Approaches to Data Assimilation within GODAE

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Abstract – The main purpose of this paper is to review some key issues and challenges for ocean data assimilation in the perspective of GODAE. This includes the “high-resolution challenge” and simultaneous trend towards the use of dynamically-consistent methods, the problem of modelling multivariate error covariances in “simple” OI-type schemes, verification of physical consistency, internal consistency checks via the calculation of residual (analysis minus observation) statistics, further extraction of information by adaptive algorithms, effect of assimilation on unobserved variables, forecasting skill, error dynamics in “advanced” schemes, as well as considerations on the performance of the observational network. GODAE is expected to boost the intercomparison exercises between assimilating systems, as well as to provide a forum to discuss the areas where progress is needed in the next years.

1 Introduction

Climate prediction (e.g. Stammer et al., 2001), as well as coastal and shelf seas applications are major customers of large-scale ocean estimation and prediction products (e.g. De Mey, 2001). The Large-scale Ocean Estimation and Forecasting Systems are themselves primary customers of the existing earth observation data. Ongoing projects such as FOAM in the UK, NLOM, HYCOM and ECCO in the US, and MERCATOR in France, among several others, are expected to play a pivotal role in ocean research and applications in the next decades. The potential applications of such systems are diverse and overlapping:

- The synthesis of simulations and observations of the oceanic state for climate analysis and forecast purposes
- A foundation for hypothesis testing about the ocean, and for model improvements
- A platform for assessment of global observing systems and of the utility of new ocean data sets
- Improved predictability of coastal, shelf, and regional models by providing suitable open-ocean boundary conditions
- Improved open-ocean nowcasts and forecasts (with application to search and rescue, iceberg paths, oil spills, shipping routes, fisheries, etc.)
- An understanding of the role of the ocean in the carbon cycle
- A consistent physical state estimate for use in biological models
- A model, properly initialized, for coupling to equivalent atmospheric and cryosphere models.

Although individual approaches and objectives are multiple, the Global Ocean Data Assimilation Experiment, GODAE, will provide a framework to intercompare those systems on a worldwide basis, and learn about what works and what does not (International GODAE Steering Team, 2000). In that perspective, the main purpose of this paper is to review some key issues and challenges for ocean data assimilation, concentrating mostly on the higher-resolution efforts. A secondary purpose is to examine how an exercise such as GODAE can help improve data assimilation and state estimation in these systems.
2 Some key issues and challenges for ocean data assimilation

2.1 “Simple” vs. “advanced” schemes

There are a variety of algorithms to approach the ocean assimilation problem (e.g. Ghil and Malanotte-Rizzioli, 1991; Bennett, 1992):  

- Examples of "simple" or "simplified" methods: *modifying* Blayo et al., 1994; *optimal interpolation (OI)*: Lorenc et al., 1991; Rienecker and Miller, 1991; De Mey and Benkiran, 2001.  
- Examples of "advanced" methods: *adjoint variational methods*: Courtier and Talagrand, 1990; Schröter, 1994; Morrow and De Mey, 1995; Courtier, 1997; Lee and Marotzke, 1997; Bennett et al., 1998, 2000; *adaptive and Markov chain methods*: Hoang et al., 1997; Harmon and Challenor, 1997; *ensemble and reduced-order methods*: Fukumori and Malanotte-Rizzioli, 1995; Evensen and van Leeuwen, 1996; Lermusiaux and Robinson, 1998; Brasseur et al., 1999; De Mey, 1997; Echevin et al., 2000; Auclair and De Mey, 2002.

The choice of the method is chiefly the consequence of the type and size of problem to which the state estimation approach is applied. Simplified methods are easy to set up, computationally efficient and can be easily upgraded but require external estimates of error covariances. In addition, the temporal evolution of such ad hoc solutions are not necessarily consistent dynamically and usually imply internal sinks and sources of momentum, heat and freshwater. In the advanced methods, the error covariances, the state estimates or both are more dynamically and statistically consistent, although some of these methods still require external error estimates, and of course these approaches are computationally much more demanding. We note, however, that they are needed to obtain dynamically self-consistent ocean estimates useful for understanding the physics of the system by exploiting all the information contained in the data.

In recent years, the horizontal and vertical resolution of Large-scale Ocean Forecasting Systems has increased significantly. This is for instance the case of NLOM (1/16°, 7 layers, global), FOAM (1/9°, 20 levels, North Atlantic and Indian), and MERCATOR (1/15° North Atlantic and Mediterranean, 43 levels), and in several assimilation studies such as Kamachi et al. (2001). This increase is driven by dynamical reasons, in particular a better description of ocean mesoscale processes, of their interaction with the mean circulation (Hurlburt and Hogan, 2000), and of subinertial processes in the coastal and shelf seas. The increase in resolution is also driven by observationally-related reasons (need to match the resolution of satellite altimetry and make better use of profile data) and by the needs of downstream applications (e.g. Navies, nesting of regional/coastal models). The state vector for such systems is huge : hence the use of simple, cheap data assimilation (DA) methods such as Optimal Interpolation (OI) and the practice of model nesting. The FOAM system (Bell et al., 2000) currently uses an iterative approach to OI (Lorenc et al., 1991) to assimilate temperature from SST and profiles. The Cooper and Haines (1996) scheme is used for the assimilation of altimetry data. The MERCATOR North Atlantic and Mediterranean system uses multivariate reduced-order OI (SOFA; De Mey and Benkiran, 2002). The NLOM global system uses a simple method as well; it is further described below. The main advantage of OI-based methods is their cost; however their performance highly depends on the background error covariance models used. We will come back to this later.

