Synthesis and Assimilation Systems – Essential Adjuncts to the Global Ocean Observing System

Lead author: Michele M. Rienecker
Global Modeling and Assimilation Office, NASA/GSFC, Greenbelt, MD 20771 USA
Email: Michele.Rienecker@nasa.gov
Ph: +1 301 614 5642  FAX: +1 301 614 6246

Abstract
Assimilation systems synthesize diverse in situ and satellite data streams into full four-dimensional state estimates by combining the strengths of each data set and also of the model. The resulting analysis provides an integrated view of the information in the various observations as well as derived estimates of unobserved quantities. Assimilation systems are
particularly important for the ocean where subsurface observations, even today, are sparse and intermittent compared with the scales needed to represent ocean variability and where satellites only sense the surface. Increasingly, models and assimilation systems are being used to provide information about the current observing system and to help in the design plans for new observations. Whether it is as a user of observations or a contributor to evaluation of the observing system, ocean synthesis and assimilation systems are now an integral part of the global ocean observing and information system.

Major advances have been made over the last decade under the auspices of WCRP’s Climate Variability and Predictability Project (CLIVAR) and the Global Ocean Data Assimilation Experiment (GODAE). In addition to advances in the assimilation systems, there have been major developments in the observing system, with satellite altimetry, the tropical moored buoy arrays in the Pacific and Atlantic, and more recently Argo. These developments have led to significant advances in our understanding and prediction of ocean variations at both mesoscale and climate scales. Many challenges remain. Some of these challenges lie in the observations themselves, some in the assimilation systems that, even in the more recent era of unprecedented observations from satellite altimetry and Argo, provide different views of climate variations. Yet there are many examples of successful applications from ocean assimilation products. Use of these systems for assessing the observing system helps identify the strengths of each observation type, and indicates that none of the current observations is redundant. Indeed, the indication is that the ocean remains under-sampled and that further improvements in the observing system are needed for both climate monitoring and prediction. Future developments will be increasingly towards consistent analyses across components of the Earth system using, e.g., coupled atmosphere-ocean models.

1. Introduction

Data assimilation provides powerful constraints on predictive models. In assimilation, models are used to synthesize diverse in situ and satellite data streams into a single product (an analysis or state estimate) that combines the strengths of each data set and also of the model. The resulting analysis provides an integrated view of the information from the various observations as well as derived estimates of unobserved quantities such as currents, property transport, overturning circulations, etc. Assimilation systems are particularly important for the ocean where subsurface observations, even today, are sparse and intermittent compared with the scales needed to represent ocean variability and where satellites only sense the surface.

Assimilation products are used to initialize predictive models for both operational oceanography and climate applications. The synthesis also provides estimates of the history of the three-dimensional state of the ocean, documenting the variability of ocean circulation and improving understanding of the ocean’s role in climate. The products, with appropriate measures of uncertainty, offer a means for monitoring the state of Earth’s climate. In some cases, they provide information on precursors to climate variations such as the build up of warm water in the western equatorial Pacific prior to an El Niño event (see Xue et al., 2009 for a discussion of several such precursors).

Increasingly, models and assimilation systems are being used to provide information about the current observing system and to help in the design plans for new observations. Whether it is as a user of observations or a contributor to evaluation of the observing system, ocean synthesis and assimilation systems are now an integral part of the global ocean observing and information system.

In spite of the major advances made over the last decade under the auspices of WCRP’s Climate Variability and Predictability Project (CLIVAR) and the Global Ocean Data Assimilation Experiment (GODAE), many challenges remain. Some of these challenges lie in the observations themselves,
some in the assimilation systems that, even in the more recent era of unprecedented observations from satellite altimetry and Argo, provide different views of climate variations.

The prospects for future advances lie in improved models and better estimates of error statistics for both models and observations. With improvements in ocean modeling and assimilation and also in the atmospheric and coupled systems, the ultimate goal of consistent analyses across the components of the Earth system seems within reach. Several groups are now beginning to make progress in this new endeavour, with the promise of better initialization of climate prediction models and also better estimates of the air-sea fluxes needed to understand climate variations and trends.

This paper builds on the community white papers by Balmaseda et al., Bourassa et al., Breivik et al., Donlon et al., Fairall et al., Freeland et al., Goni et al., Griffies et al., Heimbach et al., Hurrell et al., Kwok et al., Le Traon et al., Lagerloef et al., Lee et al., McPhaden et al., Oke et al., Palmer et al., Snowden et al., Stammer et al., Trenberth et al., Wilson et al., and Xue et al.

Section 2 provides a brief overview of the state of the art of ocean data assimilation, and section 3 the challenges being faced particularly for ocean syntheses of the climate record. Section 4 provides a view of emerging developments and the path forward for the ocean data assimilation as an integral part of the global ocean observing and information system.

2. The current global synthesis efforts

Ocean state estimation comes from a synthesis of the available observations in the context of a physical model driven with specified surface fluxes. A wide variety of estimation methods are being used to perform ocean state estimation on a routine basis, ranging from relatively simple and computationally efficient sequential or filter methods such as optimal interpolation (OI), asymptotic Kalman filters, and the 3-dimensional variational (3DVar) method, to sophisticated and computationally intensive methods, including ensemble methods that provide state-dependent estimates of the multivariate forecast error covariances, Kalman smoothers, and the four-dimensional variational (4DVar) method. Surface fluxes may come from various sources, but widespread use is made of those from atmospheric reanalyses.

The international cooperation and organization under the auspices of GODAE had an indelible impact on the routine generation of synthesis products and the outreach to user communities (Bell et al., 2009). GODAE not only demonstrated the feasibility of global ocean data assimilation but also made important contributions to the establishment of an effective and efficient infrastructure for global operational oceanography that includes the required observing systems, data assembly and processing centers, modeling and data assimilation centers and data and product servers. Many successful applications from GODAE systems are highlighted in Le Traon et al., (2009): monitoring and prediction of marine pollution (such as oil spills), forecasts for safety and effectiveness of operations at sea, information and tactical decision aids to assist Naval operations, operational use of upper ocean heat content information to forecast the intensity of tropical cyclones, and ocean initialization of coupled climate forecast systems.

