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K Fennel

M Gehlen

P Brasseur

CW Brown

C Ciavatta

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Authors
K Fennel, M Gehlen, P Brasseur, CW Brown, C Ciavatta, G Cossarini, A Crise, CA Edwards, D Ford, MAM Friedrichs, and et al

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frontiers in Marine Science

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Advancing Marine Biogeochemical and Ecosystem Reanalyses and Forecasts as Tools for Monitoring and Managing Ecosystem Health

Katja Fennel[1]*, Marion Gehlen[2], Pierre Brasseur[3], Christopher W. Brown[4], Stefano Ciavatta[5], Gianpiero Cossarini[6], Alessandro Crise[6], Christopher A. Edwards[7], David Ford[8], Marjorie A. M. Friedrichs[9], Marilaure Gregoire[10], Emlyn Jones[11], Hae-Cheol Kim[4,12], Julien Lamouroux[13], Raghu Murtugudde[14], Coralie Perruche[13] and the GODAE OceanView Marine Ecosystem Analysis and Prediction Task Team

[1] Department of Oceanography, Dalhousie University, Halifax, NS, Canada, [2] UMR8212 Laboratoire des Sciences du Climat et de l'Environnement (LSCE), Gif-sur-Yvette, France, [3] Université Grenoble Alpes, CNRS, IRD, Grenoble INP, IGE, Grenoble, France, [4] National Oceanic and Atmospheric Administration (NOAA), College Park, MD, United States, [5] National Centre for Earth Observation, Plymouth Marine Laboratory, Plymouth, United Kingdom, [6] Istituto Nazionale di Oceanografia e di Geofisica Sperimentale (OGS), Trieste, Italy, [7] Ocean Sciences Department, University of California, Santa Cruz, Santa Cruz, CA, United States, [8] Met Office, Exeter, United Kingdom, [9] Virginia Institute of Marine Science, William & Mary, Gloucester Point, VA, United States, [10] MAST-FOCUS, Department of Astrophysics, Geophysics and Oceanography, Liége University, Liége, Belgium, [11] Commonwealth Scientific and Industrial Research Organisation (CSIRO), Hobart, TAS, Australia, [12] I.M. Systems Group, Inc., Rockville, MD, United States, [13] Mercator Océan, Ramonville-Saint-Agne, France, [14] Department of Atmospheric and Oceanic Science, University of Maryland, College Park, MD, United States

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Sanae Chiba, Japan Agency for Marine-Earth Science and Technology, Japan

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John Patrick Dunne, Geophysical Fluid Dynamics Laboratory (GFDL), United States
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***Correspondence:**
Katja Fennel
katja.fennel@dal.ca

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Ocean ecosystems are subject to a multitude of stressors, including changes in ocean physics and biogeochemistry, and direct anthropogenic influences. Implementation of protective and adaptive measures for ocean ecosystems requires a combination of ocean observations with analysis and prediction tools. These can guide assessments of the current state of ocean ecosystems, elucidate ongoing trends and shifts, and anticipate impacts of climate change and management policies. Analysis and prediction tools are defined here as ocean circulation models that are coupled to biogeochemical or ecological models. The range of potential applications for these systems is broad, ranging from reanalyses for the assessment of past and current states, and short-term and seasonal forecasts, to scenario simulations including climate change projections. The objectives of this article are to illustrate current capabilities with regard to the three types of applications, and to discuss the challenges and opportunities. Representative examples of global and regional systems are described with particular emphasis on those in operational or pre-operational use. With regard to the benefits and challenges, similar considerations apply to biogeochemical and ecological prediction systems as do to physical systems. However, at present there are at least two major differences: (1) biogeochemical observation streams are much sparser than physical streams presenting a significant hinderance, and (2) biogeochemical and ecological models are largely unconstrained because of insufficient observations. Expansion of biogeochemical and ecological observation systems will allow for significant advances in the development and application of analysis and prediction tools for ocean biogeochemistry and ecosystems, with multiple societal benefits.

