Provided for non-commercial research and education use.
Not for reproduction, distribution or commercial use.

Volume 76, issues 1–2 20 February 2009 ISSN 0924-7963

ELSEVIER

Special Issue
Skill Assessment for Coupled Biological/Physical Models of Marine Systems

edited by
Daniel R. Lynch, Dennis J. McGillicuddy, Jr. and Francisco E. Werner

JOURNAL OF
MARINE
SYSTEMS

This article appeared in a journal published by Elsevier. The attached copy is furnished to the author for internal non-commercial research and education use, including for instruction at the authors institution and sharing with colleagues.

Other uses, including reproduction and distribution, or selling or licensing copies, or posting to personal, institutional or third party websites are prohibited.

In most cases authors are permitted to post their version of the article (e.g. in Word or Tex form) to their personal website or institutional repository. Authors requiring further information regarding Elsevier's archiving and manuscript policies are encouraged to visit:

http://www.elsevier.com/copyright

Author's personal copy

Journal of Marine Systems 76 (2009) 16–33

Contents lists available at ScienceDirect

Journal of Marine Systems

journal homepage: www.elsevier.com/locate/jmarsys

Skill assessment in ocean biological data assimilation

Watson W. Gregg [a,*], Marjorie A.M. Friedrichs [b], Allan R. Robinson [c], Kenneth A. Rose [d], Reiner Schlitzer [e], Keith R. Thompson [f], Scott C. Doney [g]

[a] NASA/Goddard Space Flight Center, Global Modeling and Assimilation Office, United States
[b] Virginia Institute of Marine Science, College of William and Mary, United States
[c] Department of Earth and Planetary Sciences, Harvard University, United States
[d] Department of Oceanography and Coastal Sciences, Louisiana State University, United States
[e] Alfred Wegener Institute for Polar and Marine Research, Germany
[f] Dalhousie University, Canada
[g] Marine Chemistry and Geochemistry, Woods Hole Oceanographic Institution, United States

ARTICLE INFO

Article History:
Received 28 September 2007
Received in revised form 5 January 2008
Accepted 2 May 2008
Available online 24 May 2008

Keywords:
Data assimilation
Ocean biology models
Ocean biogeochemistry models
Skill assessment
Fisheries data assimilation
Fisheries models

ABSTRACT

There is growing recognition that rigorous skill assessment is required to understand the ability of ocean biological models to represent ocean processes and distributions. Statistical analysis of model results with observations represents the most quantitative form of skill assessment, and this principle serves as well for data assimilation models. However, skill assessment for data assimilation requires special consideration. This is because there are three sets of information in data assimilation: the free-run model, data, and the assimilation model, which uses information from both the free-run model and the data. Intercomparison of results among the three sets of information is important and useful for assessment, but is not conclusive since the three information sets are intertwined. An independent data set is necessary for an objective determination. Other useful measures of ocean biological data assimilation assessment include responses of unassimilated variables to the data assimilation, performance outside the prescribed region/time of interest, forecasting, and trend analysis. Examples of each approach from the literature are provided. A comprehensive list of ocean biological data assimilation and their applications of skill assessment, in both ecosystem/biogeochemical and fisheries efforts, is summarized.

Published by Elsevier B.V.

1. Introduction

Data assimilation is an emerging field in ocean biology. As biological in situ data sets become more extensive and satellite ocean color time series reach decadal scales, data assimilation is becoming a viable means to exploit the richness of these resources. The advantage of data assimilation over conventional numerical modeling is that it provides an improved representation of biological variables, where the errors and deficiencies of both models and data are reduced in a complementary fashion. Data typically provide highly accurate representations of natural variables, but are limited by poor coverage in time and space (Fig. 1). Numerical models can provide more complete time and space distributions of the variables of interest, but the accuracy is much lower. Data assimilation combines the strengths of each representation, providing the space/time coverage of models and the accuracy of data, and thus leading to an improved representation with lower overall errors (Fig. 1).

Skill assessment of data assimilation models in ocean biology has typically been less than comprehensive. Rigorous skill assessment is critical for understanding assimilation model performance, leading to improved methodologies and approaches. As described in Stow et al. (2009-this issue), it facilitates understanding of the relative usefulness among various models and methods, assisting monitoring agencies and policy officials in choosing the appropriate model and

---

* Corresponding author.
E-mail address: watson.gregg@nasa.gov (W.W. Gregg).

0924-7963/$ – see front matter. Published by Elsevier B.V.
doi:10.1016/j.jmarsys.2008.05.006

Author's personal copy

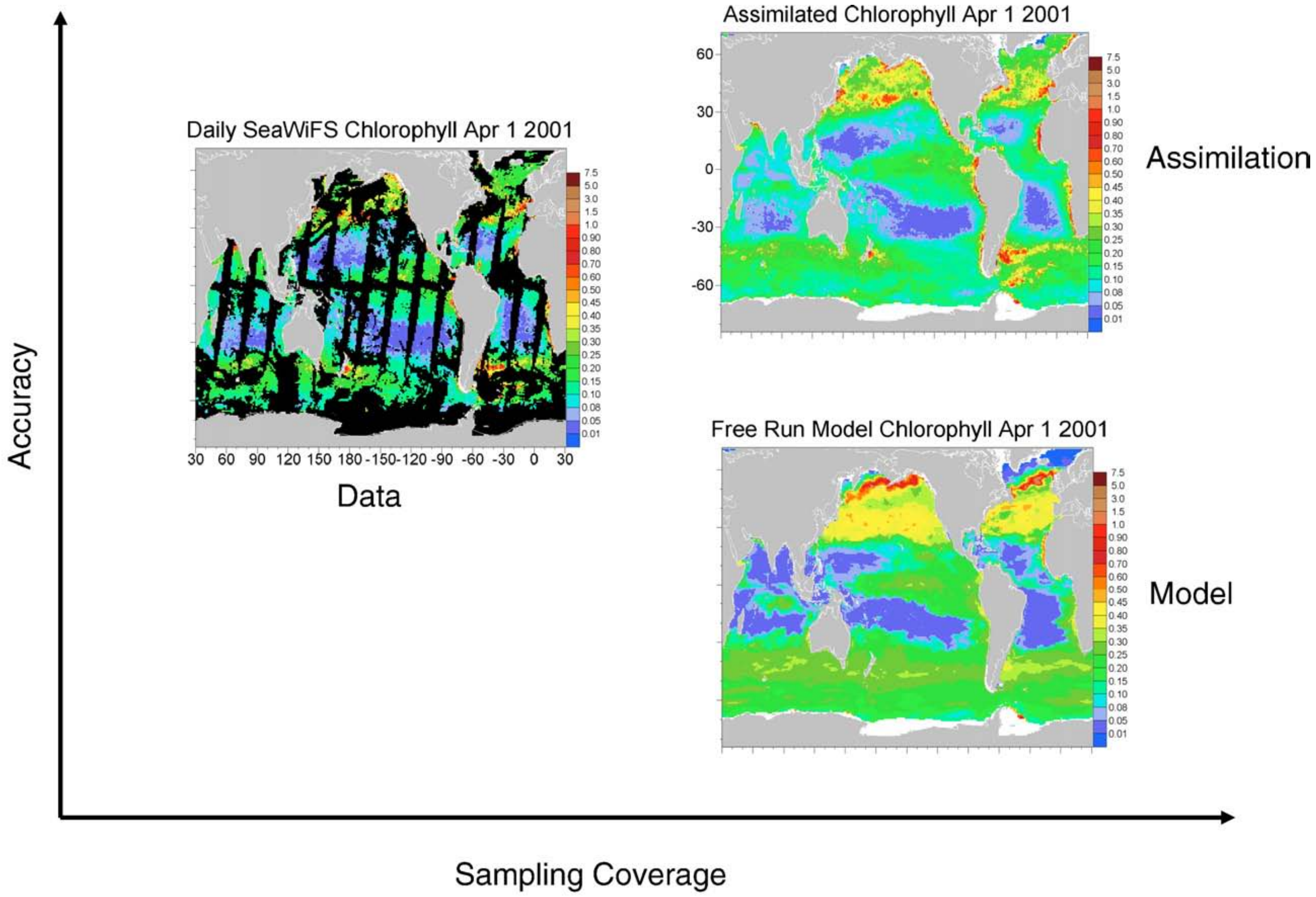

Fig. 1. Idealized representation of the relationships between data, models, and data assimilation in the context of accuracy and sampling. Based on Fig. 1 from the Introduction to this issue, from D.R Lynch, personal communication.

making the right decisions on the stewardship of natural resources.

A comprehensive, quantitative skill assessment of ocean biological data assimilation begins with the methods and approaches for conventional models, described in Stow et al. (2009-this issue). However, skill assessment for data assimilation requires special consideration. This is because there are three sets of information in data assimilation:

1) the free-run numerical model (also called reference, unconstrained, control, or unassimilated model), which integrates a set of equations forward in time to produce a representation of biological variables based on a set of parameters and processes,
2) data, or observations, and
3) the assimilation model, which uses information from both the free-run model and the data, where data are used either to modify the parameters of the free-run model, or to adjust (constrain) the outputs of the model.

This provides an opportunity to intercompare results among the three sets of information, but caution is needed because the three forms are intertwined and not independent.

In the free-run modeling approach, there are only two types of information, the free-run model and the data, and they are independent of one another. This enables use of data as an independent source of quantitative information to test the model. In the assimilation model, it is problematic to define an objective measure of skill assessment for the assimilation results, since the data needed for assessment are actually used in the assimilation.

Our purpose here is to define procedures, methods, and strategies for objective, quantitative, and comprehensive skill assessment for data assimilation in ocean biology. However, as an emerging field, it is useful here to discuss the general classes of assimilation used in ocean biology applications (Section 2) and the importance of model and data errors and how they fit into an idealized assimilation scheme (Section 3). Section 4 is a review of data assimilation efforts in the literature, encompassing ecosystem, biogeochemical, and fisheries applications, with emphasis on how skill assessment has been approached in the past. Recommended skill assessment strategies, methods, and examples are described in detail in Section 5.

2. Classes of data assimilation used in ocean biology

In contemporary ocean biology, data assimilation can be categorized by two broad classes: (1) inverse methods (Anderson et al., 2000) that minimize a cost function (defined as the sum of the weighted least square model-data differences (Schartau and

Author's personal copy

Oschlies, 2003)) and (2) sequential methods that that re-initialize the model at periodic assimilation events, typically occurring with the availability of data. The inverse methods have been used in ocean biology data assimilation mostly for parameter optimization. Re-initialization and forecast approaches using inverse methods such as 3 and 4-dimensional variational assimilation are common in meteorological applications (Kalnay, 2003) but have not found broad usage in ocean biology at the present time. Sequential methods have been used mostly for state and flux estimation in ocean biological applications. A complete description of the specific methods is beyond the scope of this paper. However, we provide a brief overview to help distinguish the types because they occasionally require different skill assessment approaches.

The practical difference between the two types, and that relates directly to the application of skill assessment, is that the data information is applied in a different sequence. In the inverse class, the data are applied in a series of activities prior to integration of the assimilation model to obtain the best set of parameter values to match the observations. The parameters are then inserted into the model and integrated forward in time just like a free-run model. This process is represented in an idealized case in Fig. 2. Skill assessment applies to the outputs of this previously optimized model integration.

In sequential data assimilation, there are no activities occurring prior to the integration of the model. Rather, the model is integrated forward in time until data are available. The model results are modified by the data, typically using statistical procedures. The model is re-initialized and integrated forward in time to the next data assimilation event. These methods are used mostly for state and flux estimation, and only rarely for parameter optimization (e.g., see Losa et al., 2003). The goal is simply to provide the best state estimate by driving model outputs toward the data through constant confrontation with data. This process is illustrated in Fig. 3. Skill assessment involves applying procedures to the outputs of the model with assimilation events incorporated in a stop-and-re-start fashion.