Ocean climate analyses have been undertaken for the initialization of seasonal forecasts since the mid-1990’s (e.g., Ji et al., 1995; Behringer et al., 1998, Ji et al., 1998, Segschneider et al., 2000). During the last decade, seasonal forecasting has reached a mature state, with several operational centers around the world issuing routine seasonal forecasts produced with coupled ocean-atmosphere models (see Balmaseda et al., 2009a). To provide meaningful forecast anomalies, the coupled model forecast drift has to be removed, requiring retrospective forecasts (hindcasts). These ocean reanalyses and re-forecasts also provide information for forecast calibration and skill assessment. Advances in assimilation systems for the ocean, the organization of the archive of historical in situ data and the
onset of the era of high quality altimetry, and, most importantly, the availability of atmospheric reanalyses spurred the generation of historical ocean climate reanalyses for the study of climate variability (e.g., Ji et al., 1995, Stammer et al., 2002, Carton and Giese, 2008, inter alia). Today, a suite of global ocean climate synthesis products is available, some extending for a duration of 50 years, others focusing on the data rich period of the ocean satellite era, roughly from 1993 to the present. The number of studies using these products for oceanographic and climate-related studies covers a wide range of topics, as highlighted in Lee et al. (2009): ocean circulation studies, sea level variability, water-mass pathways, estimation of surface fluxes and river runoff, and interannual and decadal variability of the upper-ocean and heat content. They have also been applied to research in other disciplines such as biogeochemistry and geodesy.

Le Traon et al. (2009) provides a summary of GODAE and its the achievements and sets the stage for the next phase, OceanView. Cummings et al. (2009a) provides an overview of the assimilation methods used by many GODAE systems, and Dombrowsky et al. (2009) provides an overview and comparison of twelve of the systems developed/operated during GODAE. Most centres now operate systems with 1/10° or finer horizontal grid spacing, have a global capability, and make use of community ocean models (e.g., HYCOM, MOM4 or NEMO). Lee et al. (2009) and Balmaseda et al. (2009a) provide information on many of the systems used for climate applications. Because of their need to synthesize the historical data stream, climate-focused systems tend to have coarser resolution, from about 0.25° to about 2°, usually with some equatorial refinement.

Many data types are routinely synthesized to produce ocean state estimates. The most commonly used are sea-surface height (SSH) anomalies from altimeters (e.g., TOPEX/Poseidon and JASON-1, -2, see Wilson et al., 2009), in situ temperature (T) profiles from XBTs/CTDs (Goni et al., 2009), the global tropical moored buoy array (McPhaden et al., 2009), and Argo (Freeland et al., 2009), and in situ salinity (S) profiles from Argo. Sea surface temperature (SST) estimates (e.g., Reynolds et al., 2002; Donlon et al., 2009) are either assimilated directly or used as a surface boundary condition. Salinity data from CTDs and velocity data from current meters and ADCPs are usually used for validation. Gravity measurements from GRACE and the newly launched GOCE provide estimates of the geoid for use with altimetry as well as derived bottom pressure estimates (e.g., Jayne et al., 2003; Kowk et al., 2009).

Figure 1: The impact of the modern global ocean observing system on the global meridional overturning circulation (in Sv). The panels show RMS variability differences between ocean state estimates, based on bi-weekly averaged fields over the year 2006. Top left: the impact of jointly adding SST, SSH and in situ (T, S) data to a baseline estimate consisting only of hydrographic climatology. Top right, bottom left, bottom right: the impact of adding SST, SSH, and in situ (T, S) data individually.
Various studies have shown that different data types provide complementary information from the Global Ocean Observing System (GOOS). Oke and Schiller (2007) undertook analyses of the observing system for mesoscale applications (see Section 4b). They infer that all observation types are required for constraining mesoscale circulation models. An example from climate analyses is that of Forget et al. (2009, in preparation, see Heimbach et al., 2009) who incrementally added different data types to an ECCO synthesis for 2006. Figure 1 shows the differences in RMS variability of the global meridional overturning circulation from their study as different data sets are added. The results imply that overturning uncertainties would exceed 3 Sv in the absence of the modern observing capabilities. While the specific value may be particular to this experiment, uncertainties of at least this magnitude are likely to prevail in state estimates prior to the emergence of modern observing capabilities in the 1990’s. The other panels show the impact of individual data sets. Not surprisingly, the stronger constraints on the overturning circulation come from altimetry and the in situ data (mostly Argo), while SST data provides a weaker constraint.

Even the most recent atmospheric reanalyses provide different estimates of many aspects of the atmosphere’s climate, particularly in the unconstrained variables such as precipitation and cloud properties. This is also the case for the different ocean state estimates: the underlying models and assimilation approaches differ, the weights (prior background and observation error covariances) given to observations and models differ, and the data selections differ. Of course one expects that the largest differences between state estimates would occur in times of fewer observations when different surface forcing is applied (see Section 3c) and the state estimates in the deeper ocean are still influenced by the initial states.

Depending on the application, a more reliable estimate of ocean climate variability may lie in multi-model ensemble approaches. To proceed with this, one needs detailed error estimates for the estimated states, something that is difficult to obtain with most of the current assimilation implementations. Nevertheless, an important step toward improved estimates of the time-varying ocean state and its transport properties is to understand the uncertainties in each estimate, or at least the differences between products. As a cooperative effort of the CLIVAR Global Synthesis and Observations Panel (GSOP) and GODAE, many assimilation groups in the U.S., Europe, and Japan have participated in an effort to compare a suite of derived diagnostic quantities from the different products and also with observations. The analysis intercomparisons help identify commonalities (confidence) and differences (uncertainty) in the products and help identify how or when observations constrain the estimation effectively. More details can be found in CLIVAR GSOP web page http://www.clivar.org/organization/gsop/gsop.php.