Keywords: biogeochemical model, ecological model, forecasting, reanalysis, climate projection, scenario

INTRODUCTION

Ocean warming, acidification, deoxygenation and eutrophication are manifesting on global (Bopp et al., 2013; Jickells et al., 2017; Schmidtko et al., 2017) and regional scales (Breitburg et al., 2018; Claret et al., 2018; Irby et al., 2018; Laurent et al., 2018; Fennel and Testa, 2019). These profound changes in ocean physics and biogeochemistry in combination with the ever more efficient harvesting of living marine resources are driving major shifts in marine ecosystems (Cheung et al., 2010; Bianucci et al., 2016; Brennan et al., 2016; Galbraith et al., 2017) with significant societal impacts. Changes in ocean biogeochemistry and ecosystems will also complicate conservation efforts for endangered species but are rarely considered in species recovery planning (e.g., Hartman et al., 2014). Strategies for mitigation, adaptation and protection, ranging from nutrient management in watersheds, fisheries management and Marine Protected Areas, to emission reductions of CO_2 and other greenhouse gases, have to be designed, continuously assessed and revised. This process requires adequate observation of ongoing changes, combined with skillful analysis and prediction tools that provide decision makers and the public with the necessary information to assess the impact of policy decisions.

In this context, the term "analysis and prediction tool" refers to model systems that include realistic representations of ocean circulation coupled with biogeochemical or ecological models. The biogeochemical/ecological model components have a broad range of complexities from simple parameterizations, to fully explicit representations of multiple nutrients and functional groups and serve three major purposes: (1) hindcasts or reanalyses for assessment of past and current states and trends of the system, (2) forecasts ranging from short-term (days to weeks) to seasonal (months) time windows, and (3) scenario simulations including climate change projections and nutrient reduction scenarios. While operational systems are sometimes narrowly defined as only those providing short-term forecasts, we adopt a broader definition here that encompasses the provision of hindcasts and reanalyses, short-term/seasonal forecasts, and scenarios/projections.

Building on the recent review by Gehlen et al. (2015), this article focuses on the current state and future prospect of analysis and prediction tools for ocean biogeochemistry and ecosystems. While the necessity of a tight integration of these tools with observations cannot be overstated, we focus here on the tools themselves. Overviews of the necessary observing system components are given by Roemmich et al. (unpublished) and others in this issue.

CURRENT STATUS

With the goal of illustrating the current status and breadth of ecological/biogeochemical analysis and prediction systems we present a selective overview of global and regional systems. First, we briefly describe two global forecasting systems with biogeochemistry that operate in pre-operational or operational mode to produce short-term forecasts, reanalyses and climate projections (also see Gehlen et al., 2015). We then provide examples of regional analysis and prediction systems (also see **Table 1**). All produce estimates of the biogeochemical ocean state to benefit economic, environmental and public safety needs with users in academia, government, private companies and the general public.

Global Applications

NEMO-HadOCC and NEMO-MEDUSA

The United Kingdom Met Office runs an operational global physical forecasting system referred to as FOAM (Blockley et al., 2014) which is based on the NEMO hydrodynamic model (Madec, 2008), and assimilates satellite and *in situ* data using the 3D-Var NEMOVAR scheme (Waters et al., 2015). FOAM is coupled pre-operationally to two biogeochemical components: HadOCC by Palmer and Totterdell (2001) and MEDUSA by Yool et al. (2013), for reanalyses and Ocean Observing System Simulation Experiments (OSSEs). NEMO-MEDUSA is also used for climate projections as part of the UKESM1 climate model (Kwiatkowski et al., 2014).

FOAM-HadOCC and FOAM-MEDUSA are assimilating satellite chlorophyll using 3D-Var to produce an update of surface $\log_{10}$(chlorophyll), and then calculating multivariate increments for other biogeochemical variables using the balancing scheme of Hemmings et al. (2008). This computationally efficient way to perform multivariate updates has been applied for pre-operational forecasting (Ford et al., 2012) and reanalysis (Ford and Barciela, 2017). A similar approach has also been used to assimilate *in situ* pCO_2 observations into FOAM-HadOCC, by first calculating a surface pCO_2 analysis, and then multivariate balances to DIC and alkalinity (While et al., 2012). Despite the sparse observations, the assimilation produces long-lasting corrections to the model.

FOAM-MEDUSA has the capability to assimilate profiles of chlorophyll, nitrate, oxygen, and pH using 3D-Var (Wood et al., 2018). OSSEs with this coupled system have shown the positive impacts of a BGC-Argo array (Johnson and Claustre, 2016) on model results (Wood et al., 2018).

NEMO-PISCES

Mercator Ocean operationally runs a global physical NEMO model for short-term forecasts and reanalyses. The biogeochemical model PISCES (Aumont et al., 2015) is operated offline in a coarsened 1/4° version of the 1/12° operational NEMO system (Lellouche et al., 2018) for weekly analyses and delivers daily/monthly means and 10-day forecasts.