The Naval Research Laboratory (NRL) strategy for global ocean prediction is driven by the need for ocean models with high horizontal resolution required to successfully simulate the variability of mesoscale features and the high vertical resolution required near the surface to resolve the physics of the upper ocean (Harding et al., 1999). On a global scale it is not yet possible to affordably run one ocean model in real time that has the horizontal and vertical resolution needed to meet these requirements. Thus, the first generation global ocean prediction system uses a two-model approach based on the NRL Layered Ocean Model (NLOM) and the NRL Coastal Ocean Model (NCOM), Rhodes et al. (2002). The operational eddy-resolving global ocean nowcast/forecast system which uses NLOM with 1/16° resolution and 7 layers in the vertical, (Smedstad et al. 2002) has the high horizontal resolution needed for the mesoscale dynamics and serves as an effective dynamic interpolator of the altimeter data in mapping this variability. This system has been running at the Naval Oceanographic Office (NAVOCEANO) since 18 October 2000 and it became an operational product on 27 September 2001. Real-time sea surface temperature (SST) from satellite IR and satellite altimeter sea surface height (SSH) from Topex/Poseidon, ERS-2 and Geosat-Follow-On provided via NAVOCEANO's Altimeter Data Fusion Center (ADFC), are assimilated into the model. The large size of the model grid (4096*2304*7) and operational requirements makes it necessary to use a computationally efficient assimilation scheme. The assimilation consists of an optimum interpolation (OI) deviation analysis of SSH with the model as a first guess (Smedstad and Fox, 1994), a statistical inference technique for vertical mass field updates (Hurlburt et al., 1990), geostrophic balance for the velocity updates outside of the equatorial region and an incremental updating of the model fields to further reduce gravity wave generation. A spatially varying mesoscale covariance function determined from Topex/Poseidon and ERS-2 data is used in the OI analysis (Jacobs et al., 2001). The SST assimilation consists of relaxing the NLOM SST to the Modular Ocean Data Assimilation System (MODAS) SST analysis which is performed daily at NAVOCEANO.
A different perspective is given by the ECCO consortium ("Estimating the Circulation and Climate of the Ocean"), which has been formed to carry out global ocean state estimation, mostly for data synthesis and climate applications, at spatial resolutions up to eddy-permitting (Stammer and Chassignet, 2000; Stammer et al., 2002c). ECCO activities are based on the MIT general circulation model (Marshall, et al., 1997a,b), including complete mixed layer physics and an eddy parameterization scheme, and a set of advanced data assimilation tools including 4D-var. One of ECCO's products is of fairly high resolution (1-deg telescoping to 0.3-deg within 10-deg of the Equator, and with 10m resolution in the upper 150m). Model error is explicitly modeled in the form of errors in external forcing, and calibrated, along with data error, by comparing the differences of the control run (simulation) and observations with their theoretical expectations ("covariance matching", Fu et al., 1993).

In addition to the global state estimates (Stammer et al., 2002a,b,c), ECCO is also using regional models that are nested into the global results and that make estimates with significantly higher resolution than is now possible globally. For example, the North Atlantic and the Tropical Pacific are estimated at 1/6° horizontal resolution or higher. Both open and closed boundary conditions are used.

One interesting new approach to solve large estimation problems is to partition them into series of separate smaller calculations using a partitioned Kalman filter and smoother (PKF and PS; Fukumori, 2002). The smaller dimension of each cell renders estimation of the larger problem much more practical than otherwise. In particular, the approximation makes high resolution global eddy-resolving Kalman filtering and smoothing computationally viable. In the example above, the reduced state, and equivalently the process estimated, consists of perturbations of the barotropic and first five baroclinic modes, defined in eight overlapping cells covering the globe, representing the adiabatic errors associated with errors in wind that are estimated.

Other examples of simple and advanced schemes will be given in the next sections. Let us also give a few examples of recent “hybrid” approaches that cannot be easily categorized: optimal interpolation with an adaptive loop in Testut et al., 2000; prediction of 3D-var error statistics with an Ensemble method (Hamill and Snyder, 2000; De Mey and Auclair, pers.comm., 2002); joint use of Markov chain modelling and an Ensemble method to identify ecological model parameters (Harmon and Challenor, 1997).