As one of the outcomes of this intercomparison, Stammer et al. (2009) compares the variability in state estimates from multi-decadal syntheses (Balmaseda et al., 2008; Behringer, 2007; Carton and Giese, 2008; Domingues et al., 2008; Ingleby and Huddleston, 2007; Köhl and Stammer, 2008; Martin et al., 2007; Masina et al., 2004; Smith and Haines, 2009b; Smith and Murphy, 2007; Sun et al., 2007; Weaver et al., 2003). There is a large spread in the various estimates of some quantities such as global upper ocean heat and freshwater content (Figure 2), with an even wider spread in transport estimates (not shown). Although the spread is, to some extent, due to different approaches or underlying data sets, it is somewhat surprising that the spread increases toward the end of the data record characterized by the largest number of observations. Stammer et al. (2009) shows more detail, with estimates in the individual basins. The agreement in heat content is much better in the well-observed Atlantic Ocean. The spread in freshwater content variability between all estimates is very large, suggesting a general problem of existing ocean simulations in determining the salt content from observations. This affects estimates of many climate indices, including global sea level rise.

Some of the differences and issues with the estimates in global metrics such as heat and freshwater content lie in the atmospheric forcing used. Atmospheric reanalyses, or other sources of surface forcing, are not constrained to conserve quantities such as energy and water. Trenberth et al. (2009)
find that global mean biases in surface fluxes can exceed 10 W m\(^{-2}\), with much bigger biases locally and in individual components. See Section 3b for further discussion.

Historical ocean state estimates rely on conventional ocean observations such as XBTs. It was shown recently that XBT data are contaminated by previously undetected errors in the assumed drop rate (Gouretski and Koltermann, 2007). Several new data-only analyses have been made of the ocean heat content based upon corrected XBT fall rates and other adjustments to the basic data. These updated analyses tend to remove a lot of decadal variability (Domingues et al., 2008; Wijffels et al., 2008; Ishii and Kimoto, 2009; Levitus et al., 2009). The Domingues et al. (2008) estimate is included in Figure 2a. Continued efforts are needed to address observational biases and, as a corollary, continued efforts are needed to improve ocean reanalyses by using the updated observation databases.
Sea level or SSH is an important climate variable whose variations have enormous impact on coastal communities. Figure 3 shows three synthesis estimates of local thermosteric and halosteric SSH changes, representing the spread from the syntheses presented in Stammer et al. (2009). SODA (Carton and Giese, 2008) uses in situ profiles to correct the model’s T/S structure locally in space and time. Altimetry is projected on synthetic T/S changes and only the latter are used as constraints. The GECCO results (Köhl and Stammer, 2008) represent the adjoint-family of approaches. Also shown are results from the ECMWF system (Balmaseda et al., 2008), which is tuned to improve SI forecasts. Results are shown for the periods 1962 – 2001 and 1992 – 2001, respectively.

Estimated trends over the entire 40-year period from these three products differ substantially, especially between SODA and GECCO. This is obvious for temperature but holds equally well for salinity. Over large parts of the world ocean, GECCO results suggest that SSH changes induced by heat content changes and changes in salinity counterbalance to some extent. Such a counter balance is less visible in the SODA analysis. For the more recent period, the three estimates of large-scale drifts in the thermosteric SSH are in much closer agreement although there are still notable differences in the Atlantic Ocean. Halosteric estimates also tend to converge but again there remain substantial differences, e.g., in the subpolar North Atlantic.

Understanding the differences between the analysis products and making further improvements in assimilation capabilities may require a concerted comparison effort wherein runs are undertaken with the same data and forcing and the analysis diagnostics are expanded to look at innovations and the details of data impacts.

3. Challenges

Perhaps the two greatest challenges for ocean data synthesis as a climate data record are the historical data themselves and the ability to make uncertainty estimates for the synthesis products. With the former, the severe under-sampling of the water column and of most regions of the ocean in the early periods, the issues of biases/uncertainties in air-sea fluxes (Trenberth et al., 2009b) and model biases (Griffies et al., 2009) take on greater importance.

3a The Observing System

Along with the view from synthesis comparisons noted above and in the plenary paper by Balmaseda et al. (2009b), Carson and Harrison (2008) provide another view of estimated trends in ocean temperature and issues faced by the climate community because of the uneven observational coverage in both space and time. They find that the estimated 50-year trends over most of the ocean are not significant at the 90% confidence level (CL). In fact at 50 m, only 30% of the ocean has a statistically significant trend with 90% CL, and the percentage decreases significantly with increasing depth. The estimated 50-year trends have a lot of spatial structure, with areas of strong warming and strong cooling. Together with major temporal and spatial sampling limitations, they suggest that upper ocean heat content integrals and integral trends may be substantially more uncertain than has yet been acknowledged and that further exploration of uncertainties is needed.

Some of the issues with data distribution are obvious from Figures 4a and b, showing the non-stationarity of the observing system, the under sampling of the deeper ocean even in the last two decades, and the decline of the in situ observing system in the marginal seas. The apparent horizontal strata reflect the successive influence of 450-m XBTs, 750-m XBTs, 500-m tropical moored buoys and 1000-m and 2000-m Argo floats. The importance of Argo to the ocean observing system is obvious (Freeland et al., 2009). The sampling situation is markedly worse for salinity observations (not shown), and the importance of Argo is magnified (e.g., Figure 6 below). However, Argo does not currently help in observing the marginal seas, so an alternative such as gliders (e.g., Testor et al.,
2009), is needed to address the observing system decline there.

![Figure 4a: The number of global temperature observations per month as a function of depth. The data sources are XBTs, the global tropical mooring arrays and Argo floats.](image)

![Figure 4b: As for Figure 4a, but data counts are restricted to the Gulf of Mexico and the Caribbean. Note the difference in colour scale from Figure 4a.](image)

These changes in the GOOS over time have an impact on estimates not only of trends but also of decadal variability even when the estimates are made through assimilation of the historical record. The changes also impact the ability to confidently assess and calibrate seasonal climate forecast skill.

One source of differences and/or deficiencies in the various ocean synthesis products is the input data stream. Different choices are made in data selection, and even different data sources are used. Systematic data errors have been identified and different approaches developed for reducing those biases, particularly in XBT temperatures, as mentioned above. For Argo, the issues concern float pressure sensors and salinity sensor drift (e.g., Freeland et al., 2009). Systematic errors of even 1 dbar are a concern if trying to detect slow signals of global climate change. High quality CTD transects provide the standard for assessing data quality in profiling floats. Much work is yet to be done in assembling available shipboard datasets and analyzing them jointly with Argo to identify and correct systematic errors. Assembling the best-quality data is a multi-year endeavour (Freeland et al., 2009).