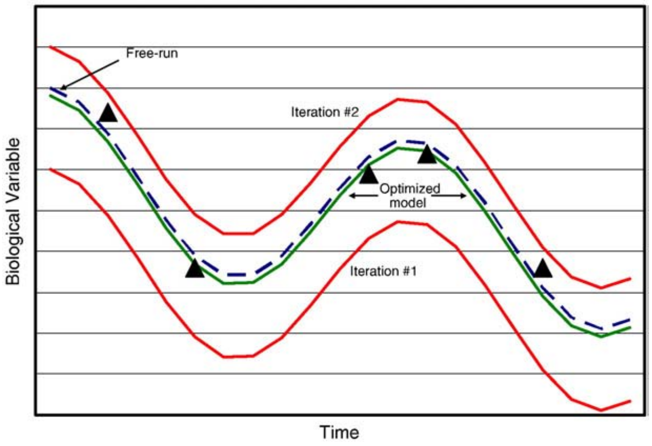

Fig. 2. Idealized representation of inverse data assimilation for parameter optimization in ocean biology. Data is represented by filled triangles, and the free-run model by the dashed blue line. In this example, two iterations of parameter optimizations (solid red lines) were tried before settling on the final optimization (solid green line), which is run forward in time and referred to as the assimilation model. Note the absence of discontinuities in the assimilation model.

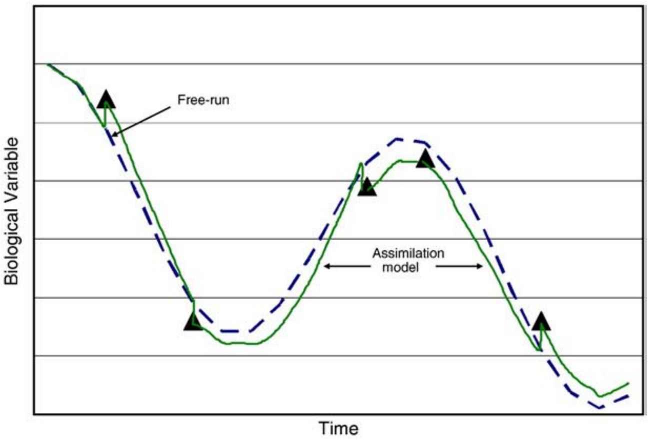

Fig. 3. Idealized representation of sequential data assimilation in ocean biology. Data is represented by filled triangles, and the free-run model by the dashed blue line. The assimilation model runs forward just as the free-run model, until data become available. Then the model integration stops while data and model are combined using (typically) statistical methods. This can result in a discontinuity when the model re-starts from this new re-initialization state.

Inverse methods for parameter optimization have historically been the most popular in ocean ecosystem data assimilation, accounting for approximately 64% of the assimilation efforts surveyed (see Table 1) but less so in fisheries (18%; Table 2). The methods are quite varied in ocean biological studies, including gradient steepest descent (Natvik et al., 2001), conjugate gradient method (Fasham et al., 1995, 1999), simulated annealing (Hurtt and Armstrong, 1996; 1999), and a micro-genetic algorithm (Schartau and Oschlies, 2003), among others, but the most widely used is the variational adjoint method (e.g., McGillicuddy et al., 1998), comprising 61% of the parameter optimization class in ecosystems and fisheries combined.

Sequential data assimilation has been used less often, but is growing in popularity since about 2000. Examples of this type of assimilation for biological oceanographic applications include direct data insertion (Ishizaka, 1990), which is probably the simplest form, nudging (Armstrong et al., 1995), optimal interpolation (Popova et al., 2002), and various implementations of the Kalman filter (Allen et al., 2002; Hoteit et al, 2003; Triantafyllou et al., 2003). Sequential data assimilation is common in fisheries applications (82%; see Table 2).

3. Model and data errors, and their relationship to assimilation methods

Central to the concept of data assimilation are errors, error estimation, and error modeling. Ocean observations have errors arising from various sources, e.g., instrumental noise, environmental noise, sampling, and the interpretation of sensor measurements. All oceanic dynamical models are imperfect, with errors arising from: the approximate explicit dynamics, parameterized sub-grid scale dynamical processes and the discretization of continuum dynamics into a computational model. Further, ocean models are forced with meteorological variables that may have their own error

Author's personal copy

characteristics. For the physical fluid dynamics of the ocean, the Navier Stokes equations provide fundamental continuum dynamics and the approximate explicit and parameterized dynamics are derived from them for scale restricted processes. There is no counterpart of the Navier Stokes equations for fundamental ocean biological dynamics, and the treatment of many biological state variables as continuum concentration density fields is not mathematically rigorous. However, the issues of approximate explicit and parameterized dynamics for scale restricted processes still apply. The very large number of variables involved in describing a realistic ocean ecosystem necessitates aggregation of some variables and neglect of other variables, with associated errors. Lack of compatibilities between models and the data, as well as between the simulated biology and the physics, are additional error sources.

In the general process of state and parameter estimation, measurement models link the state variables of the dynamical model to the sensor data. Dynamics interpolates and extrapolates the data. Dynamical linkages among state variables, reaction rates and fluxes, and parameters allow unknowns to be estimated from a subset of the state variables and rates, i.e., those more accessible to existing techniques and prevailing conditions. Error estimation and error models play a crucial role. For Gaussian errors, the data and dynamics are melded with weights inversely related to their relative errors. The final estimates should both agree with the observations within the data error bounds and satisfy the dynamical model within model error bounds. Thus the melded estimate does not degrade the reliable information of the observational data, but rather enhances that information content.

To understand the overriding importance of accurately specifying the observation and model errors in data assimilation, consider the following time-stepping model:

$$\phi_n = f_n(\phi_{n-1}, \eta_n) \tag{1}$$

where ϕ_n is a vector of state variables at time step n, f_n is a dynamical operator that carries the state forward one time step, and $\boldsymbol{\eta}_n$ is a vector of model errors.

Assume the observations at time step n are stored in the vector $\boldsymbol{y}_n$ and related to the state according to

$$\boldsymbol{y}_n = h_n(\phi_n, \boldsymbol{\varepsilon}_n) \tag{2}$$

where h_n is an observation operator that relates the state and contemporaneous observations subject to an observation error vector denoted by $\boldsymbol{\varepsilon}_n$.

Taken together, Eqs. (1) and (2) provide a very general representation of a time-stepping model and observation process. Note that the model and observation operators can be nonlinear and the errors are not necessarily additive or Gaussian. All of these features are of particular relevance when assimilating data into biogeochemical models.

To meld the information in the observations and model we must specify the statistical form of the errors. We will assume that the probability density of $\boldsymbol{\eta}_n$ has been specified and this has allowed us to obtain from Eq. (1) the conditional density of ϕ_n given ϕ_{n-1}. We will denote this conditional density by $p(\phi_n/\phi_{n-1})$. Similarly, assume the probability density of $\boldsymbol{\varepsilon}_n$ has been specified thus giving, from Eq. (2), the conditional density of $\boldsymbol{y}_n$ given ϕ_n, .i.e., $p(v_n/\phi_n)$. Routine application of Bayes' rule gives the following formula for updating the probability density of the state given all observations up to and including time step $n(Y_n)$:

$$p(\phi_n|Y_n) \propto p(y_n|\phi_n)\int p(\phi_n|\phi_{n-1})p(\phi_{n-1}|Y_{n-1})\mathrm{d}\phi_{n-1} \tag{3}$$

The conditional density $p(\phi_n/Y_n)$ contains all the information on the state given the available observations; Eq (3) shows how this conditional density can be updated sequentially as more observations become available. Eq. (3) can readily be modified to cover forecasting, and also reconstructing the state at earlier times (i.e. hindcasting).

This deceptively simple updating equation is the basis of all practical sequential data assimilation schemes including nudging, Kalman filters, and particle filters. Although Eq. (3) is not suitable for practical implementation it does highlight the critical importance of accurately specifying two types of error when assimilating data: the model and observation errors. Unrealistic specification of either error will lead to unrealistic hindcasts, nowcasts and forecasts.

To focus the discussion on the assimilation of data into biological-physical models, we will now move to a specific model defined in continuous time. Consider the 3-dimensional deterministic advective–diffusive–reactive equations for the biological state variables ϕ_i extended to include additive stochastic forcings $\mathrm{d}\eta_i$. The subscript now refers to a variable rather than time.

$$\mathrm{d}\phi_i + v\cdot\nabla\phi_i\boldsymbol{d}t - \nabla\cdot(K_i\nabla\phi_i)dt = B_i(\phi_1,\ldots,\phi_i,\ldots\phi_n)dt + d\eta_i \tag{4}$$

$$\mathrm{d}P_i = C_i(\phi_1,\ldots,\phi_i,\ldots,\phi_n)\mathrm{d}t + \mathrm{d}\zeta_i \tag{5}$$

$$y_j = H_j(\phi_i,\ldots,\phi_i,\ldots,\phi_i) + \varepsilon_j \quad (j = 1,\ldots,m) \tag{6}$$

$$\min_{\phi_i,P_i} J(\mathrm{d}\eta_i, \mathrm{d}\zeta_i, \varepsilon_j, q_\eta, q_\zeta, q_\varepsilon) \tag{7}$$

(Robinson and Lermusiaux, 2002). In Eq. (4) $\boldsymbol{v}$ is the advecting velocity, K_i is the diffusivity and B_i is the generally nonlinear biological dynamics (reaction). The model parameters (diffusivities, biological rates, etc.), $P_i=\{K_i, R_i,\ldots\}$, are also represented by an equation with additive stochastic forcings $\mathrm{d}\zeta_i$ (5), where C_i are functionals that describe the deterministic evolution of the parameters with time and space. The state variables ϕ_i are related to the data y_j via measurement models, with additive observation errors ε_j (6). The assimilation or melding criterion (7) involves, in general, the minimization of a functional J of the stochastic or error forcings $\mathrm{d}\eta_i$, $\mathrm{d}\zeta_i$, and ε_j, and of their a priori statistical properties or weights denoted by q_η, q_ζ, and q_ε (4), subject to the constraints of Eqs. (4)–(6).

The three sets of Eqs. (4)–(6) and the assimilation criterion (7) define the assimilation problem. In Eq. (5), the C_is are often assumed constant and (5) then simply states that parameters are known a priori up to a certain uncertainty $d\zeta_i$. In Eq. (6) the measurement models are denoted by H_j. These can depend, as do B_i and C_i, on the values of parameters. For example, if the parameter P_i is

Author's personal copy

measured directly then $y_i = P_i + \varepsilon_j$. Similarly, if a state variable ϕ_i is measured, (6) is simply $y_j = \phi_i + \varepsilon_j$. In Eq. (7) the functional J is often called the cost or penalty function. Using Eqs. (4) to (6) to substitute for $d\eta_i$, $d\zeta_\mathrm{i}$, and ε_j, in (7), J is expressed as a function of the state variables ϕ_i and parameters P_i, and known a priori information, the data y_i, and weights q_η, q_ζ, and q_ε. The subsequent minimization (7) subject to Eq. (4) to Eq. (6) by a chosen assimilation scheme leads to optimum estimates of ϕ_i and P_i, denoted by $\phi\ _i$ and $P\ _i$. For state estimation ($\phi\ _i$), we refer to the estimates just before and just after data assimilation as a priori and a posteriori, respectively. For parameter estimation ($P\ _i$), prior and posterior estimates refer to parameter values at the beginning and at the conclusion of the optimization. Data residuals or data-model misfits refer to the differences between the data and model estimated values of the data, $y_j - H_j(\hat{\phi}_1,\ldots,\hat{\phi}_i,\ldots,\hat{\phi}_i$. If the models or data are used as strong constraints (e.g., model structures and functionality are assumed perfect without errors), the terms $d\eta_i$, $d\zeta_\mathrm{i}$, and ε_{jj} are set to zero. If the model or data are used as weak constraints, their errors, or the probability distribution of the stochastic forcings, are specified and utilized in the assimilation criterion (7). This will usually be the case for biological models. Since assimilation calculations can be costly and time consuming, suboptimal methods that only approximately minimize the error norm are often necessary.

In accord with the above Bayesian analysis, our discussion of assimilation of data into stochastic advection–diffusion equations again brings home the importance of specifying the probability distributions of the observation and model errors. In general the attribution, representation, and propagation of errors require the careful specification of error models, and a variety of quantitative metrics for the evaluation of results and for relative weights of data and dynamics. This is a most important area of current data assimilation research. Error covariances, multivariate correlations, and probability distribution functions are all required. Determining efficient biological cost functions is important. Absolute, relative, square-root, quadratic, and likelihood cost measures have already been utilized with real biological data as well as Bayesian estimation. Many biophysical processes are multivariate and have multiscales, with strong correlations between variables and parameters. There is thus a need to investigate multivariate error covariances, by combination of data and dynamics. The direct calculation of error covariance matrices requires very large data sets which are generally costly to obtain and which generally, if available, would require excessive computational resources and computing time. Thus it is useful to model covariances with approximate structures and a few parameters after separating the errors into a bias and random uncertainty.