2.2 Modelling background error covariances in “simple” schemes

Generally speaking, state estimation and prediction require three elements linked to a common state vector: (1) deterministic prognostic equations (“the numerical model”), (2) a stochastic model of errors (probability density functions, covariances), and (3) observations. A control vector is defined and the three elements are integrated in a minimum variance/maximum likelihood principle, which is defined even for the simplest schemes (such as nudging), albeit in a hidden way.

In practice, data assimilation schemes use dynamical, statistical and cross-variable interpolation to mix observations with model estimates. This interpolation is performed in the error subspace. In general, the error subspace is modelled in a particular way (e.g. De Mey, 1997). When considering a new observation system, the question of what particular physics this observation system can help correct in the model is central, and will translate in questions on the way the error subspace and hence the error covariances are to be modelled.

For instance, it is generally agreed that error in mid-latitude ocean GCMs occur predominantly in two "components" which have different horizontal and vertical scales and arise from different sources: (1) a "synoptic" scale component, from atmospheric forcing errors, and (2) a “mesoscale” component, from errors in the internal model dynamics, such as instability processes. The FOAM group has calculated inhomogeneous, three-dimensional statistics using the method of Hollingsworth and Lönnerberg (1986). Collocated model and observation values from a 3 year integration of the 1/3° North Atlantic FOAM system were used to calculate the statistics. A combination of two second-order auto-regressive (SOAR) functions were fitted to the observed-minus-forecast covariances as a function of separation, resulting in estimates of the variances and length scales for the two components. It was also assumed that each of the two error components could be separated into horizontal and vertical parts.

Satisfactory estimates of some of the open parameters of OI schemes, such as correlation scales, can also be obtained via trial-and-error methods such as simple sensitivity assessment. The FOAM group has calibrated their background error spatial correlation scales by comparing rms SST errors to satellite data. They found that using a range of correlation scales (500km-100km) fit independent data more closely than analyses made using a single 300km scale.

Faucher and De Mey (pers. comm., 2002) present and discuss altimetric assimilation experiments in the MERCATOR North Atlantic 1/3° configuration using isopycnal EOFs to model the background error covariances in an OI scheme (De Mey and Benkiran, 2001). In a previous work, Faucher et al. (2002) showed from a set of historical hydrographic
data that the dominant isopycnal EOF accounts for most of the surface dynamic height variability in the North Atlantic ocean. In addition, the reduced-order observability problem for altimetry is more naturally studied in isopycnal coordinates because the displacement of isopycnals is the largest contribution of deep ocean dynamics to the sea-level changes. Isopycnal EOFs seem very efficient in propagating the surface altimeter signal to the deep ocean layers.

Another promising approach to explore and calibrate components of the background error is Monte-Carlo forecasting (a different approach to the Ensemble Kalman Filter, an "advanced" scheme described below). This approach has been used for instance to estimate the forecast error structure and growth due to forcing errors in coastal/shelf models (Auclair et al., 2002) and in the upper ocean (Andreu-Burillo et al., 2002; Figure 1). Some of the background error components can be considered fixed, and some updated, as in Hamill and Snyder (2000). The above authors now intend to compare the dominant Ensemble EOFs with singular vectors and bred modes as an alternative in the modelling of the structure and order reduction of the background errors.

![Figure 1: Approximate representer function for SST onto T(y,z) from Monte-Carlo method across Azores Front in October, 1993, after Andreu-Burillo et al. (2002). About 100 ensemble members were used. Atmospheric heat fluxes were perturbed. The vertical section spans the distance between N and S open boundaries at 24.16°W. The SST measurement is at 33.64°N within the section. The result shows that the potential influence of the measurement is largest at the base of the seasonal thermocline and North of the Azores Front in the case studied.](image)

2.3 Correcting the model bias

It is important to note that ocean models are very likely to be biased and that some of the impact of data assimilation will be to counter the tendency of the model to drift. This is particularly true for hydrographic profile data assimilation because models do not usually maintain a good thermocline and this is a common problem in seasonal forecasting applications. All of the optimal assimilation schemes assume that the model background is unbiased which is a major drawback. It is possible to treat model bias by extending the state vector (e.g. Dee and da Silva, 1998; Bell et al. 2000) but this area has received insufficient attention in the environmental data assimilation literature up to now.

2.4 Verification: physical consistency and effectiveness of use of observations

Data assimilation applications always need observations for verification. Normally the observations which are assimilated serve less purpose for validation than independent observations. The reason is that most assimilation schemes will pull the model closer to an assimilated observation, although the advanced schemes will minimize a global data misfit, in a way prescribed by the prior error information.

One interesting verification measure is if the impact of the observation is correct, i.e., is the model prediction and the observation weighted correctly in a statistical sense when computing the analysis? When comparing with the assimilated observations, the results will appear better the closer they are to the observations. However, an assimilation scheme should not just interpolate the observations but rather smooth them consistently with the prior error statistics of the observations and the model state. This is discussed in the “Internal consistency” section.