Operational assimilation of satellite chlorophyll using a SEEK filter (Lellouche et al., 2013) is being implemented with the goal of constraining simulated large-scale structures including chlorophyll amplitudes, extension of oligotrophic gyres, and large-scale blooms. The multivariate scheme is able to provide surface corrections of simulated phytoplankton groups and nutrient concentrations, which are then projected vertically throughout the mixed layer.

NEMO-PISCES is also used for climate projections (Séférian et al., 2012; Bopp et al., 2013) contributing to IPCC assessments. In retrospective forecasts, the multi-year predictability of ocean

TABLE 1 | Examples of analysis and prediction tools for ocean biogeochemistry and ecosystems.

Model acronym, reference	Region[1]	Mode[2]	Product class[3]	Type of DA (if any)	Data used for DA	Data used validation	Link to products
NEMO-PISCES[a]	Global	O, PO, RD	P, R, S	NA	No assimilation of biogeochemical data	Ocean color; *In situ* nutrients, chlorophyll, oxygen, pCO_2, pH	marine.copernicus.eu
NEMO-ERSEM[b]	NWS	O, PO	P, R, S	3D-Var	Ocean color total chlorophyll and PFT chlorophyll; DA for spectral PFT absorption and glider and float data is under development	Ocean color; *In situ* nutrients, chlorophyll, oxygen, fCO_2, pH	marine.copernicus.eu
POLCOMS-ERSEM[c]	NWS	RD	R	EnKF	Ocean color: total chlorophyll; PFT chlorophyll; spectral diffuse light attenuation coefficient	Ocean color; *In situ* nutrients, chlorophyll, oxygen, fCO_2, pH	portal.ecosystem-modelling.pml.ac.uk
ROMS-NEMURO[d]	CCS	PO, RD	P, R	4D-Var	Satellite chlorophyll, physical data	*In situ* chlorophyll, nutrients, oxygen, rates	oceanmodeling.ucsc.edu
eReefs[e]	GBR	PO, RD	R	EnKF	Spectral ocean color	Chlorophyll fluorescence from gliders, *in situ* nutrients	www.ereefs.info
ROMS-ECB[f]	CB	PO, RD	P, R	none	No assimilation of biogeochemical data	Satellite chlorophyll, *in situ* nutrients, oxygen	www.vims.edu/hypoxia; oceansmap.maracoos.org; comt.ioos.us
ROMS-DO[g]	GoMex	PO	P	none	No assimilation of biogeochemical data	*In situ* oxygen	pong.tamu.edu/tabswebsite
ROMS-Fennel[h]	GoMex	RD	R, S	none	No assimilation of biogeochemical data	Satellite chlorophyll, *in situ* nutrients, oxygen, rates, DIC, alkalinity, pCO_2	comt.ioos.us
OGSTM-BFM[i]	Med	O	R, P	3D-Var	Satellite chlorophyll; BGC-Argo chlorophyll and nitrate (in PO mode); Physical data	*In situ* chlorophyll, nutrients (N and P), oxygen, DIC and Alkalinity	marine.copernicus.eu; medeaf.inogs.it/forecast
MITgcm-BFM[k]	NAdr	PO, RD	P	none	No assimilation of biogeochemical data	*In situ* chlorophyll, nutrients (N and P) and oxygen	medeaf.inogs.it/adriatic
GHER-BAMHBI[j]	Black Sea	O	R, P	SEEK filter	Argo oxygen	Satellite chlorophyll, Argo oxygen, *in situ* nutrients	marine.copernicus.eu

[1]Regional acronyms: NWS, northwest European Shelf Seas; CCS, California Current System; GBR, Great Barrier Reef; CB, Chesapeake Bay; GoMex, Gulf of Mexico; Med, Mediterranean Sea; NAdr, Northern Adriatic Sea; [2]Mode refers to research-driven (RD), pre-operational (PO), operational (O); [3]Product class refers to reanalysis (R), prediction (P), scenarios (S); [a]Aumont et al., 2015; Lellouche et al., 2018; [b]Edwards et al., 2012; O'Dea et al., 2017; Skákala et al., 2018; [c]Ciavatta et al., 2014, 2016, 2018; [d]Song et al., 2016a,b,c; Mattern et al., 2017; [e]Baird et al., 2016, 2018; Jones et al., 2016; [f]Feng et al., 2015; Da et al., 2018; Irby et al., 2018; Irby and Friedrichs, 2019; [g]Hetland and DiMarco, 2008; Yu et al., 2015; [h]Fennel et al., 2011; Laurent et al., 2012; [i]Lazzari et al., 2016; Teruzzi et al., 2018; Cossarini et al., 2019; [j]Grégoire et al., 2008; Capet et al., 2016; [k]Cossarini et al., 2019.

productivity has been explored following decadal prediction protocols (Séférian et al., 2013). The model also has options to represent higher trophic levels of the marine food web allowing investigations of climate change impacts on the whole ecosystem (Lefort et al., 2014).