The changing set of observation databases poses another challenge for the assimilation community. This is particularly so when different data sets are used in different systems. The time to re-synthesize
data sets with the more sophisticated data assimilation methods precludes rapid refresh of synthesis products with potentially frequent updates in data corrections. This issue also highlights the importance of attention to the organization of data sets and the use of metadata and version control in the archive of all data. Snowden et al. (2009) proposes that the community adopt standards for describing and versioning metadata, quality control, and observational data.

Another source of differences between products is the different quality control procedures used. Data quality control is a fundamental component of any analysis/forecast system. Quality control must correctly identify observations that are obviously in error, as well as the more difficult process of identifying measurements that fall within valid and reasonable ranges, but nevertheless are erroneous. It is likely that decisions made at the quality control step affect the success or failure of the entire analysis/forecast system. Effective quality control requires a set of pre-established, standardized test procedures, with results of the procedures clearly associated with the data values. At present, there are few agreed-upon standards for ocean data quality control and very few cases where the procedures and results from the oceanographic centers have been compared. The GODAE Quality Control Intercomparison Project (see Cummings et al., 2009b) is taking the first step by comparing the outcomes of profile data quality control procedures from five oceanographic centers. The results are available on the US GODAE server: http://www.usgodae.org/ftp/outgoing/godae_qc.

Figure 5: Vertical integrals of zonal average temperature and salinity trends, translated into density trends (abscissa, units in kg/m²/yr) as a function of latitude (ordinate), from the updated ECCO-GODAE solution v3.73 (Wunsch and Heimbach, 2007). Black: full water column; dark blue: 0-848 m; red: 848-1975 m; green: 1975-2450 m; cyan: 2450-5450 m.

Even with the marked improvement in the global in situ data coverage with Argo, the current GOOS has a number of serious shortcomings. In addition to the decline in the marginal seas noted above, the deep ocean (below 2000 m) and ice-covered regions remain largely unobserved. The need to observe the ocean over the full water column is evident from ocean analyses. Figure 5, from Heimbach et al. (2009) (see also the discussion in Palmer et al., 2009), shows that changes are not restricted to the upper ocean. Abyssal trends are apparent, especially in the Southern Ocean region, but these would be missed in most of the current in situ observations. Repeat observations from WOCE indicate that some areas in the Southern Oceans have warmed significantly between 700 and 3000 m (Palmer et
al., 2009), so it is not clear that the current ocean state estimates are constrained well enough at depth. In general, the deep ocean can be expected to grow in importance with the time-scale of interest.

Currently, the only full-depth ocean observations come from dedicated hydrographic cruises that can only sample a very small area of the deep ocean. In the future, these hydrographic cruises must be augmented by an array of deep floats, moored instruments, gliders, or a combination thereof. Improvements in remotely sensed measurements of vertically integrated ocean mass (or equivalently bottom pressure, see Jayne et al., 2003) such as from the proposed GRACE-II mission could also help constrain the deep density field when combined with sea level and upper ocean information.

To improve estimates of climate variations, we also need to enhance information about boundary currents and transports through key regions, and pursue the satellite-derived sea-ice thickness from CryoSat-2 and ICESat-2 (e.g., Kwok et al., 2009). For the Arctic, Kwok et al. (2009) makes the case for water temperature and salinity observations within the upper 800 m in the deep parts of the Arctic Ocean in addition to observations for monitoring riverine freshwater fluxes.

In addition to new observations, important satellite measurements such as altimetry, gravity (bottom pressure), SST from both microwave (all-weather) and infra-red (high resolution) sources, scatterometer winds, sea-ice concentrations, and ocean colour must be maintained. Even with Argo, other elements of the in situ observing system also need to be maintained and enhanced. In particular, the global tropical moored buoy array is essential for its provision of high frequency observations for short-term climate forecast initialization (for which consistency of the observing system over time is an issue in the calculation of drifts and calibration of forecast skill). The planned tropical moored buoy array in the Indian Ocean, RAMA, needs to be completed, not only for the Indian Ocean variability itself, but also to aid forecasts of intraseasonal variations that play a role in the evolution of El Niño events. In the Pacific, additional moored buoys east of 95°W are needed to constrain model biases in the far eastern basin. Skillful seasonal forecasts remain a challenge in the tropical Atlantic so the enhancements of the PIRATA mooring array (Bourlès et al., 2008) should be maintained for sufficient duration that the impacts on seasonal forecasts can be established. As with the TAO/TRITON array, any velocity data at the mooring arrays would be helpful for independent evaluation of the assimilation products. Of course the ocean velocity field, at all depths, is poorly observed. Any velocity observations throughout the water column would be helpful not just for validation but also for input to high resolution, operational oceanography applications.

Lastly, new satellite measurements like sea surface salinity from space will be available soon and need to be pursued in the future. The upcoming SMOS (end 2009) and Aquarius (2010) mission will provide for the first time a quasi-synoptic view of ocean surface salinity that should be beneficial to ocean synthesis. This will be an additional constraint on the large-scale surface density field but also on the mixed layer salinity budget.

Most importantly, we need to continue to evolve ocean state estimation as an integral part of the ocean observing and information system.

3b Surface Forcing

Long atmospheric reanalyses have been a critical source of forcing for ocean model simulations and analyses. These reanalyses face similar issues to the ocean historical analyses – changing observing systems and lack of error estimates – that only compound the problem for climate analyses and predictions. The previous generation reanalyses (e.g., NCEP/NCAR and ECMWF/ERA-40) had major global imbalances in basic climate parameters of importance to the ocean (heat and freshwater fluxes). The latest generation, MERRA (Bosilovich et al., 2006) and ERA-Interim (Dee and Uppala, 2008), are significant improvements on the earlier analyses but are relatively short for ocean climate analyses, covering only from 1979 and 1988, respectively, to the present. Although improved from
previous reanalyses, they still show impacts of the changing observing system on global water and energy variations, and retain some global heat and freshwater imbalances. For real-time oceanographic analyses, it is the real-time Numerical Weather Prediction (NWP) analyses and forecasts that provide the needed forcing.