A second issue is to ensure that the analyzed model state is physically and dynamically acceptable, i.e., when assimilating observations of one model variable, the rest of the model state needs to be updated consistently using a multivariate analysis scheme. Typical and relevant examples relate to the computation of the vertical impact when
assimilating ocean surface observations, and also the impact on salinity or density when assimilating vertical profiles of temperature data. This is discussed in the “Need for balanced increments” section.

A third issue is to ensure that the assimilation system (observations + model + assimilation scheme) has skill in forecasting important properties of the ocean. This is discussed in the “Forecasting skill” section.

The present section deals with how ocean estimates derived from data assimilation are validated, and to which observations they are compared. It only provides a few examples since a complete discussion of model verification will be given by other speakers at the GODAE Symposium.

In principle, accuracy of state estimation is a non-decreasing function of the amount of data that is assimilated. A degradation caused by assimilation generally indicates inaccurate assumptions in the assimilation scheme, not model nonlinearities or insufficient observations. Comparisons with independent observations provide a means to assess the goodness of the assimilation, and the assumptions that underlie them. For sequential assimilation methods, the innovation sequence, relative to model-data differences of the non-assimilated control run, provides a readily available comparison with independent observations (i.e., data that is yet to be assimilated). The innovation vector is the difference between observations and model forecasts based on assimilating prior measurements. When available, formal uncertainty estimates provide yet another measure of consistency through comparisons with residual model-data differences (e.g., Fukumori et al., 1999; see next section).

The NRL nowcast/forecast system is routinely compared to independent observations. SST and temperature profiles from buoys are used to monitor the performance of the system as well as the frontal position of the Kuroshio, Gulf Stream and the Loop Current in the Gulf of Mexico determined from an independent analysis of MCSST observations. Comparison to tide gauge observations are in the process of being added to the system.

The ECCO consortium global state estimation efforts have produced results that are considered acceptable for first scientific applications and analyses. The quality of results has been tested against independent data (in particular the TAO moorings in the Tropical Pacific, as well as XBTs, WOCE hydrographic lines, drifters, PALACE data) and surface flux fields. Within ECCO, a particular science focus is on the determination of transports and the budgets of mass, heat, freshwater, and energy in various regions of the global domain. The state estimates are also being examined to assess the accuracy of various estimates of air-sea fluxes of momentum, heat, and freshwater; to quantify the relative impact of different observing systems; to study ocean dynamics; and to improve forecasting skills.

The regional and global ocean data assimilation systems at Kyoto University/FRSGC have been applied to short-range forecasting of the energetic Kuroshio around Japan and accurate estimates of the global ocean state, respectively, focusing on better description of the state of a dynamic system in the North Pacific Ocean. The global ocean data assimilation system using a free-surface ocean general circulation model (with the resolution of 1° horizontally and 34 levels vertically) and the 4D-var method provided a comprehensive 4D data set with good dynamical consistency by assimilating temperature and salinity data from World Ocean Database 1998 and TOPEX/POSEIDON altimetric anomaly data. In doing so, net air-sea heat and freshwater fluxes from World Ocean Atlas 1998 and wind stress from NCEP were used as the initial forcing. The results show the efficiency of the assimilation system in reproducing the detailed features similar to those of ocean circulations reported so far. For instance, a low salinity distribution associated with the North Pacific Intermediate Water (NPIW) is reproduced quite accurately. It is worth noting that the NPIW is a good implication of the subsurface circulation in the North Pacific and that some important aspects of ocean circulations particularly in subsurface layers are not well represented even in current sophisticated assimilation systems. Furthermore, the accuracy of estimated heat and freshwater fluxes is also better than that by the flux correction method used in most ocean-atmosphere coupled models.

\section*{2.5 Internal statistical consistency of data assimilation systems}

In an "advanced" assimilation scheme such as 4D-var (e.g. Weaver et al., 2002) and the Ensemble Kalman Filter (EnKF, e.g. Evensen and van Leeuwen, 1996), one can consistently use the assimilated data for verification. This is done by comparing the innovation statistics and analysis-minus-observation (AmO) residuals to the predicted error statistics from the assimilation scheme. This provides a test whether the prior error statistics have been prescribed correctly to properly represent the actual errors in the model and the observations. One example with the EnKF is given in Haugen and Evensen (2002), which conclude from such a test that the error statistics have been prescribed correctly.