Regional Applications

Hindcasts and Short-Term Forecasts for the Northwest European Shelf Seas

The Northwest European Shelf Seas (NWS) in the northeast North Atlantic Ocean hosts productive ecosystems of significant interest to several European nations. An operational prediction system for the NWS (Edwards et al., 2012; O'Dea et al., 2017) is maintained by the United Kingdom Met Office. It is based on NEMO (Madec, 2008), and includes a biogeochemical component based on ERSEM (Blackford et al., 2004; Butenschön et al., 2016). The operational forecasting system assimilates physical data using 3D-Var NEMOVAR (King et al., 2018) and provides daily analyses and 6-day forecasts of physical and biogeochemical variables. Assimilation of satellite chlorophyll is currently used for reanalyses and will be implemented for short-term forecasting in the near-future.

Besides total chlorophyll, the system can assimilate a regional ocean-color product for phytoplankton functional types (PFTs, Skákala et al., 2018), which has been shown to improve the plankton community structure and air-sea carbon fluxes in a multi-annual reanalysis (Ciavatta et al., 2018). Developments to allow direct assimilation of ocean color spectral data (Ciavatta et al., 2014) and assimilation of glider and float observations are ongoing.

Reanalysis and Short-Term Forecasts for the Mediterranean Sea

The semi-enclosed Mediterranean Sea is of significant importance to several European, Middle-East and African nations for fisheries, tourism, etc. Decadal reanalyses and short-term predictions for the Mediterranean are produced by an operational NEMO system (Tonani et al., 2014) that is coupled off-line with an assimilative biogeochemical system (Cossarini et al., 2015; Lazzari et al., 2016; Teruzzi et al., 2018). The system uses 3D-Var data for assimilation of physical fields (Dobricic and Pinardi, 2008) and satellite chlorophyll (Teruzzi et al., 2018).

Currently, assimilation of BGC-Argo data is in pre-operational mode (Cossarini et al., 2019) and shows the positive impact of observed chlorophyll and nitrate profiles on simulated vertical phytoplankton distributions throughout the year. A decadal reanalysis with assimilation of physical variables and satellite chlorophyll has shown trends and anomalies in nutrients and air-sea CO_2 fluxes in the Mediterranean (von Schuckmann et al., 2018).

Hindcasts and Short-Term Forecasts for the California Current System

The California Current System (CCS) is a productive upwelling region encompassing waters of the eastern Pacific off the US west coast. A data-assimilative physical-biogeochemical forecast system for this region operates quasi-operationally at the University of California, Santa Cruz (Moore et al., 2013). The system uses ROMS (Shchepetkin and McWilliams, 2005; Haidvogel et al., 2008) with a horizontal resolution of 1/10° (Veneziani et al., 2009) and meteorological forcing from COAMPS (Hodur et al., 2002). A 4D-Var method (Moore et al., 2011a,b) is applied to assimilate multiple remotely sensed and *in situ* physical data.

The biogeochemical component is based on NEMURO (Kishi et al., 2007; Fiechter et al., 2014) and constrained using a lognormal form of 4D-Var (Song et al., 2012) to account for the non-Gaussian statistics of biogeochemical observations (see Song et al., 2016a,b,c; Mattern et al., 2017, for more details). Presently only satellite-derived chlorophyll is assimilated, because of its high temporal and spatial coverage.

The system has also been used to produce a 30-year reanalysis (Broquet et al., 2009; Neveu et al., 2016) enabling analyses of regional climate variability (Jacox et al., 2014, 2015, 2016; Crawford et al., 2017) and the identification of habitats for marine fisheries (Schroeder et al., 2014, 2018; Scales et al., 2017) and marine mammals (Becker et al., 2016).