Data assimilation methods and schemes, the structure of dynamical, observation and error models, and observational networks and sampling strategies are all interrelated as an overall system. Accuracy, efficiency, optimality, robustness, and stability of the overall system can be achieved only by an iterative development of the system's architecture, components, linkages, and feedbacks. The assessment process for biophysical assimilation systems for various purposes will naturally involve iterative procedures.

4. Previous efforts in skill assessment of ocean biological data assimilation

4.1. Ecosystem/Biogeochemical models

Here we provide a review of data assimilation efforts in ocean ecosystems/biogeochemistry. Because our emphasis is on assessment, we only include efforts using natural observations. Twin experiments (e.g., Carmillet et al., 2001; Friedrichs, 2001), sensitivity studies (e.g., Dutkiewicz et al., 2006), and other diagnostic efforts using simulated data, while important for understanding assimilation methodological feasibility, are not included here. Table 1 lists the efforts in ocean ecosystem/biogeochemical data assimilation using observations and some of their key features, emphasizing skill assessment.

Historically, the most common form of skill assessment in ocean biological data assimilation has been graphical analysis. Most of the early work used this metric exclusively. More modern data assimilation assessment has included statistical analysis (RMS, correlation), difference fields, and Taylor diagrams (see Joliff et al., 2009-this issue). As these more comprehensive assessment methods proliferate, our ability to evaluate our data assimilation increases, leading eventually to improved data assimilation models. Here, we highlight a small number of innovative approaches used by data assimilation investigators, although an extensive list is provided in Table 1.

Ishizaka (1990) pioneered marine ecosystem data assimilation using satellite data. Using data insertion, he assimilated Coastal Zone Color Scanner (CZCS) chlorophyll into a 3D model of the southeast US coast. Immediate improvements in chlorophyll representations were observed in this multivariate assimilation, but persisted only over limited spatial domains and for short times (<2 days). Assessment involved statistical analysis (correlation and RMS with CZCS data), in addition to 2D contour maps of model and satellite chlorophyll (Table 1). Error growth after the assimilation event was tracked. These quantitative assessment methods stand out in an era near the beginning of data assimilation in ocean ecosystems.

An Ensemble Kalman filter was used in a 1D assimilation of the Cretan Sea by Allen et al. (2002). Chlorophyll and nitrate data at various depths from a buoy were assimilated separately in a pair of univariate experiments. Assimilation frequency was 2 days. Assessment involved line plots over the 200-day analysis period, involving free-run model, assimilation model, and observations. Additionally statistical analysis (RMS) of assimilated and unassimilated variables provided a quantitative estimate of the error and its growth over time.

Nerger and Gregg (2007) used the Singular Evolutive Interpolated Kalman filter to assimilate daily global satellite ocean color data. The filter was static in this application and consequently was more similar to optimal interpolation. The assimilation utilized log-transformed chlorophyll and explicit data errors were incorporated. The multi-year assimilation results were evaluated statistically using bias and RMS differences against satellite data as well as in situ data, which represented an independent data set. The assimilation results indicated lower RMS differences compared to in situ than did the satellite data in some basins, although the global assimilation RMS differences were higher. This suggested that

Author's personal copy

Table 1
Applications of ocean biogeochemical/ecological assimilation

Authors	Assimilation method	Model dimension	Location	Skill assessment
Fasham et al. (1995)	Conjugate gradient method (I)	0D	Northwest Atlantic (BATS)	*Graphical analysis*: line plot comparisons of model plankton and nutrients with observations
Matear (1995)	Simulated annealing (I)	0D	Northeast Pacific (Station P)	*Statistical analysis*: standard deviation of optimized parameters; correlation among parameters
Hurtt and Armstrong (1996)	Simulated annealing (I)	0D	Northwest Atlantic (BATS)	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations
Spitz et al. (1998)	Adjoint (I)	0D	Northwest Atlantic (BATS)	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations
Fasham et al. (1999)	Conjugate gradient method (I)	0D	Northeast Atlantic	*Graphical analysis:* line plot comparisons of assimilation model with observations
Hurtt and Armstrong (1999)	Simulated annealing (I)	0D	North Atlantic (BATS and OWSI)	*Graphical analysis*: line plot comparisons of assimilation model with observations Statistical analysis: log-likelihood of assimilation model with observations
Vallino (2000)	Adjoint (I)	0D	Arbitrary; lab data	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations
Fennel et al. (2001)	Adjoint (I)	0D	Northwest Atlantic (BATS)	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations
Schartau et al. (2001)	Adjoint (I)	0D	Northwest Atlantic (BATS)	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations. Also plots of unassimilated variable including free-run and assimilation
Spitz et al. (2001)	Adjoint (I)	0D	Northwest Atlantic (BATS)	*Graphical analysis*: line plot comparison of assimilation model with observations
Hemmings et al. (2003)	Conjugate direction set method (I)	0D	North Atlantic (30 stations)	*Graphical analysis*: maps of assimilation/observation RMS *Statistical analysis*: RMS between assimilation and observations
Losa et al. (2003)	SIR sequential importance resampling filter (S)	0D	Northwest Atlantic (BATS)	*Graphical analysis*: line plot comparisons of assimilation model with observations. Also plots of unassimilated variable vs observations
Losa et al. (2004)	Maximum data cost criterion (I)	0D	North Atlantic	*Graphical analysis*: maps of free-run and assimilation model and satellite data; line plot comparisons of free-run and assimilation models with observations of unassimilated variable
Hemmings et al. (2004)	Conjugate direction set method (I)	0D	North Atlantic (30 stations)	*Graphical analysis*: maps of assimilation/satellite observation RMS; maps of difference between assimilation and climatology *Statistical analysis*: RMS between assimilation and satellite observations; difference between assimilation and climatology
Kuroda and Kishi (2004)	Adjoint (I)	0D	Northwest Pacific	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations.
Weber et al. (2005)	Micro-genetic algorithm (I)	0D	Northwest Atlantic (BATS)	*Graphical analysis*: line plot comparisons of assimilation model with observations, including assimilated and unassimilated vaiables. Tabular representation of unassimilated variables with another study
Prunet et al. (1996a)	Adjoint (I)	1D	Northeast Pacific (Station P)	*Graphical analysis*: line plot comparisons of free-run and assimilation model with observations
Prunet et al. (1996b)	Adjoint (I)	1D	Northeast Pacific (Station P)	*Graphical analysis*: line plot comparisons of assimilation model with observations *Statistical analysis*: tabular comparison of unassimilated variable with other studies
Allen et al. (2002)	Ensemble Kalman filter (S)	1D	Cretan Sea	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations. *Statistical analysis*: RMS
Friedrichs (2002)	Adjoint (I)	1D	Equatorial Pacific	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations. *Statistical analysis*: difference between assimilation model and data for an unassimilated variable. Use of independent data set.
Hoteit et al. (2003)	Singular evolutive extended Kalman filter (S)	1D	Cretan Sea	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations. Plots of relative error (ratio) over time *Statistical analysis*: relative error (ratio)

(continued on next page)

Author's personal copy

Table 1 (*continued*)

Authors	Assimilation method	Model dimension	Location	Skill assessment
Faugeras et al. (2003)	Adjoint (I)	1D	Mediterranean Sea	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations. Tabular comparison of unassimilated variables with other efforts. Use of an independent data set.
Faugeras et al. (2004)	Adjoint (I)	1D	Mediterranean Sea	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations.
Schartau and Oschlies (2003)	Micro-genetic algorithm (I)	1D	North Atlantic (3 stations)	Tabular comparison of cost function; tabular comparison of parameters with free-run, assimilation, and typical values from other studies
Ibrahim et al. (2004)	Singular evolutive extended Kalman filter (S)	1D	Cretan Sea	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations for an unassimilated variable. Plot of RMS error growth of unassimilated variable *Statistical analysis*: RMS of unassimilated variable
Magri et al. (2005)	Singular evolutive extended Kalman filter (S)	1D	Ligurian Sea	*Graphical analysis*: line plot comparisons of RMS among free-run, assimilation model, and observations. 2D maps of free-run, assimilation model, and comparisons *Statistical analysis*: RMS
Oschlies and Schartau (2005)	Micro-genetic algorithm (I)	1D	North/Equatorial Atlantic	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations for assimilated and unassimilated variables. Use of independent data sets. 2D maps of free-run, assimilation model primary production with estimates from an algorithm. 2D maps of free-run, assimilation model nitrate with climatology. Line plot of RMS. Taylor diagram of chlorophyll with satellite and in situ climatological chlorophyll. *Statistical analysis*: RMS of free-run and, assimilation model with observations and climatologies. Correlation of assimilated chlorophyll with satellite and climatological in situ chlorophyll
Friedrichs et al. (2006)	Adjoint (I)	1D	Arabian Sea	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations for assimilated and unassimilated variables. *Statistical analysis*: cost function of free-run and assimilation models with observations
Torres et al. (2006)	Ensemble Kalman filter (S)	1D	Ria de Vigo, Spain	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations for assimilated and unassimilated variables. Plots of correlation vs normalized standard deviation, and plots of RMS of free-run and assimilation model with observations for assimilated and unassimilated variables *Statistical analysis*: RMS, correlation, normalized standard deviation between free-run and assimilation models and observations.
Friedrichs et al. (2007)	Adjoint (I)	1D	Equatorial Pacific and Arabian sea	*Graphical analysis*: line plot comparisons of assimilation models with observations; bar plot comparisons of cost function from ssimilation models with observations for assimilated and unassimilated variables. *Statistical analysis*: cost function, portability index
Raick et al. (2007)	Singular evolutive extended Kalman filter (S)	1D	Ligurian Sea	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations, Taylor diagram *Statistical analysis*: RMS, correlation, normalized standard deviation between free-run and assimilation models and observations. Forecast correlation analysis.
Lenartz et al. (2007)	Ensemble Kalman filter (S)	1D	Ligurian Sea	*Graphical analysis*: line plot comparisons of free-run and assimilation models with observations, line plot comparisons of RMS between the above and between two difference assimilation schemes, Taylor diagram *Statistical analysis*: RMS, correlation, normalized standard deviation between 2 different assimilation models assimilation and observations.
McGillicuddy et al. (1998)	Adjoint (I)	2D	Gulf of Maine	*Graphical analysis*: line plot of cost function between assimilation experiments and observations
Holfort and Siedler (2001)	Singular value decomposition (I)	2D	North Atlantic	*Graphical analysis*: scatterplots of assimilation model nutrients and other models
Ishizaka (1990)	Insertion (S)	3D	Southeast US coast	*Graphical analysis*: line plots of free- run and assimilation model correlation and RMS with satellite data; 2D contour maps of assimilation model chlorophyll and satellite chlorophyll; plots of error growth without additional assimilation *Statistical analysis*: correlation, RMS