CERFACS has developed, in collaboration with the ocean-climate modelling group at LODYC and the seasonal forecasting group at ECMWF, incremental three- and four-dimensional variational assimilation (3D- and 4D-var) systems (Weaver et al., 2002) for the rigid-lid version of the OPA OGCM (Madec et al., 1998). The systems have been applied to produce an extended set of analyses of the tropical Pacific Ocean over the period 1993-98 using \textit{in situ}
temperature observations from the Global Temperature and Salinity Pilot Programme. Figure 2a, shows the 1993-98 average of the AmO residuals as a function of depth for all the assimilated TAO data in 3D-var and 4D-var experiments (Weaver et al., 2002). For comparison, the average of the difference between the temperature field in the control run (a model integration without data assimilation) and the TAO data is also shown. The control displays a large warm bias of about 2°C just below the thermocline. This bias is largely reduced in 3D-var and almost completely absent in 4D-Var. In Figure 2b, the root-mean-square (rms) of the control shows large differences both just below the thermocline, where there are large biases, and in the thermocline, where signals associated with the seasonal cycle and interannual variability are largest. These differences are substantially reduced in both 3D-var and 4D-var. In 4D-var, the rms of the AmO is reduced over the entire water column to values less than the specified level of observation error (0.5°C). This is precisely what we wish the assimilation system to do. In 3D-var, on the other hand, the rms of the AmO exceeds 0.5°C over much of the thermocline. This better performance of 4D-var than 3D-var in fitting the data can be attributed to several factors as discussed in Weaver et al.

![Figure 2](image)

**Figure 2:** Time-averaged statistics, plotted as a function of depth, of the analysis-minus-observation (AmO) residuals for TAO data during the 1993-98 period. (a) average and (b) rms of AmO residuals. The dashed, dashed-dotted and solid curves correspond to the control, 3D-Var and 4D-Var experiments, respectively.

### 2.6 Need for balanced increments: the effect of assimilation on non-observed variables

A key virtue of data assimilation is its use as a means to estimate the complete state of the ocean from incomplete observations, including aspects of the state that are not directly measured. In simple schemes, dynamical assumptions or properties can be built in the state definition and error covariances (e.g. using isopycnal conservation: Cooper and Haines, 1996; Faucher et al., 2002). However, even in multivariate systems, it is worth checking how assimilation changes non-observed variables.

In FOAM, problems arise near the equator when assimilating temperature data into the ocean model in a simple manner. The model state is pushed out of balance by the assimilation, resulting in large time mean temperature increments which warm/cool the model ocean by more than 30°C per year. The density change caused by this large input of heat induces persistent vertical advection in the model. Two different methods have been devised which attempt to counteract these problems by attempting to restore some form of balance, details of which can be seen in Martin et al. (2002) and Burgers et al. (2002). Burgers et al. apply a generalized form of geostrophic balance appropriate near the equator to calculate increments to the zonal velocities to balance density increments from their analysis scheme. Martin et al. suggest a scheme which uses the assimilation increments to update slowly evolving bias fields. The bias fields augment the model state and affect the model's pressure gradients. These two approaches are complementary. The first reduces the initialization shock associated with unbalanced increments to the mass field whilst the second attempts to counteract biases in the vertical distribution of the momentum input from the surface wind stress.

A related effect is seen in the CERFACS 3D variational estimates in the Tropical Pacific presented above. One study compares the 1993-96 average surface zonal velocity analyses from 3D-var and 4D-var. The intensity of the North Equatorial Counter Current (NECC) is improved in both assimilation experiments: the NECC is close to 0.2 m/s in 3D-var and 4D-var, compared to 0.1m/s in the control and 0.3 m/s from climatological estimates (Reverdin et al., 1994). This improvement of the NECC intensity can be linked through geostrophy to the steepening of the meridional temperature gradient between 5°N and 10°N produced by the assimilation. More striking, however, is the large eastward bias of 0.3 m/s in the surface currents of the 3D-Var analysis observed in the central-eastern equatorial Pacific. This
bias is associated with a surging of the Equatorial UnderCurrent and spurious downwelling eastward of 110°W. These problems arise because of the univariate nature of the 3D-var system used by the authors. As we have seen above, these effects appear in other data assimilation systems such as FOAM, and are associated with a disruption to dynamical balances along the equator caused by the univariate assimilation of subsurface temperature data. These problems do not appear in the 4D-var analyses, possibly because the analysis increment is constrained to satisfy the dynamics of the tangent-linear model so that velocity and temperature corrections generated by 4D-var will already be balanced to some extent.

2.7 Forecasting skill

Testing the ability to forecast from an analyzed state is one of the most comprehensive checks of an assimilation system. It checks whether the dynamical model and assimilation scheme are consistent to each other, provides detailed insight on error growth rates, and usually gives interesting clues to what goes wrong in the system. The most commonplace test is to compare the forecast to persistence.

Construction of a nowcast/forecast system for the Kuroshio, which is the western boundary current in the North Pacific, is still a challenge because of the nonlinear nature of the Kuroshio variabilities. The time series of the analysis field obtained by the Kyoto University/ESC (Earth Simulator Center) regional assimilation system using the variational method exploited by Ishikawa et al. (2001) and the sea surface height field (Kuragano and Shibata, 1997) correctly represents the Kuroshio path variabilities during the study period from 1993 to 1997 (Komori et al., 2002). For example, the $\text{rms}$ differences from the observations fall within 0.3° for the location in latitude of the current axis off Enshu-nada, where the Kuroshio path variabilities are largest, while their observed $\text{rms}$ variabilities are 0.5°. By using the resulting fields as the initial conditions, 116 cases of 90-day forecast experiments for the Kuroshio path variabilities are then performed and show that the accuracy of the forecast field around Japan is much higher than that of persistence experiments. These results and the comparison with the $\text{rms}$ variability of the analysis field enable the authors to infer that roughly 60-day forecasts of the Kuroshio path variabilities around Japan are possible.

