterbury, P.J. Turner, J.P. Montoya, E. Omoregie, G.F. Steward, A. Hansen, and D.M. Karl. 2001. Unicellular cyanobacteria fix N_2 in the subtropical North Pacific Ocean. *Nature* 412:635–638.