Author's personal copy

Armstrong et al. (1995)	Nudging (S)	3D	Atlantic	*Graphical analysis*: 2D maps of free-run and assimilation model of assimilated and unassimilated variables; 2D maps of zonal mean rations of assimilation model chlorophyll to satellite chlorophyll *Statistical analysis*: ratio
Semovski & Wozniak (1995)	Kalman filter (S) and Adjoint (I)	3D	North Atlantic	*Graphical analysis*: line plot comparisons of assimilation model with satellite data
Moisan et al. (1996)	Nudging (S)	3D	California coast	*Graphical analysis*: tabular comparison of unassimilated variable with other studies
Anderson et al. (2000)	Optimal interpolation (S)	3D	Gulf Stream	*Graphical analysis:* 2D maps of free-run and assimilation model to observe discontinuities
Schlitzer (2000)	Adjoint (I)	3D	Global	Graphical analysis: 2D contour maps of free-run and assimilated nutrient distributions
Popova et al. (2002)	Optimal interpolation (S)	3D	Northeast Atlantic	*Graphical analysis*: line plot comparisons of free-run model with observations
Schlitzer (2002)	Adjoint (I)	3D	Southern Ocean	*Graphical analysis*: 2D comparisons of export fluxes with satellite primary production estimates *Statistical analysis*: mean and RMS differences in nutrients between assimilation and observations
Besiktepe et al. (2003)	Optimal interpolation (S)	3D	Massachusetts Bay	*Graphical analysis*: line plot comparisons of free-run and assimilation models RMS with observations *Statistical analysis*: forecast RMS of free-run and assimilation models with observations
Garcia-Gorriz et al. (2003)	Adjoint (I)	3D	Adriatic Sea	*Graphical analysis*: 2D maps of free-run, assimilation model chlorophyll and satellite *Statistical analysis*: bias (misfit) between free-run and assimilation with satellite data
Natvik and Evensen (2003a,b)	Ensemble Kalman filter (S)	3D	North Atlantic	*Graphical analysis*: 2D maps of free-run, assimilation model chlorophyll and satellite; 2D maps of differences between free-run, assimilation model and satellite data. Line plots of skewness and kurtosis of free-run and assimilation model *Statistical analysis*: skewness and kurtosis
Schlitzer (2004)	Adjoint (I)	3D	Global	*Graphical analysis*: Comparisons of carbon exports with other efforts, tabular and textual
Hoteit et al. (2005)	Semi-evolutive partially-local extended Kalman and singular fixed partially local extended Kalman filters (S)	3D	Cretan Sea	*Graphical analysis*: 2D contour maps of free-run and assimilation model chlorophyll *Statistical analysis*: relative RMS between assimilation models and free-run
Tijputra et al. (2007)	Adjoint (I)	3D	Global	*Graphical analysis*: 2D contour maps of free-run and assimilation model chlorophyll and satellite, difference maps between assimilation and free-run chlorophyll *Statistical analysis*: cost function of free- run, multiple assimilation experiments with chlorophyll observations
Huret et al. (2007)	Evolution strategies (I)	3D	Bay of Biscay	*Graphical analysis*: 2D maps of free-run and assimilation models and observations
Gregg (2008)	Conditional relaxation analysis method (S)	3D	Global	*Graphical analysis*: 2D maps of free-run and assimilation model chlorophyll and satellite observations, with differences; line plots of free-run and assimilation model of unassimilated variable (primary production) and estimates derived from satellite; plots of error growth under different assimilation event frequencies *Statistical analysis*: RMS and bias between free-run/assimilation models and observations; RMS and bias using an independent data set (in situ data)
Nerger and Gregg (2007, in press)	Singular evolutive interpolated Kalman filter (S)	3D	Global	*Graphical analysis*: 2D maps of free-run and assimilation model chlorophyll and satellite observations, with differences; line plots of free-run and assimilation model of unassimilated variables(primary production) and estimates derived from satellite, and assimilated nitrate with free-run *Statistical analysis*: RMS and bias between free-run/assimilation models and observations; RMS and bias using an independent data set (in situ data)

I indicates inverse assimilation and S indicates sequential. The table is ordered by model dimension and then date of publication.

Author's personal copy

Table 2
Applications of fisheries data assimilation

Authors	Assimilation method	Location	Assessment method
Ussif et al. (2005)	Adjoint (I)	Northeast Arctic Cod *(Gadus morhua)*	Compared mean and standard deviation of estimated parameter values; plotted time series of observed, predicted using the new assimilation method, and predicted using a simpler assimilation method.
Schnute (1991)	Kalman filter (S)	Generic	Little attention given to skill assessment
Schnute (1994)	Kalman filter (S)	Generic	Little attention given to skill assessment
Pella (1993)	Kalman filter (S)	Generic	Little attention given to skill assessment
Kimura et al. (1996)	Kalman filter (S)	Eastern Pacific Yellowfin tuna *(Thunnus albacares)*	Compared bias, variance, and RMSE of parameter values estimated with assimilation versus least squares; plotted parameter likelihood surface; plotted time series of model outputs for assimilated parameter estimates and least squares-estimated parameter values; plotted histograms of residuals between predicted and observed output variables.
Punt (2003)	Kalman filter (S)	Northern Namibia Hake *(Merluccis capensis)*	Compared box plots showing the probability distributions of the median absolute relative error and relative error of parameter estimates and model outputs.
Sullivan (1992)	Kalman filter (S)	Gulf of Alaska Walleye Pollack *(Theragra chalcogramma)*	Compared parameter estimates, their standard errors, and their correlation structure for different estimation methods; plotted predicted and observed frequency histograms of model output variables.
Holt and Peterman (2004)	Kalman filter (S)	British Columbia and Alaska Sockeye salmon (*Oncorhynchus* spp.)	Compared the ratio of the MSE of model outputs for assimilated parameter estimates to MSE values from a simpler model; Also plotted ratio of percent bias.
Huiskes (1998)	Adjoint (I)	Pacific halibut *(Hippoglossus stenolepis)*	Plotted a cost function over iterations and between model outputs using assimilation and a simpler model; compared 3-dimensional surface plots of model outputs obtained with assimilation versus observed, and also plotted their absolute difference.
Gronnevik and Evensen (2001)	Ensemble Kalman, ensemble smoother, and ensemble Kalman smoother (S)	Icelandic cod *(Gadus morhua)*	Plotted output variables and their error variances for three assimilation methods and the free-run case.
Walters (2004)	Kalman filter (S)	General fish population	Plotted differences in predicted output that used a complex model prediction for year t and a prediction that used a complex model prediction for year $t-1$ plus data for year t.

I indicates inverse assimilation and S indicates sequential.

some places. Primary production estimates derived from the assimilation model were compared to the Behrenfeld and Falkowski (1997) algorithm, as a test of an unassimilated variable, and showed major improvements over the free-run model. Additionally, a side-by-side plot of nitrate fields (also an unassimilated variable) from the assimilation model were shown with the free-run model nitrate fields.

Oschlies and Schartau (2005) used a micro-genetic algorithm at three stations in the North Atlantic, and applied the resulting parameter values to a simulation of the entire basin. The assimilation involved 5 observational types: dissolved inorganic and particulate organic nitrogen, chlorophyll, primary production, and zooplankton biomass. Primary production results from the assimilation model compared favorably with estimates using CZCS data, but agreement of spatial patterns and temporal variability of chlorophyll between the model and SeaWiFS 5-year mean chlorophyll (1997–2002) was lacking. An impressive skill assessment was employed, including RMS evaluations of the free-run and assimilation models against in situ nitrate climatologies with depth, correlations and standard deviations of free-run and assimilation chlorophyll against SeaWiFS and in situ climatological chlorophyll. The in situ nitrate and chlorophyll and the satellite chlorophyll were not used in the assimilation and represented independent data sets for comparison. Graphical analysis was extensive, including line plot comparisons of free-run and assimilation models with observations for both assimilated (chlorophyll) and unassimilated (primary production) model primary production with estimates from the algorithm of Antoine et al. (1996), derived from satellite chlorophyll data. A Taylor diagram of chlorophyll with satellite and in situ climatological chlorophyll was included. The improvement of the optimized model over the free-run model was clearly evident in the comprehensive skill assessment.

In a 1D multi-model study, Friedrichs et al. (2007) used the variational adjoint method to optimize 12 ecosystem models characterized by varying levels of complexity using common data from the equatorial Pacific and the Arabian Sea. Multivariate assimilation involved in situ observations of dissolved inorganic nitrogen, chlorophyll, primary production, export, and zooplankton concentrations. When a single region was considered, the simplest models were found to fit the data as well as those with multiple phytoplankton functional groups. However, when the models were required to simulate both regions simultaneously using identical parameter values, those with greater phytoplankton complexity produced lower misfits. One type of assessment strategy was a cross-validation experiment in which data were assimilated from one site, and the resulting optimal parameters were used to generate a simulation for the second site.

4.2. Fisheries

While the term “data assimilation” has not yet become mainstream in fisheries, fisheries modeling analyses have used some of the major concepts associated with data

Author's personal copy

assimilation. Formal data assimilation has been incorporated into some fisheries applications (Table 2). These examples have generally involved either data assimilation used to improve the predictions of other non-fisheries models whose outputs are used as inputs to fisheries predictions or models, or directly with fisheries models but in a demonstration mode. Data assimilation has not yet been incorporated into fisheries modeling used for stock assessment whose predictions are actually used in fisheries management. There are examples of data assimilation being applied to the fisheries models themselves, but most all of these were presented as demonstration or example analyses. As with ecosystems data assimilation, we do not consider simulated data or twin experiments (e.g., Ussif, 2002, 2003) here.

Perhaps the most commonly used data assimilation technique used with fisheries models is Kalman filtering in order to separate the effects of measurement error and process error. Schnute (1991, 1994) and Pella (1993) laid out the theoretical basis for using Kalman filtering with fisheries models, but presented simple examples without much attention to skill assessment of the assimilated results. Kimura et al. (1996) applied Kalman filtering to a simple difference model of annual biomass (termed delay-difference) under a variety of assumptions about process error and measurement error. They used time series of catch and relative abundance of yellowfin tuna in the eastern Pacific Ocean as the basis of their analysis. They compared the traditional least squares approach with Kalman filtering, and concluded that the both generated similar estimates when there was only measurement error and that Kalman filtering outperformed least squares when there was also process error present. Interestingly, they also concluded that both methods yielded positively biased biomass predictions that could affect management advice. For the application to yellowfin tuna, they plotted the likelihood surface for the two parameters estimated by Kalman filtering (a third parameter was allowed to vary randomly), and presented time series plots of annual biomasses based on parameters estimates from least squares and Kalman filtering.

Other examples of Kalman filtering include application to other formulations of biomass-based models (Pella, 1993), a comparison with the more general state-space estimation (Punt, 2003), with age-structured models (Sullivan 1992), and with spawner-recruit and time series regression models (Peterman et al. 2003; Holt and Peterman 2004). Skill assessment in these examples varied greatly. Sullivan (1992) simply reported parameter estimates and standard errors, while Punt (2003) included box plots and median absolute relative error of model parameter estimates and outputs such as spawning stock biomass, maximum sustainable yield (MSY), and the ratio of current fishing rate to the desired fishing rate at MSY (i.e., F_t/F_{MSY}). Perhaps the most sophisticated skill assessment was the retrospective analysis used by Holt and Peterman (2004). They used mean squared error and mean percent bias computed over the predicted and observed recruitments accumulated by sequentially using the first n years to predict the recruitment in year $n+1$. They analyzed 24 sockeye salmon stocks and contrasted the MSE and percent bias of predicted recruitments (relative to observed) estimated without Kalman filtering and estimated with Kalman filtering. They found that Kalman filtering resulted in lowered MSE for about 35% of the stocks and had bias closer to zero for 54% to 94% (depending on the age-classes modeled) of the stocks.

Huiskes (1998) used the adjoint methods for parameter estimation of a commonly used age-structured fisheries model called virtual population analysis (VPA). VPA is widely used for making short-term (a few years) forecasts of stock size, fishing mortality, and catch (NRC, 1998). They demonstrated the approach using data from the Pacific halibut fishery and compared the results to a standard VPA (without assimilation). Skill assessment included plots of observed catch by age from 1938 to 1976 and predicted catch using the adjoint method. They compared the plots by computing the averaged absolute difference between the observed and predicted catches. The averaged absolute difference of the VPA with data assimilation was about 20% versus 35% based on the standard VPA. They also presented a frequency histogram of numbers by age predicted by the standard and assimilated VPA for a typical cohort.

Gronnevik and Evensen (2001) used data assimilation for state estimation in the context of fisheries modeling and stock assessment. They used three data assimilation techniques (ensemble Kalman filter, ensemble smoother, and ensemble Kalman smoother) with an age-structured population model applied to catch-at-age data for Icelandic cod. They also included a pure ensemble approach that had no data assimilation to serve as a benchmark for comparison. The youngest age class was started at a fixed abundance each year (i.e., fixed recruitment assumption). They plotted the estimated annual values, and their error variances, of fishable stock (sum of age-4 through age-10), abundance and fishing mortality rates of age-7 fish, and total catch over time among the four methods (no assimilation and the three assimilation methods). The two Kalman-based assimilation techniques generated similar estimates that differed somewhat from the ensemble smoother, and all three generated estimates that differed greatly from the no-assimilation case.