Short-Term Forecasts for Australia's Great Barrier Reef System

The Great Barrier Reef off northeast Australia is a world heritage site but under pressure from agricultural runoff, coral bleaching, crown of thorns starfish outbreaks, ocean warming and acidification, and mechanical damage from tropical cyclones. The eReefs biogeochemical modeling system (Baird et al., 2016) was developed to capture key processes related to water quality including carbonate chemistry (Mongin et al., 2016), bio-optics and bleaching (Baird et al., 2018).

The eReefs system uses a 100-member Ensemble Kalman Filter to assimilate ocean color spectral bands (Jones et al., 2016). The model predicts inherent and apparent optical properties through direct simulation of 17 optically active constituents at 8 spectral bands. This allows for prediction of remote sensing reflectances of the 8 MODIS ocean-color bands and avoids representation errors by directly simulating observed quantities. A reanalysis is available from June 2013 to October 2016. Relative to the assimilation of chlorophyll, forecast errors are reduced by up to 50%, and representation of glider-derived fluorescence and *in situ* observations of nutrients, both withheld from assimilation, is improved by 45 and 20–30%, respectively.

Reanalyses, Short-Term Forecasts and Scenarios for Chesapeake Bay

Chesapeake Bay is a large, productive estuary in the United States that suffers from severe eutrophication and hypoxia. Real-time nowcasts and 2-day forecasts of temperature, salinity and oxygen are produced using the ROMS-based Estuarine, Carbon and Biogeochemistry (ECB) model (Feng et al., 2015; Da et al., 2018; Irby et al., 2018; Irby and Friedrichs, 2019). The forecast system, based in large part on earlier developments by NOAA and the University of Maryland (Brown et al., 2013), uses operationally available forcing from the North American Mesoscale Forecast System and USGS river fluxes. The system of Brown et al. (2013) also predicts the occurrence of several noxious species including jellyfish, harmful algal blooms and water-borne pathogens. While the biogeochemical variables are forecast mechanistically, the species predictions are generated using multivariate empirical habitat suitability models of the target species.

Input from stakeholder meetings has revealed that the ecological forecasts are useful to end-users whose lives and livelihoods depend on Chesapeake Bay, e.g., by guiding recreational and commercial fishermen to productive fishing grounds. The forecasts also inform the Annual Chesapeake Bay Hypoxia Report Card (https://www.vims.edu/research/topics/dead_zones/forecasts/report_card/index.php) which helps managers and the public in assessing water-quality improvements of Chesapeake Bay.

The model has also been used for reanalysis studies quantifying the impact of atmospheric nitrogen deposition (Da et al., 2018) and the uncertainties associated with hypoxia mitigation due to recent nutrient reductions (Irby and Friedrichs, 2019) and future climate change (Irby et al., 2018).

Short-Term Forecasts, Reanalyses and Scenarios of Hypoxia in the Northern Gulf of Mexico

The northern Gulf of Mexico shelf receives large inputs of freshwater and anthropogenically derived nutrients leading to the formation of a large hypoxic zone every summer. A suite of models have been developed to improve understanding of the underlying mechanisms and for operational uses ranging from short-term and seasonal predictions, seasonal and multi-year hindcasts to scenario simulations and climate change projections.

A multi-model intercomparison (Fennel et al., 2016) indicated that a skillful physical model combined with a simple oxygen model (Hetland and DiMarco, 2008; Yu et al., 2015) is sufficient for short-term predictions in this system. A ROMS-based short-term prediction system for dissolved oxygen is run pre-operationally at Texas A&M University[1]. Longer hindcast and scenario simulations use more comprehensive biogeochemical models. The physical-biogeochemical model of Fennel et al. (2011) and Laurent et al. (2012) has been used for multi-year hindcasts to inform fisheries management (Langseth et al., 2014), simulations of nutrient reduction scenarios (Fennel and Laurent, 2018), and future projections of hypoxia and pH conditions (Laurent et al., 2017, 2018). These inform the Hypoxia Taskforce, a multi-agency, multi-state entity charged with devising strategies for reduction of the hypoxic zone and monitoring progress toward this goal (Task Force, 2001).

POTENTIAL BENEFITS, CURRENT STATUS AND CHALLENGES

Ocean biogeochemical and ecological analysis and prediction systems rely on skillful models of ocean physics. Thus, many of the same considerations that apply to operational systems for ocean physics do also apply for biogeochemical and ecological applications but there are important differences.

Potential benefits of biogeochemical/ecological operational systems include (1) the generation of dynamically and internally consistent reanalyses, nowcasts and forecasts through melding of observations with a dynamical model, (2) provision of oceanographic context for observations (from event scale to long-term trends and shifting baselines), (3) estimation of system properties that are not directly observable but can be inferred from dynamical models (e.g., biogeochemical fluxes), and (4) spatial and temporal coverage not attainable by direct observation.