The operational NLOM system routinely calculates statistics showing the skill of the weekly 30-day forecasts. $\text{Rms}$, anomaly correlation and skill score for SSH and SST are calculated globally and for several sub regions. Both persistence and climatology are used in the evaluation of the forecast skill. Similar statistics are calculated by FOAM and MERCATOR as well.

2.8 Error dynamics and adaptive schemes

A key scientific issue that needs to be examined during GODAE relates to the capacity of assimilation systems to produce consistent error statistics about the ocean state estimates, and to propagate those error statistics properly from one assimilation cycle to the next. In the linear Kalman filter, the specification of the system noise ($Q$), the observation error ($R$) and the background error covariance at the initial time ($P_0$) perfectly determines the subsequent evolution of the error statistics throughout the assimilation sequence. This is because the observations do control the trajectory of the model state, but they have no impact on the evolution of the error statistics (except through the definition of the observation network $H$). As a result, imperfections in the specification of the $P_0$, $Q$ and $R$ matrices can affect the stability of the filter and trigger drifts of the assimilation system.

The assimilation error dynamics has been investigated using the SEEK filter, which is a reduced-order Kalman filter developed to assimilate multivariate satellite and in situ data into numerical models of the ocean circulation and ecosystem dynamics (e.g., Verron et al., 1999; Carmillet et al., 2001). The basic theory has been established and illustrated by Pham et al. (1998) using a quasigeostrophic model of the mid-latitude ocean circulation. The analysis step of the SEEK filter is achieved in a sub-space of small dimension which contains the assumed dominant directions of the background error. The adoption of a reduced-rank error covariance matrix further simplifies the computation of the forecast error and makes the scheme tractable for problems of very large size. The initialization of the error sub-space can be expressed in terms of singular vectors, breeding modes or multivariate EOFs of a prior model run. A comparison between implementations of the SEEK algorithm, the Ensemble Kalman Filter (described above) and the Ensemble Kalman Smoother is discussed by Brusdal et al. (2002).

Using twin experiments with a primitive-equation model of the Gulf Stream in idealized configurations, Ballabrera et al. (2001) examine how the evolutive nature of the SEEK filter is affected by an imperfect specification of the statistics of the background error. They observe that the truncation error doesn’t impact the control of the solution when at least one of the three following conditions is verified: (i) the initial error is perfectly described by the reduced space; (ii) the truncation error is dynamically uncoupled with the error components of the reduced space; (iii) the reduced space must contain all the components of the growing error during the forecast time period.
As these constraints are never perfectly satisfied in real situations, an adaptive estimation approach was investigated in order to introduce some feedback between the data and the estimation error. Several approaches exist to restore the consistency between the forecast errors diagnosed by the filter and the statistics of the innovation vector. The adaptive algorithm proposed by Brasseur et al. (1999) updates the error subspace of the SEEK filter along the geostrophic attractor by extracting information left in the innovation vector after each analysis step. Using a statistical approach, Brankart et al. (2002) and Testut et al. (2002) implemented an adaptive mechanism to tune the model error parameterization according to the local innovation variance, and thereby account for regional properties of the ocean dynamics.

The well-posedness of this mechanism has been validated in the context of hindcast experiments conducted during the 1993-1996 period with two different models: the 1/3° North Atlantic OPA model of the MERCATOR prototype system, and the Atlantic/Arctic MICOM model of the European DIADEM system. Sea-surface temperature from the NASA Pathfinder project and altimetric data from the ERS and Topex/Poseidon missions were assimilated in both systems every 10 days. Testut et al. (2002) study the distribution of the 10-day forecast error in the North Atlantic once the assimilation experiment has reached an asymptotic regime. The largest forecast errors are found along the Gulf Stream path between Cape Hatteras and 40°N, where the standard deviation exceeds 20 cm in some places. Local maxima are also detected in the North Atlantic Current extension and along the Azores Current at 35°N. The relevance of this error distribution was demonstrated by examining the internal consistency of the assimilation scheme. Brankart et al. (2002) compare the estimated innovation variance with the sum of the observation and forecast error variance diagnosed by the filter in a zonal section across the Gulf Stream region (at 30°N). These authors show that the adaptive mechanism is able to bring them in fairly good agreement one with the other.

In order to objectively validate the results of these hindcast experiments, the misfits between the temperature fields of the 10–day forecasts and independent XBT profiles collected during the assimilation period were calculated in the upper 700 meters of the water column. A similar behavior is observed in the OPA and MICOM assimilation experiments, with a reduction of the misfit in the surface layer and between 300 and 700 meter depth. The impact of the assimilation at intermediate depth is less significant, suggesting that the control of the mixed layer depth still needs to be improved.