Walters (2004) also suggested data assimilation methods can be used for state estimation in fisheries. He illustrated how Kalman filtering can be used to provide relatively quick and efficient estimates of current fish stock biomass, an important metric for management, that mimic the predictions from the more complex stock assessment models.

5. Skill assessment strategies in data assimilation

In our review of previous work in ocean biological data assimilation, we have seen that skill assessment methods vary considerably, with many efforts utilizing only simple graphical analysis of assimilated variables and data. Quantitative comparisons are often lacking, although recent efforts show progress. The diversity of skill assessment methods can be considered an attribute, especially when accounting for the complexity of many biological models, but understanding the capability of data assimilation models requires at least a small set of common quantitative analyses. We set forth here a number of skill assessment methods that are important in data assimilation evaluation, and provide examples of relevant application when possible.

Statistical analysis of comparisons between data assimilation and a reference is the most important method for skill

Author's personal copy

assessment (see Stow et al., 2009-this issue). In the skill assessment of a free-run model, the statistical evaluations are derived from comparisons between the model and available data, where data serve as the reference field, and the approach is straightforward. This is a necessary procedure for assimilation models as well. Data assimilation methods typically employ data weighting schemes, model-data optimization, and compensation for data errors, which means that the data have changed in the application and skill assessment using the assimilated data is a useful exercise. Similarly, a statistical comparison between the assimilation model and the free-run model can provide useful information on the behavior of the assimilation process, which differs from the free-run model through the intimate use of data.

Although we consider statistical analysis a requirement for skill assessment in ocean biological data assimilation, the requirement is not intended to be an impediment to research and publication. “Good” statistical results are not necessary for scientific progress. The requirement stands because it enables an objective approach for understanding assimilation model capability and the ability to compare the results with other efforts. Statistical analysis can serve as a means to understand advantages and drawbacks in different assimilation investigations, in a quantitative manner, and facilitate future progress.

5.1. The need for independent data sets

Skill assessment using assimilated data lacks the independence necessary for a comprehensive, objective evaluation. This is because the data needed for model assessment are also typically an integral component of the data assimilation. Independent data sets, however, can provide an extra level of objective skill assessment beyond the data assimilated, and provide an improved measure of assimilation model skill. Such independent data sets can be those from a different area or time than where the model parameters were derived, a different depth, or preferably, a different source. An obvious example of a different source is using remote sensing data for assimilation and in situ data for skill assessment.

Sometimes no such alternate data set is available. A conundrum arises, since a comprehensive, objective assessment of the assimilation skill is not possible when all data are assimilated.

In these cases it is recommended to withhold data simply for the purpose of assessment. The entire data set can still be used in the assimilation, but separate analyses can be performed where some data are withheld. The amount of data needed to be withheld is dependent upon the nature of the problem, and a balance must be struck that achieves both a representation of the assimilation model and the quality of the assessment statistics. This balance can be difficult to determine in advance and requires judgment on the part of the investigator. How much data should be withheld? We suggest starting with no withheld data to get a sense of the skill of the assimilation model in its (hopefully) optimal configuration. Then withhold 50% of the data and observe the deterioration of assimilation performance relative to improvement in assessment statistics simultaneously. Whether the right balance has been achieved is ultimately up to readers, and an honest explanation of the problems and results is likely to promote confidence in the choice. Withholding can only provide a partial measure of assimilation model skill, but it achieves the requirement of a quantitative, independent assessment.

5.2. Graphical analysis of assimilation results

The simplest and most popular method for evaluating performance in data assimilation is *graphical analysis*. This can include line plots, bar charts, maps, 2D images, or any other graphical depiction of the data assimilation results and observations. For two-dimensional applications and higher, this includes observation of spatial discontinuities. These analyses can be quantified by use of variance or standard deviation, but usually severe departures are readily apparent by inspection. Rose et al. (2009-this issue) propose promising new methods for spatial mapping to assist skill assessment.

Side-by-side plots of the data along with the a priori and a posteriori simulated distributions provide the most information. Difference fields are instructive. Use of common scales is critical. For 2D and 3D spatial applications, this means color scales must be the same for both the assimilation and the data. An example is from Oschlies and Schartau (2005), where primary production from a free-run, assimilation, and an algorithm derived from data are shown together (Fig. 4). Difference fields, or ratio fields, are essential, but a different scale is of course necessary (Fig. 5). The color scales should use many values to fully capture the variability, as used in these examples.

5.3. Responses of unassimilated variables to the data assimilation

Ocean biological models can be very complex a dozen state variables (e.g., Aumont et al., 2003; Moore et al., 2004). Typically there are insufficient data available for many of these state variables for assimilation. It is instructive to evaluate how the assimilation process affects these unassimilated model components. The effects can be different depending upon the data assimilation class employed.

In a free-run model, all state variables satisfy the governing equations precisely. For sequential data assimilation, when data are assimilated, changes are made to the instantaneous values for certain state variables, and these variables will no longer satisfy the governing equations precisely. By definition, the assimilated variable represents observations more closely in the assimilation. But the unbalance between the adjusted variable and others that have dependence on it can be important and must be assessed. The adjustments can produce either positive or negative results.

Consider a simple case of a model with just chlorophyll, a single nutrient (say nitrate), and detritus. Assume a situation where chlorophyll and nitrate are too high as compared to observations, but in balance of course, as required by the model equations. Sequential data assimilation of chlorophyll reduces the chlorophyll. But now there is less chlorophyll to uptake the nitrate, and the nitrate becomes higher. This is repeated every assimilation event. The result is that the lack of balance caused by the assimilation produces overestimates of nitrate, despite the improvement in chlorophyll estimates. This situation is an important data assimilation assessment

Author's personal copy

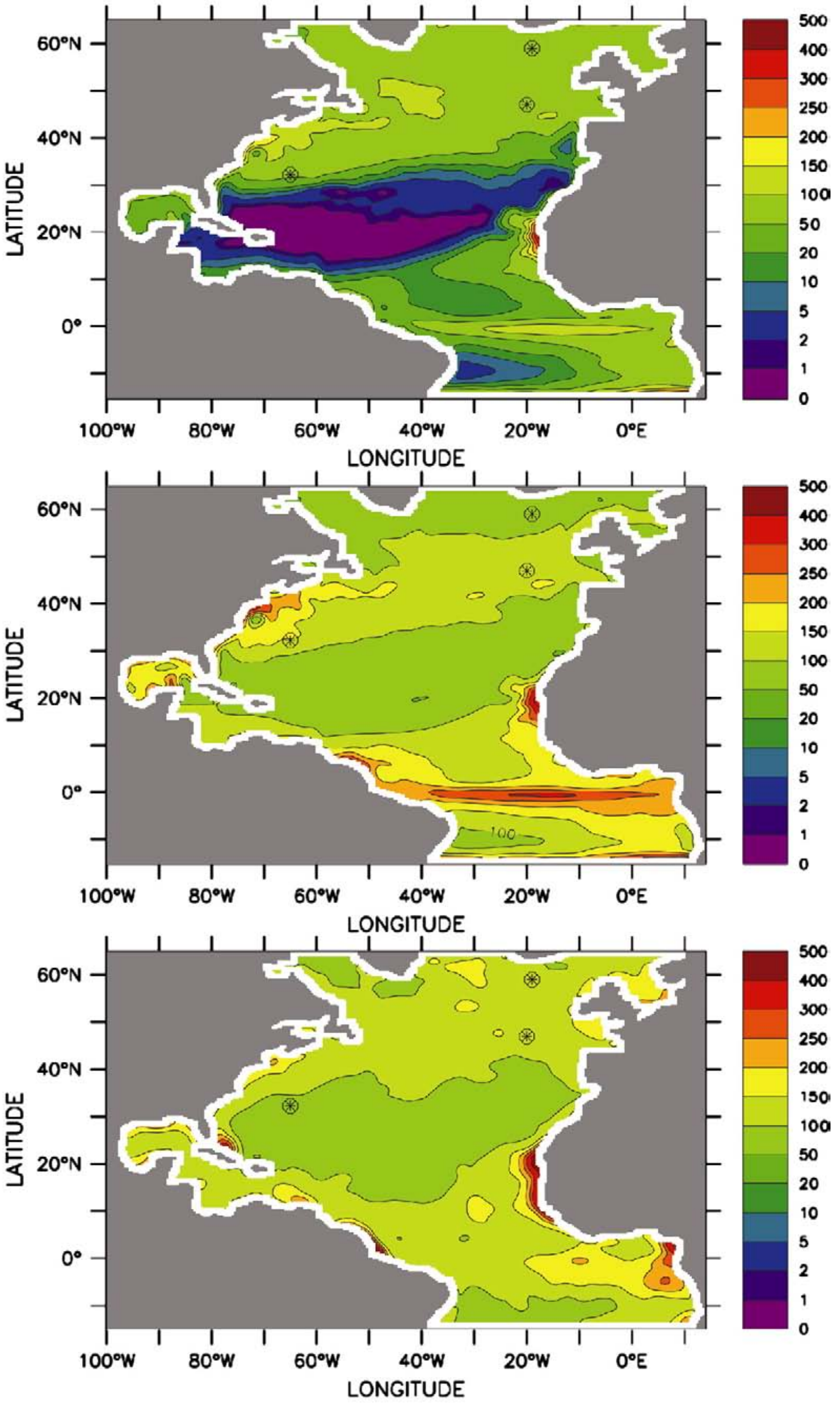

Fig. 4. Comparison of primary production from a free-run model (top), an optimized model (middle), and estimates from an algorithm (Antoine et al., 1996) using SeaWiFS data (bottom). From Oschlies and Schartau (2005) with author's permission.

issue, illustrating the importance of monitoring the behavior of unassimilated variables, nitrate in this case.

This scenario can actually become catastrophic for the assimilation in a low chlorophyll-low nitrate case. Assimilation in this case will lead to higher chlorophyll, which in turn leads to lower nitrate. If the discrepancy between the observations and the model is very large, and the assimilation is persistent, the high chlorophyll can uptake more nitrate than is available for a given time step, and cause the model to become unstable (i.e., "blow-up"). Gregg (2008) found this problem near the outflow of the Congo River, where satellite estimates of chlorophyll were contaminated by chromophoric dissolved organic matter. In this case, it was diagnosed as a problem of data error, and the assimilation scheme was manipulated to account for these data errors.