Currently there are only a few operational forecasting systems (i.e., systems maintained by an operational agency with strict commitment to routinely provide forecasts) that assimilate biogeochemical variables and several pre-operational systems (i.e., those run by academics or operational agencies as demonstrations but without commitments for continuous operation). Some will transition to operational mode in the near future (see Section "Current Status" and **Table 1**).

Two main challenges hinder the implementation of biogeochemical and ecological forecasting and analysis systems: data availability, and adequacy of data-assimilation methods. Obviously adequate biogeochemical and ecological observation streams are required in addition to physical ocean observations. Access to biogeochemical observations at meaningful spatial and temporal scales is still limited, especially when required in real-time or near-real time. Currently, the main biogeochemical data stream used in assimilation is satellite ocean color, but this measurement is limited to the surface ocean and provides an imperfect proxy of phytoplankton biomass that, by itself, is insufficient for constraining the multiple biogeochemically active pools in the euphotic zone. Efforts are being made to maximize the benefits of ocean color observations, e.g., by assimilating spectral bands (Baird et al., 2016, 2018; Jones et al., 2016) or satellite-derived PFTs (Xiao and Friedrichs, 2014a,b; Ciavatta et al., 2018; Skákala et al., 2018). The limited availability of observations is especially serious in coastal applications where altimetry and ocean color measurements are compromised by bathymetry and a variety of optical constituents.

Another major difference from physical ocean models is that established assimilation methods (see, e.g., Moore et al., 2019) cannot be applied to biogeochemical and ecological variables in a straightforward manner. Reasons for this include the non-Gaussian characteristics of biogeochemical observations, the strong non-linearity of biogeochemical models and the frequent lack of direct correspondence between convenient observables and model variables. Also, experience has shown that assimilation of physical observations in coupled models often does not improve but degrades the biogeochemical state. Methods for accommodating non-Gaussian distributions are being developed (Song et al., 2012). The strong non-linearity can only be addressed by broadening the suite of observed biogeochemical variables. Although the biogeochemical assimilation schemes described above are multivariate, i.e., assimilation of one variable (e.g., chlorophyll) results in updates to other variables (e.g., nutrient concentrations), the adequacy of these updates hinges on the accuracy of biogeochemical models and is not well tested. Rigorous validation of biogeochemical models and tests of their predictive skill will require increased information content in available data streams. The degradation of biogeochemical fields during physical assimilation appears to arise at least partly when physical and biogeochemical variables are updated independently in violation of property-property relationships and can be substantially reduced by accounting for their correlation (Yu et al., 2018).

In principle, schemes are available for assimilating properties other than ocean color products and data types other than surface observations (e.g., from floats and gliders), but thus far they have mostly been used in OSSE-type twin experiments where synthetic observations are used (Wood et al., 2018; Yu et al., 2018). The

[1] http://pong.tamu.edu/tabswebsite/

true test of these methods has to await better availability of biogeochemical observations.

The prospect of a global BGC-Argo array (Johnson and Claustre, 2016) holds great promise for open ocean applications by expanding the suite of observed properties and extending observations from the surface ocean into its interior (Fujii et al., this issue) but requires careful calibration and verification. BGC-Argo observations will allow for a rigorous validation of biogeochemical models and will provide much better constraints on their dynamics and vertical structure as shown by Cossarini et al. (2019) in the Mediterranean Sea model.

New observations may also elucidate previously unrecognized shortcomings in the dynamical models and prompt modifications/refinements of model structure/formulations. Our best hope for reducing models' structural uncertainty and improving their robustness and predictive skill is model development guided by an expanded observing system in concert with process studies, application of theory, and synthesis of other available information. Data assimilation is best used to correct stochastic variability in state estimates produced by structurally sound models, rather than trying to correct for biases or inappropriate model structures.

CONCLUSION

The potential benefits and scope of applications of biogeochemical/ecological analysis and prediction systems are broad. Presently, the availability of relevant observations is limited, which is a major impediment and explains why biogeochemical/ecological operational systems are still in their infancy compared to physical ocean forecasting. An expansion of ocean observing systems to include more biogeochemical/ecological parameters is crucial for expanded operational services and operational models can help in the design of expanding observing systems.

AUTHOR CONTRIBUTIONS

KF wrote the manuscript with contributions from all authors.

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