The development of improved atmospheric datasets to force global ocean-ice climate models is a key area that needs continual attention. The ocean modeling community has tended to tackle this task itself. Three examples are the following: the forcing data set prepared for a global ocean-ice model comparison, the Coordinated Ocean-ice Reference Experiments (CORE) (Griffies et al., 2009a) using the atmospheric forcing dataset (based on the NCEP/NCAR Reanalysis) compiled by Large and Yeager (2004) and updated by Large and Yeager (2009); an analogous dataset based on ECMWF reanalysis by Röseke (2006); and the DRAKKAR Forcing Set 3 (DFS3, Brodeau et al., 2009; Smith and Haines, 2009a) based on ERA-40 and tuned to fit the needs of the DRAKKAR model configurations. The Objectively Analyzed air-sea Fluxes (OAFlux, Yu and Weller, 2007) is an example of a blended product that is based on NWP and satellite data and uses in situ data to guide the weights used in the blend. Fairall et al. (2009) point out that all these products also suffer from changes in the observing system and, possibly, changes in the operational NWP system. Hence, the problem of inhomogeneity remains in diagnostics of decadal variability and trends. Problems can also arise with a mismatch of scales when data from different sources are combined in flux algorithms.

The continuation of surface observations from space is essential to the estimation of air-sea fluxes. Scatterometer missions are essential to the goal of constraining surface momentum and turbulent heat fluxes. Improvements needed for the coming decade include improved sampling at high wind speeds and rain conditions (Fairall et al., 2009; Bourassa et al., 2009) and, ideally, resolution of the diurnal and inertial forcing. Remote sensing of latent and sensible heating remain a challenge (Liu and Curry, 2006) with considerable uncertainty in how to remotely estimate near-surface air temperature and humidity (Jackson et al. 2006). An additional challenge is estimation of fluxes through sea ice, where the ocean surface climate is noticeably different from the open ocean. Continued measurements of surface shortwave radiation, and its penetration into the upper ocean, are essential to support simulations of interactions between ocean biology and physics. Rainfall measurement missions are essential for freshwater flux estimates. The uncertainty in precipitation over the ocean is large – differences between satellite estimates and NWP product can be greater than 10mm month\(^{-1}\) in the tropics. The planned GPM mission should help reduce precipitation uncertainties in the future.

In situ surface measurements are particularly important for calibration of satellite-derived fluxes and evaluation of NWP and reanalysis flux estimates. Fairall et al. (2009) summarize the various in situ sources of fluxes. They recommend expansion of the surface flux reference network under OceanSITES, especially in higher latitudes and in areas with severe weather conditions, and expanding the ship-based measurement program. The increased coverage would help improve NWP products as well as the estimation of uncertainty in these products. The in situ measurements are also critical for climate quality calibration of satellite observations.

It is possible that constraints on fluxes will come more from assimilating ocean data than from direct estimates, however the entanglement of model error with forcing error is strong and care is needed in the interpretation of such inferred fluxes. Certainly progress is needed in consistent estimation of air-sea fluxes using constraints from observations in the atmosphere and the ocean, perhaps in coupled models. This is discussed more in Section 4a.

3c Modeling and Assimilation Challenges

Other challenges for ocean data assimilation lie in covariance modeling of the background or forecast fields and of observation errors, including representation error, and in the ability of the observations
to constrain the mesoscale ocean variability. Of course improving the models themselves is also a high priority.

The estimates of model and data errors dictate the outcome of the estimation product. Therefore, the ocean state estimation community needs to work closely with observationalists to obtain robust estimates of data errors (including biases), an important issue that is often left to assimilation groups. Of course representation error is a function of the model, its resolution, and the phenomena of interest in the analysis. Little attention has been paid to the representation errors for in situ data to date; some progress is being made with satellite data which is much more amenable to analysis because of its better sampling characteristics (e.g., Kaplan et al., 2009; Miller, 2009). The new air-sea flux data set by Berry and Kent (2009) includes estimates of representativeness errors due to sampling and includes the representativeness errors for subdaily variability in its random error estimates.

An important part of the assimilation procedure is the preparation or screening of the input through quality control software. Here too, collaboration between the assimilation and observational community is important. Particular care needs to be given to the clear documentation of the procedures employed, as in Ingleby and Huddleston (2007) and Gaillard et al. (2009).

A close collaboration between the assimilation and modeling communities is needed to understand model errors better. A close collaboration is also needed between the climate modeling and observational communities to assess where observations and models diverge, and develop methodologies to resolve differences. Griffies et al. (2009b) discusses origins of biases and differences between model simulations and between models and observations: shortcomings in grid resolution, both horizontal and vertical; improper numerical algorithms; incorrect or missing subgridscale parameterizations; improper representation of other climate components such as the atmosphere, cryosphere, ocean biogeochemistry, and land runoff; and possibly other reasons not yet identified. The authors suggest that comparisons would be substantially aided if observations collected on pressure surfaces were retained in that form rather than, or in addition to, being translated to depth coordinates.

Observational studies are useful for refining and evaluating parameterizations in various regions, e.g., overflows, interior mixing, mesoscale eddies (where surface expressions are sampled byaltimeters, and the interior by Argo). Climatologies of the mixed layer formed from in situ data are valuable for evaluating model mixed layer and submesoscale parameterizations. The Repository for Evaluating Ocean Simulations (REOS, http://www.clivar.org/organization/wgomd/reos/reos.php) is a centralized source for data and a location for the observational community to advertise new products of use for modelers.

Of central importance to ocean state estimation is the ability to correct both temperature and salinity and maintain dynamical balances. This has been achieved through multivariate assimilation schemes using empirical orthogonal functions (Maes et al., 2000; Fujii and Kamachi, 2003; Testut et al., 2003; Usui et al., 2006) or temperature–salinity covariances from asymptotic Kalman filter/smoothers (e.g., Fukumori, 2002) or ensemble-based filters (e.g., Zhang et al., 2007; Keppenne et al., 2008) that are well suited to handle the nonstationary stochastic processes like climate variations in which the error structure of flows is highly anisotropic and time-varying. These multivariate relationships can also be important to effective assimilation of altimeter data (e.g., Keppenne et al., 2008). In their study, Zhang et al. (2007) show that with the multivariate covariances from an ensemble filter salinity errors at the equator are reduced by 45%, vertical motion errors by 81%, and the undercurrent errors by 50% compared with univariate assimilation of temperature only. Balmaseda et al. (2009b) discuss the importance of multivariate corrections to temperature, salinity and sea level and the positive impact on seasonal forecast skill. Yang et al. (2009a, b) show that state-dependent multivariate covariances can be effectively estimated with coupled breeding approaches and that improvements in the salinity
state estimates and density stratification have an impact on forecast skill. Of course 4D-var approaches implicitly include flow-dependent relationships and balances but still require estimates of the background and model error statistics.