Sequential assimilation shows improved performance in cases where chlorophyll is low compared to observations and nitrate is high, or vice versa. In the former case, assimilation of chlorophyll should increase concentrations, leading to increased uptake of nitrate, producing improved fields for both variables. This can occur in models where irradiance availability is inadequate, or of course incorrect model parameterization, among others. The inverse case, too-high chlorophyll and too-low nitrate is typical in iron-limited

Author's personal copy

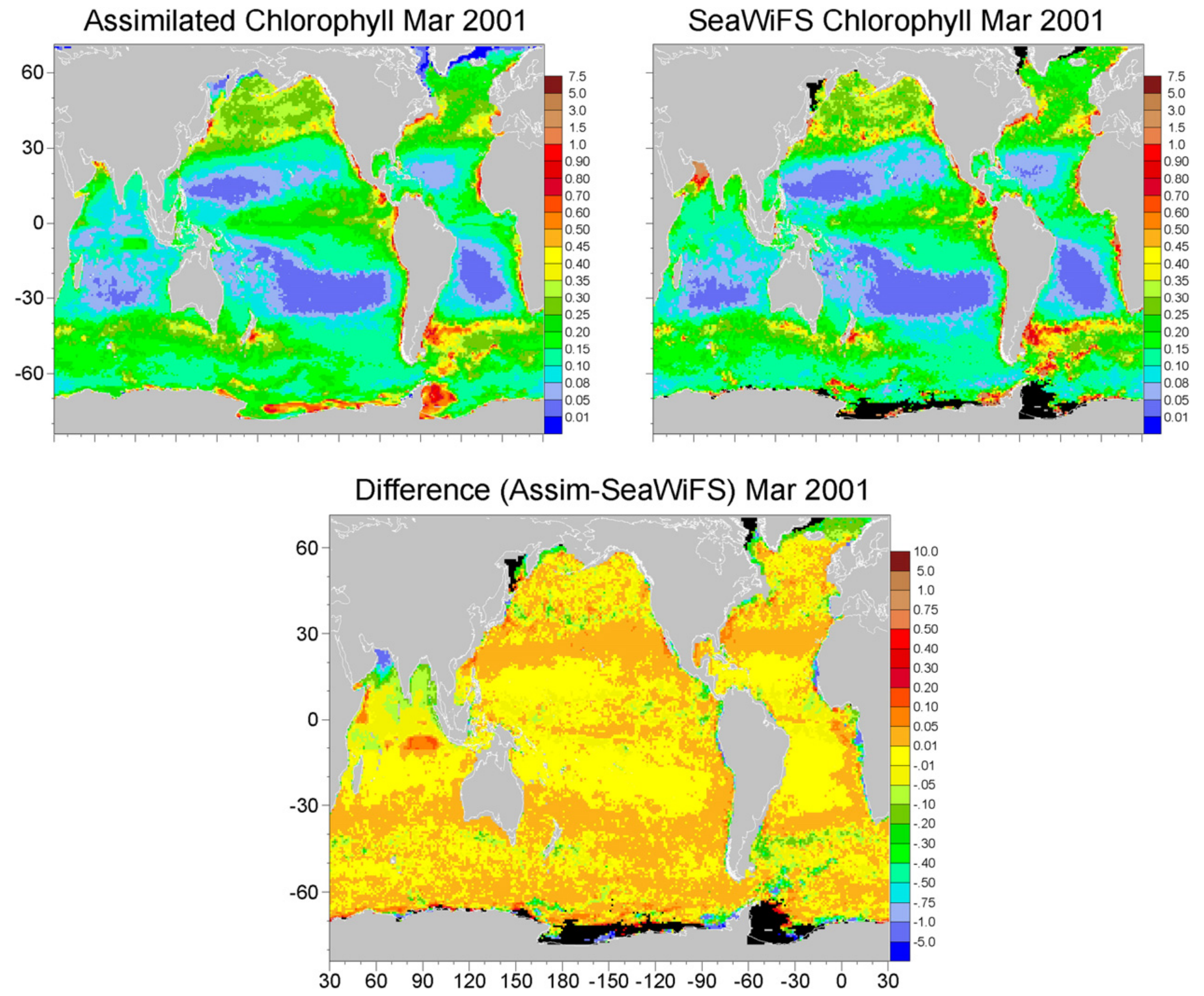

Fig. 5. Assimilation model chlorophyll (mg m^{-3}), SeaWiFS mean chlorophyll, and the difference (Assimilation-SeaWiFS, in chlorophyll units) for March 2001. From Gregg (2008).

regions, if iron limitation is not included as in our hypothetical model. Again a well-performing assimilation method will improve both the assimilated variable and the unassimilated one (decreasing the chlorophyll leading to increased nitrate), producing an overall superior representation.

Scenarios are quite different for inverse assimilation methods. However, the importance of monitoring unassimilated variables remains. Parameter optimization can absorb errors in the physical model, unknown processes, etc. into the parameters. While agreement is observed in the state variables whose parameters have been optimized, unassimilated variables can show poor behavior. As an example, consider optimized growth rates for phytoplankton in the simple model described above. The chlorophyll values are likely to agree with observations, but primary production may not because of an erroneous growth rate compensating for errors elsewhere in the system.

The point is that assessment of unassimilated variables is important for understanding the overall skill of an assimilation model. A similar situation occurs for depth distributions in a model with only surface observations available for assimilation, as is the case for remote sensing data assimilation efforts.

5.4. Assessment outside the prescribed region/time of interest

In inverse data assimilation, the procedure is to establish agreement between the data and optimized parameter set as it is integrated over a region and time of interest. Skill assessment involves providing evidence of that agreement. Assuming there are no large imbalances between assimilated and unassimilated variables leading to persistent errors that cannot be addressed by adjusting parameters, the assimilation can produce a more realistic representation than the free-run model. However, outside of the assimilation area or time of interest, the assimilation may have difficulty. Understanding when, where, and how this occurs is important for skill assessment of data assimilation systems. While the investigator may not care about the performance outside the area/time of interest, it provides important information on the

Author's personal copy

reliability, robustness, and skill of the assimilation within the area/time of interest. This procedure also typically meets the independent data set criterion discussed in Section 5.1 and has been shown to be very beneficial in parameter optimization assimilation studies.

In an example of applying an adjoint assimilation model in a different time of interest, Friedrichs (2002) optimized parameters for the Equatorial Pacific during normal conditions, i.e., vigorous upwelling in the eastern portion providing nutrients for moderate phytoplankton growth and abundances. The abnormal conditions associated with the 1997 El Niño produced changes in the underlying biological and physical fields (Chavez et al., 1998), specifically reduced upwelling of nutrients to the surface resulting in poor phytoplankton growth and low abundances. There is also evidence of a shift in phytoplankton species resulting from the lower nutrient condition (Chavez et al., 1999). As a result, the previously optimized parameters were no longer valid and assimilation model performed poorly during this time, from about Oct 1997. When La Niña replaced the El Niño in May 1998, upwelling of nutrients to the surface resumed, and were even enhanced as La Niña is associated with stronger winds. Under these new conditions, that resembled the normal conditions more than El Niño, the optimized parameters were valid and the assimilation results improved. This experimental approach provided an assessment of the skill of the parameter optimization, but also the conditions under which it was likely to break down, providing information on the general applicability of the model scheme and assimilation methodology. Note that this information would not have been available had the author not extended her assimilation outside the time of interest, namely normal conditions in the Equatorial Pacific, and conclusions on the generality of the model and assimilation scheme would otherwise have been misleading.

Another example of parameter optimization assimilation, this time relating to a different region of interest, was Oschlies and Schartau (2005). Parameters were optimized at three time-series stations in the North Atlantic. Then these optimized parameters were applied at a different location in the same basin. Model-data differences at this different location showed measurable improvement. This exercise exemplified the robustness of the assimilation model and suggested confidence in a 3D application across the entire basin.

5.5. Forecasting

Forecasting as skill assessment involves running the assimilation model forward in time and then assessing statistics of the comparison with data at that future time. It is a special case of the concept to the procedure of testing an assimilation model outside the time of interest (Section 5.4). Although the future aspect of forecasting is inherent, the method can easily be performed using past time increments, running the assimilation from a past time to a forward time. Forecasting assessment derives its value from the time interval run and the comparison with observations at a second, more forward time step (Fig. 6). Much value can be gained from increasing the time interval and deriving statistics with observations. Forecasting in biological data

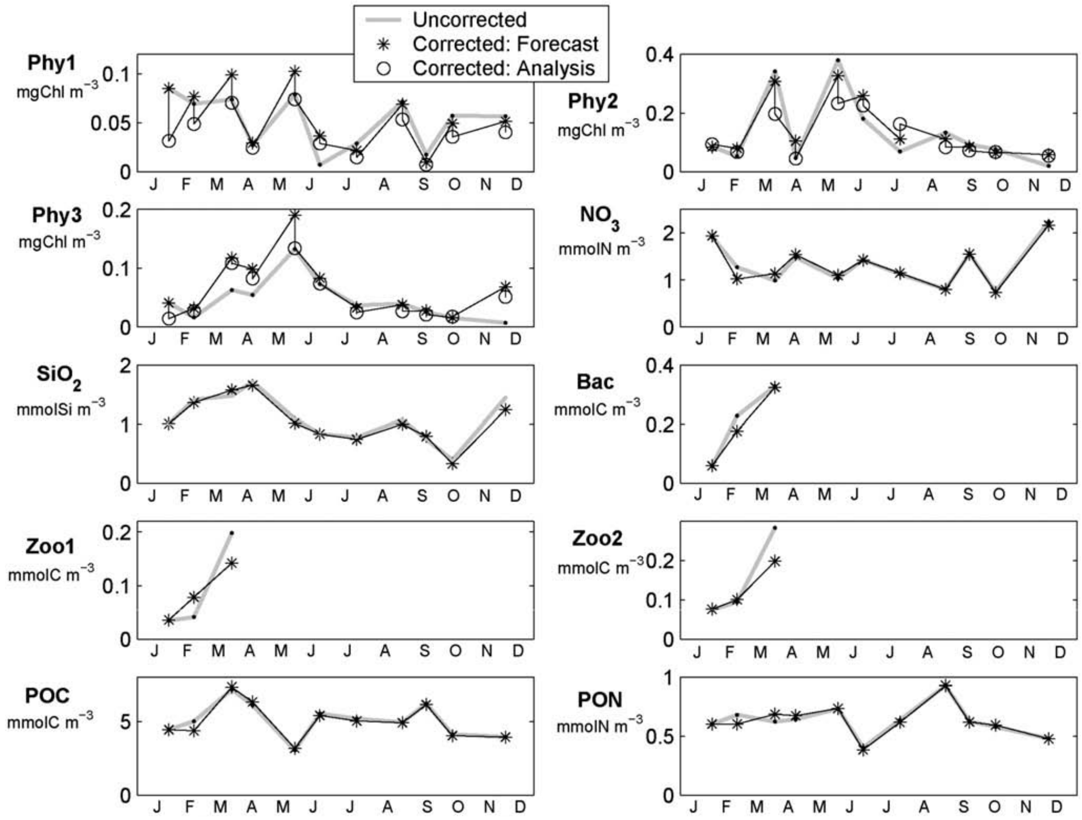

Fig. 6. Example of forecast error analysis from the Singular Evolutive Extended Kalman filter assimilation in the Ligurian Sea. From Raick et al. (2007) with author's permission.

Author's personal copy

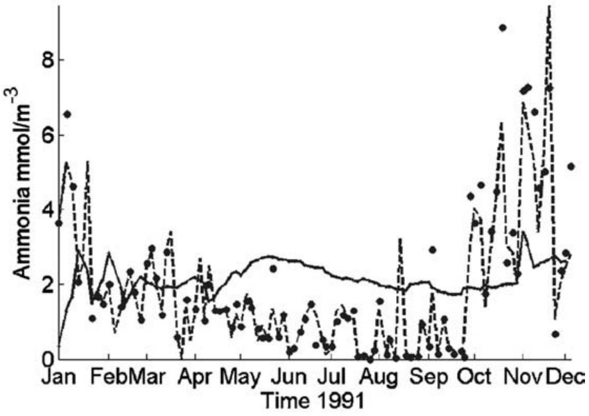

Fig. 7. Comparison of free-run model (solid line), assimilation model (dashed line) and observations (dots) for ammonium. Note the discontinuities in the assimilation model compared to the free-run, which can be characteristic of sequential assimilation. However, note how the assimilation shows much better comparison with data. From Torres et al. (2006) with author's permission.

assimilation (e.g., Robinson et al., 1999; Raick et al., 2007) is not common, at least so far, but it is the subject of much ongoing activity.

5.6. Trend analysis

Trend analysis is another important method for evaluating the performance of assimilation. This can be valuable in detecting temporal discontinuities that result from the shock of assimilation events (Fig. 7), particularly for sequential data assimilation. The sharp and frequent discontinuities in this example suggest that the data are subject to short-term influences that are not adequately captured by the model, by virtue of model design flaw, data error, or more likely forcing data. The example also shows that the assimilation is capable of repairing much of the problem, whatever the source, enabling useful information about the behavior of this system to be derived from the assimilation.

In inverse data assimilation, discontinuities associated with assimilation events are not common because of the nature of the approach, and consequently short-term trend analysis is less useful. Longer-term trends, are more useful for this type of data assimilation, and may indicate unstable parameterization.

Trend analysis can be especially useful in diagnosing problems associated with assimilation of physical data into a coupled biological-physical assimilation model. Anderson et al. (2000) found that sequential assimilation of physical data produced cross-frontal fluxes of nutrients, along with spurious vertical velocities, that affected the balance between the physical and biological models. These discontinuities were observed in trend plots of the biological variables. Use of trend analysis is similarly useful for detecting the effects of errors in the physical model in biological assimilation.