A simple adaptive scheme for the specification of error statistics in the assimilation of gridded altimeter data was presented by Fox et al. (2000). Following Dee (1995) an adaptive deduction of errors in model sea level was derived based on altimeter-model misfits. The scheme uses the property that the innovation statistics must be consistent with the errors in the observations (assumed known) and the errors in the model (unknown). Fox et al. use this to calculate a low resolution measure of model sea level error which is then used to assimilate altimeter maps into the global 1/4°, 36-level OCCAM model.

The Ensemble Kalman Filter (EnKF) allows for the prediction of multivariate, dynamically-consistent error statistics. The EnKF has proven successful with OGCMs and is currently used in several applications which includes a real time forecasting system for the North Atlantic and the Arctic Oceans (DIADEM/TOPAZ) and a hindcast application for the Indian Ocean (Haugen and Evensen, 2002). An advantage of using advanced schemes like the EnKF is that they simplify the multivariate assimilation of different types of observations. For instance, when assimilating a temperature profile the salinity and vertical stratification is also being consistently updated through the multivariate covariance functions. With “simple” schemes such as OI and 3D-var, one has instead to build that multivariate character “by hand” into the scheme, and carefully check any catastrophic unbalance in the increments, while that character is consistently satisfied by most advanced methods such as the Ensemble and adjoint (4D-var) methods.

2.9 Observational array performance and design

Unprecedented volumes of measurements will be collected during and after the GODAE period, including for instance an extensive ARGO drifter program, and new instruments such as imaging altimeters will come next. It is very important to be able to diagnose the observing system performance in the existing forecasting systems, if possible before the observing systems are set up and the measurements start to flow in. Data assimilation can be used to provide with such performance assessment.

Indeed, data assimilation has many purposes besides estimating the state of the ocean and its parameters. The diagnostics produced by data assimilation include posterior error moments, significance test for the priors, and analyses of the conditioning of the fit to dynamics and data. The last mentioned of these is no less than an assessment of the efficiency of the measurement system or “array”, for observing the hypothetical ocean.
The hypothetical ocean consists not only of bathymetry, equations of motion, initial conditions and boundary conditions, but also probabilistic descriptions of the errors in all these pieces of information. The descriptions are usually in the form of means and covariances, implying that the errors are jointly normal. The specification of the array similarly includes prior means and covariances for the observations, that is, error moments hypothesized before receiving the data.

Even if the dynamics are in continuous form, the algorithm for the least-squares best fit to the dynamics and to the data is always reducible to a linear finite dimensional equation. The dimension of the equation equals the number $M$ of data. Linearity is assured, if the dynamics and measurement processes are linear. [If they are not both linear, the nonlinear least-squares best fit may be found as the limit of a sequence of linearized least-squares best fits]. The $M$-by-$M$ coefficient matrix for the finite-dimensional linear equation is entirely and uniquely determined by the hypothetical ocean (basin, linearized dynamics and error statistics) and the array (linearized measurement processes and error statistics). The conditioning of the matrix is revealed by diagonalizing, that is, by finding its eigenvalues and eigenvectors (Bretherton et al., 1976). Examples of eigenspectra are shown in Figure 3. The basin is the tropical Pacific and the dynamics are those of a linearized, coupled intermediate model. The error statistics are inferred from archived TAO data (Bennett et al., 1998, 2000), while the array is the TAO subsystem comprised of monthly-mean anomalies of SST, thermocline depth $Z20$ and surface winds $(u_a, v_a)$. It is clear that, at the assumed levels of measurement error, there are about 800 effective degrees of freedom in the 2600-component observing subsystem. Indeed, the subsystem is efficient for observing the hypothesized dynamics. Examination of the eigenvectors (not shown), associated with the largest eigenvalues, reveals those coupled circulation patterns that are the most stable to observe.

\begin{figure}[ht]
\centering
\includegraphics[width=\textwidth]{spectrum.png}
\caption{Spectrum of stabilized representor matrices. The number of observations $M$ is 2624 for Episode 1 (April 1994-March 1995, a moderate El Nino event) and 2644 for Episode 2 (April 1995-March 1996, a mild La Nina event). All three types of measurement (SST, $Z20$, $(u_a, v_a)$) have been included, and the measurement errors have been assumed uncorrelated. The measurements and their standard errors (0.3K, 3m, (0.5m/s, 5m/s)) have been scaled by r.m.s. anomaly values (2K, 50m, (5m/s, 2m/s)). The steps in the spectra arise from the different scaled standard errors. Note the striking similarity of these spectra for Episodes 1 and 2, even though they are derived from dynamics linearized about real nonlinear estimates of the ocean state during each episode. Thus, composite El Nino and La Nina estimates would have sufficed as backgrounds for linearization, and these spectra could have been derived a priori. Reducing the standard error of measurement of SST from 0.3K to 0.1K still leads to about 800 effective d.o.f., indicating that the scaled measurement errors for $Z20$ and for $(u_a, v_a)$ are more critical to the smoothing process.}
\end{figure}

The preceding array analyses used dynamics linearized about real ocean estimates, that were in turn made by assimilating real TAO data for major El Nino events into the nonlinear coupled model. The analyses could instead have been made with dynamics linearized about composite El Ninos, for example; that is, the analysis could have been made before deployment of the TAO array.