A sense of the critical nature of the treatment of salinity in the pre-Argo era, and the importance of Argo, can be gained from Figure 6, where the ECMWF ocean data assimilation system (S3, Balmaseda et al., 2008) has been used to assess the impact of Argo salinity observations on a global salinity analysis in the upper 300 m (S300). There are many areas where the effect of temperature on S300 is contrary to the direct effect of using salinity. S3 uses the Haines et al. (2006) algorithm to correct salinity along isotherms to maintain important water mass properties. Haines et al. (2006) show that this \( S(T) \) assimilation algorithm should have error covariance properties that allow the longer temporal and spatial scales of water mass variability to be used to increase the impact of observations. Smith and Haines (2009) show that assimilating salinity along isotherms improves upon conventional depth-level assimilation.

![Figure 6: Impact of Argo on the average salinity in upper 300 meters (S300, in psu) in the ECMWF S3 analysis.](image)

The quantification of model errors for the specification of forecast error covariances in 3DVar or Kalman filter/smooth approaches is only one area that needs attention. The identification of model error sources is also critical to estimation based on control theories. Some model errors are attributable to multiple sources. For example, a biased SST estimate in the equatorial Pacific cold tongue could be related to errors in wind, surface heat flux, or mixing parameterizations and advection (also related to resolution). Determination of the appropriate “controls” and correct attribution of error sources are important to the fidelity of the estimation products.

The uncertainty in the analysis solution arising from assumptions made about the cost function – the imposition of balance and other constraints, error specifications, the controls – is as yet an unexplored area of investigation. A related question is the impact on the solution of requiring that the model equations be satisfied so that budgets can be balanced. For some climate applications, it has been argued that forcing the balance is necessary. Most ocean assimilation systems do not follow this approach. For atmospheric assimilation systems, the tendency has been to use the extent of imbalance
as one measure of the quality of the system. Ocean assimilation systems would benefit from being evaluated in a similar vein. The impacts of some of these choices will only be understood through controlled intercomparisons where the same model, data, QC, and forcing are used.

Although many of the assimilation efforts for operational oceanography applications are at resolutions of about 1/10°, most of the state estimation products for climate applications have resolutions that are too coarse to represent mesoscale eddies. As these eddies affect the climate through their interaction with the larger scales, it is imperative that ocean state estimation efforts move towards eddy-permitting resolutions. An important issue is that the in situ data are not adequate to constrain the mesoscale and the emphasis is placed on multiple sources of altimeter data to capture eddy variability. The future Surface Water Ocean Topography (SWOT) mission (Fu et al., 2009) is expected to provide new insight to ocean variations at scales smaller than the ~100km scale currently possible. Increased horizontal model resolution is also needed to take better advantage of the fine spatial scales of the next generation NWP surface forcing.

Le Traon et al. (2009) outlines other issues related to resolution for operational oceanography as the user community is looking to extend models inshore, across the shelf, and into bays and estuaries. Attention is needed for better methods for nesting models, or for variable resolution and adaptive model grids. In addition, depending on the relevant dynamics of the situation (e.g., local topographic effects, wind wave, tidal currents, land freshwater input, etc.), assimilation methods have to be developed to constrain not only the large-scale (quasi-) geostrophic field but also fields influenced by small-scale nonlinear processes. Of course, the extension of data-assimilation systems inshore assumes that coastal observing systems will be developed to support them. Cost-effective in situ coastal observing systems will be a challenge. Many satellite observations also have issues near shore; further work is needed to improve satellite technology and capability in this environment.

4. The future

Ocean data assimilation has matured in significant ways over the last decade. The deficiencies in the historical data collections cannot be rectified. However, with the advances made with satellite altimetry, Argo and the global tropical moored buoy arrays, and the upcoming observations such as the completion of the RAMA array in the Indian Ocean (McPhaden et al., 2009) and satellite measurements of surface salinity (Lagerloef et al., 2009), we can be certain that further significant advances will emerge in the coming decade. Some exciting advances, like the contributions being made to observing system evaluation/design and the developments of assimilation in coupled ocean-atmosphere models, are already underway.

4a Integrated Earth System Analyses

The various observations of Earth’s environment are currently assimilated through analysis or state estimation techniques that typically involve individual components of the Earth’s climate system. As such, the state of one component is not adequately constrained by the observations and dynamics of other components and the resulting state estimates are not necessarily consistent across the various components. This hampers research on the attribution of causes of the variability and changes within the coupled system and limits the skill of climate prediction. In 2003, the report from the “Workshop On Ongoing Analysis of the Climate System” (Arkin et al., 2004) recognized the importance of consistent analyses, perhaps through the coupling of components during analysis: “One essential aspect of a comprehensive climate observing system is the capability to synthesize observations into a coherent, internally consistent depiction, or analysis, of the evolution and present state of global climate.” For the ocean, the issue is not just coupling with the atmosphere, but also with sea-ice and ocean biology, and also with the land surface.
There are many issues to be addressed in tackling this problem, not least of which are the differences in time scales for the ocean and atmosphere, both processes and observations. Another area of concern is the biases in coupled models (see Griffies et al., 2009b). These will have a detrimental impact on state estimates during periods that are observation-challenged. However, biases are significantly reduced at high resolution and it is the role of data assimilation to compensate for errors, including biases if the appropriate formulation is used.

There are a few groups pioneering this new horizon of estimation using coupled ocean-atmosphere models. None of the current implementations actually undertakes the very complex task of assimilating atmospheric observations. Zhang et al. (2007) use an ensemble Kalman filter implementation and assimilate a pre-existing atmospheric analysis along with the ocean observations. Sugiura et al. (2008) use a 4DVar implementation to estimate drag (coupling) coefficients used in the calculation of momentum and heat fluxes between the ocean and atmosphere, along with the ocean initial state. Fujii et al. (2009) assimilate ocean observations into a coupled model and find an improvement in several atmospheric fields over those from an atmosphere-only run using observed SSTs. Coupled estimation efforts are expected to evolve markedly as the climate community continues to improve initialization for seasonal climate prediction and embarks on decadal prediction.