Use of trend analysis need not be restricted to plots of biological variables. Trend analysis of errors can also be very useful. Gregg (2008) tracked the growth of chlorophyll error as a function of assimilation frequency using the annual bias and uncertainty (Fig. 7), in a sequential data assimilation effort. Using daily assimilation, the annual bias and uncertainty were 5.5% and 10.1%, respectively. The error grew as the assimilation frequency decreased: if the assimilation occurred every 5 days, the bias remained <15% and the uncertainty was <30%. At very low assimilation frequencies, the annual bias and uncertainty approached the free-run model: at an assimilation frequency of once per year (every 183 days), the error was indistinguishable from the free-run model (Fig. 8).

This provides information about the stability of the assimilation system, and the strengths and weaknesses of the underlying free-run model. It also provides an understanding of how often assimilation events must occur, which can be an important consideration for the computational cost of the assimilation system and methodology.

6. Summary

Skill assessment for ocean biological data assimilation is more difficult than for free-run models. First, there are more types of information (free-run model, data, and assimilation model) that should be inter-compared. Second, the data sets needed for

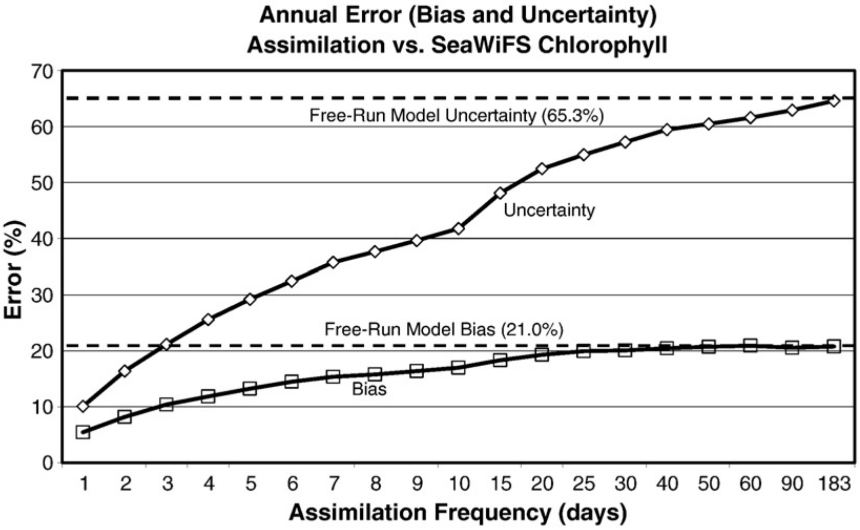

Fig. 8. Annual bias and uncertainty for assimilation as a function of assimilation frequency (days of assimilation events, i.e., 1 is every day, 2 is every other day, etc.) assimilation is performed). The annual bias and uncertainty for the free-run model is shown. From Gregg (2008).

Author's personal copy

evaluation are often integral for the assimilation, producing a lack of independence necessary for objective assessment. Most investigators compare their assimilation results to the assimilated variables. While this is a necessary first step, it is insufficient for a comprehensive evaluation. An independent data set must be sought. If the assimilation uses all the known available data for a particular location and time of interest, as is often the case, then withholding data is recommended to achieve the independent requirement. The data can be withheld strictly for the evaluation, but used in the final assimilation.

Because data assimilation is such a relatively new field in ocean biology, most efforts at skill assessment have often been qualitative and not comprehensive. Seldom has an independent data set been considered, and the most popular assessment method is graphical analysis: a plot of the data and the assimilation results. This is important, but a next step is to apply statistical analysis, which is more quantitative step and does not require much additional effort. We urge assimilation scientists to adopt the standards of skill assessment described in detail by Stow et al. (2009-this issue) as part of a routine evaluation. Again we emphasize the importance of an independent data set. Assimilation also has special assessment considerations above and beyond those of a free-running model. These include responses of unassimilated variables to the data assimilation, performance outside the prescribed region/time of interest, forecasting, and trend analysis.

Data assimilation, while still new in ocean biology, is a method whose time has come as in situ and satellite data sets proliferate. The prospects of data assimilation for improving our ability to estimate past and present states, eventually leading to improved prediction, are exciting and achievable outcomes that can be expected in the years to come. These prospects cannot be fulfilled unless rigorous, comprehensive skill assessment approaches are utilized.

Acknowledgements

We thank Steven Pawson, NASA/GMAO, and 3 anonymous reviewers for review and commentary of the manuscript. We also thank members of the Skill Assessment Working Team (Skill Assessment for Coupled Biological/Physical Models of Marine Systems held July 11–13, 2006 and March 6–8, 2007 at Chapel Hill, NC) for insightful discussions on data assimilation and its evaluation, especially Icarus Allen, Geoffrey Evans, Dale Haidvogel, John Kindle, Daniel Lynch, Dennis McGillicuddy, Roger Proctor, and Dougie Speirs. The two workshops were sponsored by the NOAA Center for Sponsored Coastal Ocean Research. We thank Andreas Oschlies, Caroline Raick, and Ricardo Torres for permission to use figures. This work was partially supported by the NASA Modeling, Analysis and Prediction Program (to WWG and SCD) and NASA Ocean Biology and Biogeochemistry Program (to MAMF).

References

Allen, J.I., Eknes, M., Evensen, G., 2002. An ensemble Kalman filter with a complex marine ecosystem model: hindcasting phytoplankton in the Cretan Sea. Annales Geophysicae 21, 399–411.

Anderson, L.A., Robinson, A.R., Lozano, C.J., 2000. Physical and biological modeling in the Gulf Stream region: I. Data assimilation methodology. Deep-Sea Research I, 1787–1827.

Antoine, D., Andre, J.-M., Morel, A., 1996. Oceanic primary production 2. Estimation at Global scale from satellite (coastal zone color scanner) chlorophyll. Global Biogeochemical Cycles 10, 57–69.

Armstrong, R.A., Sarmiento, J.L., Slater, R.D., 1995. Monitoring ocean productivity by assimilating satellite chlorophyll into ecosystem models. In: Powell, Steele (Ed.), Ecological Time Series. Chapman and Hall, London, pp. 371–390.

Aumont, O., Maier-Reimer, E., Blain, S., Monfray, P., 2003. An ecosystem model of the global ocean including Fe, Si, P colimitations. Global Biogeochemical Cycles 17, 1060. doi:2001GB001745.

Behrenfeld, M.J., Falkowski, P.G., 1997. Photosynthetic rates derived from satellite-based chlorophyll concentrations. Limnology and Oceanography 42, 1–20.

Besiktepe, S.T., Lermusiaux, P.F.J., Robinson, A.R., 2003. Coupled physical and biogeochemical data-driven simulations of Massachusetts Bay in late summer: real-time and postcruise data assimilation. Journal of Marine Systems 40, 171–212.

Carmillet, V., Brankart, J.-M., Brasseur, P., Drange, H., Evensen, G., Verron, J., 2001. A singular evolutive extended Kalman filter to assimilate ocean color data in a coupled physical-biochemical model of the North Atlantic ocean. Ocean Modelling 3, 167–192.

Chavez, F.P., Strutton, P.G., McPhaden, M.J., 1998. Biological–physical coupling in the central equatorial Pacific during the onset of the 1997–1998 El Nino. Geophysical Research Letters 25, 3543–3546.

Chavez, F.P., Strutton, P.G., Friederich, G.E., Feely, R.A., Feldman, G.C., Foley, D.G., McPhaden, M.J., 1999. Biological and chemical response of the Equatorial Pacific to the 1997–98 El Nino. Science 286, 2126–2131.

Dutkiewicz, S., Follows, M.J., Heimbach, Marshall, J., 2006. Controls on ocean productivity and air–sea carbon flux: an adjoint model sensitivity study. Geophysical Research Letters 33, L02603. doi:10.1029/2005GL024987.

Fasham, M.J.R., Evans, G.T., Kiefer, D.A., Creasey, M., Leach, H., 1995. The use of optimization techniques to model marine ecosystem dynamics at the JGOFS station at 47 degrees N 20 degrees W. Philosophical Transactions of the Royal Society of London B 348, 203–209.

Fasham, M.J.R., Boyd, P.W., Savidge, G., 1999. Modeling the relative contributions of autotrophs and heterotrophs to carbon flow at a Lagrangian JGOFS station in the Northeast Atlantic: the importance of DOC. Limnology and Oceanography 44, 80–94.

Faugeras, B., Levy, M., Memery, L., Verron, J., Blum, J., Charpentier, I., 2003. Can biogeochemical fluxes be recovered from nitrate and chlorophyll data? A case study assimilating data in the Northwestern Mediterranean Sea at the JGOFS-DYFAMED station. Journal of Marine Systems 40–41, 99–125.

Faugeras, B., Bernard, O., Sciandra, A., Levy, M., 2004. A mechanistic modeling and data assimilation approach to estimate the carbon/chlorophyll and carbon/nitrogen ratios in a coupled hydrodynamical–biological model. Nonlinear Processes in Geophysics 11, 515–533.

Fennel, K., Losch, M., Schroter, J., Wenzel, M., 2001. Testing a marine ecosystem model: sensitivity analysis and parameter optimization. Journal of Marine Systems 28, 45–63.

Freidrichs, M.A.M., 2001. A data assimilative marine ecosystem model of the central equatorial Pacific: numerical twin experiments. Journal of Marine Research 59, 859–894.

Freidrichs, M.A.M., 2002. Assimilation of JGOFS EqPac and SeaWiFS data into a marine ecosystem model of the central equatorial Pacific Ocean. Deep-Sea Research II 49, 289–320.

Friedrichs, M.A.M., Hood, R.R., Wiggert, J.D., 2006. Ecosystem model complexity versus physical forcing: quantification of their relative impact with assimilated Arabian Sea data. Deep-Sea Research II 53, 576–600.

Friedrichs, M.A.M., Dusenberry, J.A., Anderson, L.A., Armstrong, R.A., Chai, F., Christian, J.R., Doney, S.C., Dunne, J., Fujii, M., Hood, R., McGillicuddy, D.J., Moore, J.K., Schartau, M., Spitz, Y.H., Wiggert, J.D., 2007. Assessment of skill and portability in regional marine biogeochemical models: role of multiple planktonic groups. Journal of Geophysical Research 112, C08001. doi:10.1029/2006JC003852.

Garcia-Gorriz, E., Hoepffner, N., Ouberdous, M., 2003. Assimilation of SeaWiFS data in a coupled physical–biological model of the Adriatic Sea. Journal of Marine Systems 40–41, 233–252.

Gregg, W.W., 2008. Assimilation of SeaWiFS ocean chlorophyll data into a three-dimensional global ocean model. Journal of Marine Systems 69, 205–225.

Gronnevik, R., Evensen, G., 2001. Application of ensemble-based techniques in fish stock assessment. Sarsia 86, 517–526.

Hemmings, J.C.P., Srokosz, M.A., Challenor, P., Fasham, M.J.R., 2003. Assimilating satellite ocean-colour observations into oceanic ecosystem models. Philosophical Transactions of the Royal Society of London A-Mathematics, Physics, and Engineering Science 361, 33–39.

Hemmings, J.C.P., Srokosz, M.A., Challenor, P., Fasham, M.J.R., 2004. Split-domain calibration of an ecosystem model using satellite ocean colour data. Journal of Marine Systems 50, 141–179.

Holfort, J., Siedler, G., 2001. The meridional oceanic transports of heat and nutrients in the South Atlantic. Journal of Physical Oceanography 31, 5–29.

Author's personal copy

Holt, C.A., Peterman, R.M., 2004. Long-term trends in age-specific recruitment of sockeye salmon (*Oncorhynchus nerka*) in a changing environment. Canadian Journal of Fisheries and Aquatic Sciences 61, 2455–2470.

Hoteit, I., Triantafyllou, G., Petihakis, G., Allen, J.I., 2003. A singular evolutive extended Kalman filter to assimilate real in situ data in a 1-D marine ecosystem model. Annales Geophysicae 21, 389–397.

Hoteit, I., Triantafyllou, G., Petihakis, G., 2005. Efficient data assimilation into a complex, 3-D physical–biogeochemical model using partially-local Kalman filters. Annales Geophysicae 23, 3171–3185.