Several of these ocean estimates have been made, with real TAO data from several ENSO episodes. However, in every episode the significance test statistic was excessively large. It had to be concluded that the priors for the dynamical errors and data errors were wrong, and so it was unsound to have based an array assessment upon them.
Arrays should be designed using proven models, yet models cannot be proven until an array has been designed and deployed. The design requires some working hypothesis about the phenomena which are to be observed. The testing of models and the assessment of arrays are inextricably intertwined.

3 Perspective: intercomparison of data assimilation approaches and improvement of existing methodologies

The above list of important issues and challenges shows that, beyond the fact that the objectives are sometimes very different, common concerns are shared by many groups running large-scale ocean estimation and forecasting systems worldwide. The Global Ocean Data Assimilation Experiment offers the opportunity to intercompare the systems on some of these common issues, in particular:

- Physical consistency analysis and quality assurance (comparison to observations)
- Performance of the assimilation procedure: effectiveness of the use of observations, performance of the observational array, forecasting skill, overall control of model trajectory in error subspace, consistency check of prior hypotheses.

It is believed that two types of exercises of inter-comparing data assimilation approaches will coexist in GODAE: some of these tests will involve comparing whole systems, others just different data assimilation methods in the same model with the same data. Up until now there have not been many studies comparing different data assimilation methods in the same model configuration. In some instances, it may be possible to come up with a standard data set against which the different data assimilation methods can be tested. The time period should be at least one year so that the seasonal cycle and several different types of events are present in the data set. In addition to these types of studies, the different systems in GODAE can also be compared, but this would show more of the differences in the whole assimilation system than the data assimilation method itself. The model being used and the resolution will dictate much of the types of processes one would be able to resolve and model successfully, and it would have a great impact on the systems ability to perform successful forecast from the data assimilated initial conditions.

Other papers in this meetings address in detail the issue of common diagnostics. Recently Fox and Haines (2002) have developed diagnostics of heat and water volume budgets based on data assimilation statistics in an attempt to diagnose the reasons for model bias. They show that, during a 5 year (1992-96) assimilation experiment with the global OCCAM model, the impact of temperature profile assimilation over the North Atlantic region is largely to compensate for poor air-sea heat fluxes in maintaining water masses such as 18°C mode waters. This is quantified as a water transformation rate induced by the integrated effect of all the data assimilation events over the period and placed within the context of a Walin (1982) water budget. This is a step towards using data assimilation to learn about the deficiencies in models and further diagnostics of this type should be developed as GODAE proceeds.

Applications of “advanced” data assimilation schemes are expensive in terms of CPU and impose constraints on the model resolution one can afford to use. On the other hand, they provide a more consistent result at the resolution it is used, and one can also learn much about the behavior of the multivariate error statistics which vary as a function of time and space. Such information is also extremely useful when designing “simple”, OI-type schemes. In fact, it may be advantageous to first develop an advanced system and then use the information from this to improve the design of simpler and computationally more efficient schemes. Based on the previous discussion one can clearly justify the further development of both simple OI schemes and more sophisticated assimilation methods. Based on the actual application and its CPU requirement one will need to make a decision if an advanced scheme is affordable or if a simpler scheme must be used.
To move forward, progress is needed in the following areas in the GODAE time frame:

- Agreement on list of data assimilation-related diagnostics for each of us to look at -- including: innovation statistics per observation type, geographic region and depth, residual statistics, forecasting skill, cross-validation statistics (withheld data), statistical consistency checks
- Progress on modelling the model process noise and understanding its sources (atmospheric forcing, instability processes, physics, etc.)
- Better multivariate, balanced estimates of background errors, complemented by a posteriori dynamical consistency checks of the effect of those error estimates on non-observed variables
- Practical methods to estimate (evolve) the dominant modes of errors and use these in background error modelling: reduced-order methods (SEEK, ROIF), ensemble methods, partitioning methods, bred modes, etc.
- Practical methods to estimate variable open parameters, in several types of models (GCM, ecological, coupled): adaptive methods, Markov chain methods, etc.
- Theoretical and practical methods to correct the model bias and estimate the mean state of the ocean, e.g. using Gravity Recovery and Climate Experiment (GRACE) data, external climatologies
- A much fuller exploration of the control vector space, including adjustments to internal parameters such as diffusion and viscosity coefficients, and external parameters such as the bottom topography and lateral boundary condition relationships.

It is believed that the GODAE meetings will provide a forum to discuss these issues as well as the inter-comparison exercises mentioned above.

References


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