Breivik et al. (2009) discuss the importance of data assimilation for estimating sea-ice concentrations, which, like SST, are important as lower boundary conditions for the atmosphere as well as for ocean state estimation. Simple analysis techniques have been used in weather prediction centres for some time. Now more advanced techniques (including the ensemble Kalman filter of Lisæter et al., 2003 and the variational implementation of Caya et al., 2009) are starting to emerge as ocean models and assimilation systems evolve to be truly global. Future developments will be in two main areas. The first is the development of techniques to incorporate as many observational observations as feasible. Currently, the observations that have been assimilated are those from passive microwave instruments, ice charts and ice drift. Other observations, such as active radar and satellite-derived sea-ice thickness from the future CryoSat-2 and ICESat-2, will be incorporated over the coming years. The second development area lies in improving the prior estimate provided by coupled atmosphere-ice-ocean models that propagate information from past observations.

With the growth of operational oceanography the demand has also been growing for data and information relevant to understanding the global marine ecosystem, unravelling the functions of the marine ecosystem in a changing climate, and contributing to sustainable management of marine resources. Sathyendranath et al. (2009) outlines a program for the integration of in situ and remotely-sensed data relating to ecosystems. Whereas the former can give information about, for example, the vertical structure of chlorophyll-a, main phytoplankton groups and specific rate constants (e.g., photosynthetic parameters) at a particular geographic location, the latter can provide information about the chlorophyll-a field at the regional and global scales at daily to weekly intervals. The combination of both approaches can give estimates of important ecological variables, such as of the water-column integrated primary production. Assimilation provides the best means to combine the information from both sources. As examples of ocean colour assimilation, Nerger and Gregg (2007) and Gregg (2008) have undertaken global synthesis of satellite-derived chlorophyll-a. During the next decade coupled physical-biogeochemical assimilation can be expected to emerge, providing new insights not only to ocean biological variations and the marine carbon cycle but also into the feedbacks within the physical climate system.

The pathway to an eventual fully integrated Earth system analysis will continue to proceed incrementally, with advances in coupling between two or three components at a time.
4b Realizing the potential of analyses and models in observing system design

An important and emerging role for ocean data assimilation is the assessment of the contribution of the various components of the observing system and scientific guidance for improved design and implementation of the ocean observing system. As ocean models and assimilation systems have improved in quality over the years, ocean analysis and forecasting systems and associated tools, such as adjoint sensitivity diagnostics, are powerful means to assess the impact of the observing system for particular applications, to identify gaps and thereby improve the efficiency/effectiveness of the observing system.

Observing System Experiments (OSEs) where different components of the GOOS are systematically withheld can help quantify the impact of each observation type on the quality of analyses or the skill of a forecast. Various other techniques, including observing system simulation experiments (OSSEs), adjoint- and ensemble-based approaches, can be used to aid the design and evaluation of ocean observing systems. Examples of various evaluations of the observing system can be found in Oke et al. (2009), Balmaseda et al. (2009a, b) and Heimbach et al. (2009). A couple of examples are highlighted here.

Figure 7: Preliminary estimates of the Information Content (IC; %), degrees of freedom of signal (DFS) and the number of assimilated super-observations (# Obs) for the Bluelink reanalysis system in the region 90-180°E, 60°S-equator, computed for 1 January 2006. The scale for the IC is to the left and the scale for the DFS and # Obs is to the right, from Oke et al. (2009).

One recurring result from different OSEs includes the complimentary nature of different observation types (e.g., Guinehut et al., 2004; Oke and Schiller 2007; Balmaseda et al. 2008). For example, Oke and Schiller (2007) performed a series of OSEs to compare the relative impact of Argo, SST and SLA observations on an eddy-resolving ocean reanalysis. They systematically withheld altimeter, Argo and SST observations. They found that satellite SST observations are the only observation type considered that have the potential to constrain the circulation in shallow seas and over wide continental shelves; altimetry is the only observation type that even goes close to constraining the mesoscale ocean circulation; and Argo observations are the only observation type that constrains sub-surface temperature and salinity (Figure 7). None of the observation types in the GOOS was found to be redundant. Each different observation type brings unique contributions to the GOOS and all observation types should be routinely assimilated by forecast and reanalysis products and, more importantly, maintained by the international community. The consistent use of and impact from SST observations is a credit to the GHRSSST program that provides high level quality controlled SST data in near real-time (Donlon et al., 2009).

Another result that is common to many studies is the necessity of assimilation of altimeter data to represent mesoscale variability (e.g., Oke and Schiller 2007; Martin et al., 2007; Pascual et al., 2006; Benkiran et al., 2009). Studies by Pascual et al. (2009) and Benkiran et al. (2009) have shown that four altimeters are needed in real time to get the similar quality performance as two altimeters in
delayed time. A series of OSEs using the 1/9° UK Met Office system quantify the analysis improvements from 1, 2 and 3 altimeters (Figure 8). The impact of different numbers of altimeters is assessed by comparing the analyzed sea level anomaly (SLA) with the assimilated along-track altimeter data, and the analyzed surface velocities with those derived from surface drifting buoys (which are not assimilated). The addition of the first altimeter has the greatest impact. This is consistent with the results of Benkiran et al. (2009). The results are different for different regions. Mesoscale dynamics in the Northeast Atlantic seem to be constrained better by the altimeters than in the Northwest Atlantic.

Figure 8: Anomaly correlation between forecast SLA and along-track altimetric SLA from all satellites (left) and forecast near-surface velocity and near-surface velocity derived from drifting buoys (right). The results are based on a series of OSEs that assimilate SLA data from 0-3 satellites, using the 1/9° North Atlantic FOAM configuration for the first 3 months of 2006.

The potential impact of remotely sensed sea surface salinity (SSS) from SMOS or Aquarius on the forecast skill of the Mercator Ocean system has been assessed by Tranchant et al. (2008) through a series of OSSEs. Their conclusion, that the level of observation error is critical to the impact of this new observation type, is consistent with that of Brassington and Divakaran (2009) who assessed the theoretical impact of SSS observations on an ensemble-based data assimilation system.