Huiskes, M.J., 1998. Virtual population analysis with the adjoint method. In: Funk, F., Quinn, T.J., Heifetz, J., Ianelli, J.N., Powers, J.E., Schweigert, J.F., Sullivan, P.J., Zhang, C.I. (Eds.), Fishery Stock Assessment Models, Alaska Sea Grant College Program Report No. AK-SG-98-01, Fairbanks.

Huret, M., Gohin, F., Delmas, D., Lunven, M., Garçon, V., 2007. Use of SeaWiFS data for light availability and parameter estimation of a phytoplankton production model of the Bay of Biscay. Journal of Marine Systems 65, 509–531.

Hurtt, G.C., Armstrong, R.A., 1996. A pelagic ecosystem model calibrated with BATS data. Deep-Sea Research II 43, 653–683.

Hurtt, G.C., Armstrong, R.A., 1999. A pelagic ecosystem model calibrated with BATS and OWSI data. Deep-Sea Research II 46, 27–61.

Ibrahim, H., George, T., George, P., 2004. Towards a data assimilation system for the Cretan Sea ecosystem using a simplified Kalman filter. Journal of Marine Systems 45, 159–171.

Ishizaka, J., 1990. Coupling of Coastal Zone Color Scanner data to a physical–biological model of the southeastern United-States continental-shelf ecosystem .3. Nutrient and phytoplankton fluxes and CZCS data assimilation. Journal of Geophysical Research 95, 20201–20212.

Joliff, J.K., Kindle, J.C., Shulman, I., Penta, B., Friedrichs, M.A.M., Helber, R., Arnone, R.A., 2009. Summary diagrams for coupled hydrodynamic-ecosystem model skill assessment. Journal of Marine Systems 76, 64–82 (this issue). doi:10.1016/j.jmarsys.2008.05.014.

Kalnay, E., 2003. Atmospheric Modeling, Data Assimilation and Predictability. University Press, Cambridge. 341 pp.

Kimura, D.K., Balsiger, J.W., Ito, D.H., 1996. Kalman filtering the delay-difference equation: practical approaches and simulations. Fishery Bulletin 94, 678–691.

Kuroda, H., Kishi, M.J., 2004. A data assimilation technique applied to estimate parameters for the NEMURO marine ecosystem model. Ecological Modelling 172, 69–85.

Lenartz, F., Raick, C., Soetaert, K., Grégoire, M., 2007. Application of an Ensemble Kalman filter to a 1-D coupled hydrodynamic-ecosystem model of the Ligurian Sea. Journal of Marine Systems 68, 327–348.

Losa, S.N., Kivman, G.A., Schroter, J., Wenzel, M., 2003. Sequential weak constraint parameter estimation in an ecosystem model. Journal of Marine Systems 43, 31–49.

Losa, S.N., Kivman, G.A., Ryabchenko, V.A., 2004. Weak constraint parameter estimation for a simple ocean ecosystem model: what can we learn about the model and data? Journal of Marine Systems 45, 1–20.

Magri, S., Brasseur, P., Lacroix, G., 2005. Data assimilation in a marine ecosystem model of the Ligurian Sea. Comptes Rendus Geoscience 337, 1065–1074.

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

McGillicuddy, D.J., Lynch, D.R., Moore, A.M., Gentleman, W.C., Davis, C.S., Meise, C.J., 1998. An adjoint data assimilation approach to diagnosis of physical and biological controls on *Pseudocalanus* spp. in the Gulf of Maine-Georges Bank region. Fisheries Oceanography 7, 205–218.

Moisan, J.R., Hofmann, E.E., Haidvogel, D.B., 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, 22677–22691.

Moore, J.K., Doney, S.C., Lindsay, K., 2004. Upper ocean ecosystem dynamics and iron cycling in a global three-dimensional model. Global Biogeochemical Cycles 18, GB4028. doi:10.1029/2004GB002220.

NRC (National Research Council), 1998. Improving Fish Stock Assessments. National Academy Press, Washington, DC.

Natvik, L.J., Evensen, G., 2003a. Assimilation of ocean colour data into a biochemical model of the North Atlantic. Part 1. Data assimilation experiments. Journal of Marine Systems 40–41, 127–153.

Natvik, L.J., Evensen, G., 2003b. Assimilation of ocean colour data into a biochemical model of the North Atlantic. Part 2. Statistical analysis. Journal of Marine Systems 40–41, 155–169.

Natvik, L.-J., Eknes, M., Evensen, G., 2001. A weak constraint inverse for zero-dimensional marine ecosystem model. Journal of Marine Systems 28, 19–44.

Nerger, L., Gregg, W.W., 2007. Assimilation of SeaWiFS data into a global ocean-biogeochemical model using a local SEIK filter. Journal of Marine Systems 68, 237–254.

Nerger, L., Gregg, W.W.,in press. Improving assimilation of SeaWiFS data by the application of bias correction with a local SEIK filter. Journal of Marine Systems.

Oschlies, A., Schartau, M., 2005. Basin-scale performance of a locally optimized marine ecosystem model. Journal of Marine Research 63, 335–358.

Pella, J.J., 1993. Utility of structural time series model and the Kalman filter for predicting the consequences of fishery actions. In: Kruse, G., Eggers, D.M., Marasco, R.J., Pautzke, C., Quinn, T.J. (Eds.), Proceedings of the International Symposium on Management Strategies for exploited fish populations. Alaska Sea Grant College Program Report 93-02, Fairbanks.

Peterman, R.M., Pyper, B.J., MacGregor, B.W., 2003. Use of the Kalman filter to reconstruct historical trends in productivity of Bristol Bay sockeye salmon (*Oncorhynchus nerka*). Canadian Journal of Fisheries and Aquatic Sciences 60, 809–824.

Popova, E.E., Lozano, C.J., Srokosz, M.A., Fasham, M.J.R., Haley, P.J., Robinson, A.R., 2002. Coupled 3D physical and biological modeling of the mesoscale variability observed in North-East Atlantic in Spring 1997: biological processes. Deep-Sea Research I 49, 1741–1768.

Prunet, P., Minster, J.F., RuizPino, D., Dadou, I., 1996a. Assimilation of surface data in a one-dimensional physical–biogeochemical model of the surface ocean. 1. Method and preliminary results. Global Biogeochemical Cycles 10, 111–138.

Prunet, P., Minster, J.F., RuizPino, D., Dadou, I., 1996b. Assimilation of surface data in a one-dimensional physical–biogeochemical model of the surface ocean. 2. Adjusting a simple trophic model to chlorophyll, temperature, nitrate, and pCO2 data. Global Biogeochemical Cycles 10, 139–158.

Punt, A.E., 2003. Extending production models to include process error in the population dynamics. Canadian Journal of Fisheries and Aquatic Sciences 60, 1217–1228.

Raick, C., Alvera-Azcarate, A., Barth, A., Brankart, J.M., Soetaert, K., Grégoire, M., 2007. Application of a SEEK filter to a 1D biogeochemical model of the Ligurian Sea: twin experiments and real in-situ data assimilation. Journal of Marine Systems 65, 561–583.

Robinson, A.R., Lermusiaux, P.F.J., 2002. Data assimilation for modeling and predicting coupled physical–biological interactions in the sea. In: Robinson, A.R., McCarthy, J.J., Rothschild, B.J. (Eds.), The Sea. Applying the adjoint method for global biogeochemical modeling, vol. 12. John Wiley & Sons, Inc, New York, pp. 475–536.

Robinson, A.R., McCarthy, J.J., Rothschild, B.J., 1999. Interdisciplinary ocean science is evolving and a systems approach is essential. Journal of Marine Systems 22, 231–239.

Rose, K.A., Roth, B.M., Smith, E.P., 2009. Skill assessment of spatial maps for oceanographic modeling. Journal of Marine Systems 76, 34–48 (this issue). doi:10.1016/j.jmarsys.2008.05.013.

Schartau, M., Oschlies, A., Willebrand, J., 2001. Parameter estimates of a zero-dimensional ecosystem model applying the adjoint method. Deep-Sea Research II 48, 1769–1800.

Schartau, M., Oschlies, A., 2003. Simultaneous data-based optimization of a 2D-ecosystem model at three locations in the North Atlantic: Part I—method and parameter estimates. Journal of Marine Research 61, 765–793.

Schlitzer, R., 2000. Applying the adjoint method for global biogeochemical modeling. In: Kasibhatla, P., et al. (Ed.), Inverse Methods in Global Biogeochemical Cycles. AGU Geophys. Monograph Series, vol. 114, pp. 107–124.

Schlitzer, R., 2002. Carbon export fluxes in the Southern Ocean: results from inverse modeling and comparison with satellite-based estimates. Deep-Sea Research II 49, 1623–1644.

Schlitzer, R., Usbeck, R., Fischer, G., 2004. Inverse modeling of particulate organic carbon fluxes in the South Atlantic. In: Wefer, G., Mulitza, S., Rathmeyer, V. (Eds.), The South Atlantic in the Late Quaternary—Reconstruction of Material Budget and Current Systems. Springer, Berlin, pp. 1–19.

Schnute, J.T., 1991. The importance of noise in fish population models. Fisheries Research 11, 197–223.

Schnute, J.T., 1994. A general framework for developing sequential fisheries models. Canadian Journal of Fisheries and Aquatic Sciences 51, 1676–1688.

Semovski, S.V., Wozniak, B., 1995. Model of the annual phytoplankton cycle in the marine ecosystem-assimilation of monthly satellite chlorophyll data for the North Atlantic and Baltic. Oceanologia 37, 3–31.

Spitz, Y.H., Moisan, J.R., Abbott, M.R., Richman, J.G., 1998. Data assimilation and a pelagic ecosystem model: parameterization using time series observations. Journal of Marine Systems 16, 51–68.

Spitz, Y.H., Moisan, J.R., Abbott, M.R., 2001. Configuring an ecosystem model using data from the Bermuda Atlantic Time Series (BATS). Deep-Sea Research II 48, 1733–1768.

Stow, C.A., Jolliff, J., McGillicuddy, D.J., Doney, S.C., Allen, J.I., Friedrichs, M.A.M., Rose, K.A., Wallhead, P., 2009. Skill Assessment for Coupled Biological/Physical Models of Marine Systems. Journal of Marine Systems 76, 4–15 (this issue). doi:10.1016/j.jmarsys.2008.03.011.

Author's personal copy

Sullivan, P.J., 1992. A Kalman filter approach to catch-at-length analysis. Biometrics 48, 237–257.

Tijputra, J.F., Polzin, D., Winguth, A.M.E., 2007. Assimilation of seasonal chlorophyll and nutrient data into an adjoint three-dimensional ocean carbon cycle model: sensitivity analysis and ecosystem parameter optimization. Global Biogeochemical Cycles 21, GB1001. doi:10.1029/2006GB002745.

Torres, R., Allen, J.I., Figueiras, F.G., 2006. Sequential data assimilation in an upwelling influenced estuary. Journal of Marine Systems 60, 317–329.

Triantafyllou, G., Hoteit, I., Petihakis, G., 2003. A singular evolutive interpolated Kalman filter for efficient data assimilation in a 3-D complex physical–biogeochemical model of the Cretan Sea. Journal of Marine Systems 40, 213–231.

Ussif, A.A., Sandal, L.K., Steinshhamn, S.I., 2002. Estimation of biological and economic parameters of a bioeconomic fisheries model using dynamical data assimilation. Journal of Bioeconomics 4, 39–48.

Ussif, A.A., Sandal, L.K., Steinshamn, S.I., 2003. A new approach of fitting biomass dynamics models to data. Mathematical Biosciences 182, 67–79.

Ussif, A.A., Sandal, L.K., Steinshhamn, S.I., 2005. Assimilation of time series data into a dynamic bioeconomic fisheries model: an application to the North East cod stock. Journal of Bioeconomics 7, 179–195.

Vallino, J.J., 2000. Improving marine ecosystem models: use of data assimilation and mesocosm experiments. Journal of Marine Research 58, 117–164.

Walters, C., 2004. Simple representation of the dynamics of biomass error propagation for stock assessment models. Canadian Journal of Fisheries and Aquatic Sciences 61, 1061–1065.

Weber, L., Volker, C., Schartau, M., Wolf-Gladrow, D.A., 2005. Modeling the speciation and biogeochemistry of iron at the Bermuda Atlantic Time-Series study site. Global Biogeochemical Cycle 19, GB1019. doi:10.1029/2004GBC002340.