Other than in the context of seasonal forecast skill, little has been done to assess the value of ocean observing capabilities with respect to large-scale ocean circulation diagnostics and their fluctuations on climate timescales (i.e. decadal and beyond). Some preliminary analysis of OSEs can be found in Carton and Giese (2008), Stammer et al. (2007), Baehr et al. (2004, 2008), and Forget et al. (2008). Many outstanding questions, such as the optimal ocean observing system for estimating long-term freshwater and heat transports within the global climate system, remain.

Even in the atmospheric community where OSSEs have a longer history the usefulness of OSSEs is not universally accepted. Certainly care is needed in the interpretation; and the careful simulation of the observations with realistic error characteristics from a simulation that has been validated to some extent in terms of its representation of nature is essential. Comparison of results from several systems to assess the robustness of the results is also important. The situation is no different for OSEs.

4c Monitoring the Ocean and the Observing System

Ocean data assimilation provides a comprehensive and powerful approach to monitoring the global ocean and, as such, is an important adjunct to the observing system. For the future, we envision a regular evaluation of the state of the ocean over the full water column, providing information about important ocean indices to both science and application communities on a regular basis.
In addition, it is expected that the assimilation systems and associated tools will provide routine mechanisms for evaluation of the health of the observing system. As a guide to tools that may be developed, the ocean community can look to the emerging tools in the atmospheric assimilation community. These tools represent diagnostics from analysis and forecasts systems that are relatively inexpensive to compute. For example, analysis sensitivity experiments and adjoint tools can quantify the impact of each individual observation on an analysis and forecast (e.g., Cardinali et al., 2004; Langland and Baker, 2004), albeit through a single pre-determined metric. The identification of persistent problems (e.g., negative impacts) with particular observations may indicate sensor drifts, particularly if consistent across several assimilation and forecast systems. Gelaro and Zhu (2009) show how the adjoint tools in conjunction with OSEs can provide insight into the synergy between different observation types. These tools are now being implemented into the U.S. Navy’s ocean analysis and forecast systems.

Ocean syntheses should also be used in improving data quality by, for example, providing the “background” used in statistical checks. This feedback loop could be important in ensuring that ocean syntheses provide the best possible analyses of current and past climate. It might also help refine bias corrections of observations such as those needed for historical XBTs.

Because the GOOS is constantly changing, results from OSEs quickly become obsolescent and a new paradigm is needed to monitor and evaluate the GOOS (Oke et al., 2009). The GODAE OceanView community is shifting their efforts to transition their OSE/OSSE activities towards routine monitoring of the GOOS. Some initial steps have been taken to coordinate these activities. Specifically, agreement is sought on how GODAE partners can and should move towards routine monitoring of the GOOS; agreement on how this can be coordinated between the international groups; and a staged plan for moving these activities towards routine monitoring, so that the GODAE OceanView community can have a real impact on the ongoing design and assessment of the GOOS.

5. Recommendations

Several recommendations are made to improve the GOOS, the collaborations between the assimilation and observation communities, and the assimilation systems themselves. With these improvements we can realize the potential of assimilation systems to synthesize observations so as to provide information that is more extensive than the information that can be gleaned from individual observations - for an impact on ocean and climate analysis and forecasts.

i) Systematic, sustained observations of the ocean and its forcing are critical to the improvement of decadal and longer-term ocean state estimation. At minimum, the existing GOOS must be maintained. For the global observing system, the requirement is for the maintenance of Argo as well as important satellite measurements such as altimetry, gravity (bottom pressure), microwave and infrared-based SST, scatterometer winds, precipitation, ocean colour, and microwave-based sea-ice concentration. In addition, the global tropical moored buoy arrays are essential for their provision of high frequency observations for short-term climate forecast initialization. The planned tropical moored buoy array in the Indian Ocean, RAMA, needs to be completed, and additional moored buoys east of 95°W are needed to constrain model biases in the far eastern Pacific. The enhancements of the PIRATA mooring array should be maintained for sufficient duration that the impacts on seasonal forecasts can be established. In addition to the sustained observations, the development of new observing systems such as biogeochemical Argo, and measurements of sea-ice thickness and sea surface salinity from space are encouraged.

ii) The surface flux reference network under OceanSITES, especially in higher latitudes and in areas with severe weather conditions, should be expanded along with the ship-based measurement program.
The increased coverage would help improve NWP products as well as the estimation of uncertainty in these products. Increased coverage will also improve satellite calibration.

iii) The under-sampling of the ocean ought to be addressed. To improve future ocean climate estimates, we need to extend the observing system to include full-depth Argo-type measurements, and enhance information about boundary currents, transports through key regions, and in marginal seas.

iv) Ocean state estimates should be maintained and viewed as an integral part of the ocean observing and information system.

v) Atmospheric reanalysis projects should continue to be pursued and should address climate-scale inconsistencies associated with the changing observing system.

vi) Land freshwater input to the ocean (ice melting, river runoff, ground water seepage) needs to be better determined.

vii) The input data streams: Attention needs to be paid to uncertainties in all the data sets, both input ocean observations and surface flux products. Particular care should be given to quality control of present and historical data sets, including the development of standards for QC tests. Appropriate metadata needs to be included with each observation so that its heritage and the history of corrections are available to assimilation groups. In addition to instrument and systematic errors, sampling (representation) errors need to be carefully considered. A program of targeted digitization of historical data sources could help to fill gaps in poorly sampled periods and regions.

viii) Much needs to be done over the next decade to characterize the uncertainties in each synthesis product and to improve them through improved assimilation approaches and the use of improved ocean general circulation models. Ultimately, a multi-model ensemble state estimate should take into account the uncertainty estimate.

ix) To fully understand the differences between the analysis products and to make further improvements in assimilation capabilities, a concerted comparison effort may also be needed wherein runs are undertaken with the same data and forcing and the analysis diagnostics are expanded to look at innovations and residuals and the details of data impacts.

x) Progress needs to be made in dynamically consistent coupled atmosphere/ocean/sea-ice estimation to provide both a consistent view of Earth’s climate variability and to improve the initialization for coupled climate predictions.

xi) The assimilation systems and associated tools ought to be developed as routine mechanisms for evaluation of the health of the observing system.

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