OCEAN STATE ESTIMATION FOR CLIMATE RESEARCH

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ABSTRACT

Spurred by the sustained operation and new development of satellite and in-situ observing systems, global ocean state estimation efforts that gear towards climate applications have flourished in the past decade. A hierarchy of estimation methods is being used to routinely synthesize various observations with global

ocean models. Many of the estimation products are available through public data servers. There have been an increasingly large number of applications of these products for a wide range of research topics in physical oceanography as well as other disciplines. These studies often provide important feedback to the observing systems. This white paper describes the approaches used by the estimation systems in synthesizing observations

and model dynamics, highlights the applications of their products for climate research, and addresses the challenges ahead in relation to the observing systems. Further applications to study climate variability using ENSEMBLE state estimation products are described by a white paper by Stammer et al. (2010).

1. INTRODUCTION

As satellite and in-situ observing systems for the global ocean (e.g. altimetry and Argo) progress and mature with time, there is an ever-increasing need to synthesize the diverse observations by using them to constrain state-of-the-art ocean general circulation models (OGCMs). The resulting ocean state estimation products aim to provide estimates of the time-varying, three-dimensional state of the ocean and to help understand the variability of ocean circulation and its relation to climate. They offer a tool to estimate quantities that are difficult to infer from observations alone, such as oceanic heat transport.

The vision of global ocean state estimation as a means to synthesize ocean observations into a dynamically consistent estimate of the ocean circulation was developed under the "World Ocean Circulation Experiment" (WOCE) and was further developed as part of WCRP's "Climate Variability and Predictability Project" (CLIVAR) and Global Ocean Assimilation Experiment (GODAE). As a result of this, and with the sustained commitment of various funding agencies, climate-oriented ocean state estimation efforts have flourished in the past decade. Since OceanObs'99, many ocean state estimation systems have been developed to routinely produce estimates of the physical state of the ocean that are publically available through data servers. State estimation products have been used to study a wide range of topics in physical oceanography and climate-related phenomena as well as in geodesy and biogeochemistry.

2. APPROACHES

A hierarchy of estimation methods has been adopted by various groups to perform ocean state estimation, ranging from sequential or filter methods such as objective mapping or the so-called optimal interpolation (OI), 3-dimensional variational (3D-VAR) method, and Kalman filter, to the so-called "smoother" methods such as the Green's function, Rauch-Tung-Striebel (RTS) smoother, and the adjoint method (a.k.a. Lagrange multiplier, Pontryagin's principle, 4-dimensional variational or 4D-VAR). Table 1 lists the estimation methods used by various systems, many of which have a focus on climate applications (for diagnostic analysis, initialization of climate prediction, or both).

In sequential estimation, the estimated state at a certain time is influenced by observations up to that time. In smoother methods, however, the estimated state at any time is affected by observations in the future as well as in the past and present. The sequential methods as implemented various assimilation groups by are typically computationally more efficient than smoother methods such as the adjoint. The sequential approaches allow the estimated state to deviate from an exact solution of the underlying physical model by applying statistical corrections to the state, which is often based on some basic physical constraints (such as preservation of the water mass properties, geostrophic balance, etc.). These corrections are meant to compensate a combination of various errors in model physics (including forcing), such as errors in the representation of advection and mixing, errors due to lack of resolution, erroneous bathymetry, and missing physical processes. Because they do not explicitly describe the correction of a specific physical process, these corrections imply internal sources and sinks of heat, salt, and momentum, etc., which tend to render the estimated state closer to the observations being assimilated (depending on the treatment of the model and data errors).

Adjoint-based estimation systems often demand the estimated state to satisfy the model equations exactly over a certain time interval. The optimization of the state within such a time interval is accomplished by adjusting the control variables, which are typically the initial state, surface forcing, and model parameters. Not having internal source and sink allows the so-called physical consistency, namely, the consistency of the estimated surface forcing with the estimated ocean state and the closure of property budgets, which greatly facilitates many aspects of climate research such as heat balance and diagnosis of the relative roles of different surface forcing on the ocean. The adjoint approach is adopted by the Consortium of Estimating the Circulation and Climate of the Ocean (ECCO, Stammer et al. 2002a) and Japan's K-7 project (Sugiura et al. 2008) (Tab. 1). Nevertheless, the lack of internal sources and sinks in the adjoint approach could make it more difficult for the model to fit certain aspects of the observations, especially over a long integration. In this case, it is important to identify and implement internal control variables so as to correct model error that the initial state and surface forcing cannot account for. Examples of such internal control variables include the mixing coefficients (e.g. Stammer 2005) or an "eddy stress" to represent the effect of mesoscale eddies that are not resolved by coarse resolution models. The adjoint method itself is amendable to the introduction of internal control variables.

System	Method	Data	Period	Server
ECCO-GODAE (MIT-AER), USA	Adjoint	Altimetry; scatterometry; tide gauges; gravity; SST, SSS; T & S profiles from XBT, CTD, Argo, TAO & other buoys, elephant seals (SeaOS); Florida Current; RAPID array	1992-2008	www.ecco-group.org
ECCO1, USA	Adjoint	Altimetry; scatterometry; tide gauges; geoid; SST, SSS; T & S profiles from XBT, CTD, Argo, TAO & other buoys.	1992-2001	www.ecco-group.org
G-ECCO, Germany	Adjoint	Altimetry; scatterometry; tide gauges; geoid; SST, SSS; T & S profiles from XBT, CTD, Argo, TAO & other buoys,.	1952-2001	www.ecco-group.org
ECCO-JPL, USA	Kalman filter & RTS smoother	Altimetry, T profiles from XBT/CDT, Argo, and TAO.	1993-present	www.ecco-group.org or www.ecco.jpl.nasa.gov/external
ECCO2, USA	Green's functions	Altimetry, SST, T & S profiles from XBT, CTD, Argo, TAO; sea ice data	1992-2008	www.ecco2.org
GMAO/NASA, USA	OI, ensemble Kalman filter	Altimetry, T & S profiles from XBT, CTD, Argo, TAO	1993-present	gmao.gsfc.nasa.gov/research/ocean assim/
GFDL/NOAA, USA	Coupled Data Assimilation (Ensemble Kalman Filter)	SST, T profiles from XBT, CTD, Argo, TAO & S profiles from CTD, Argo	1979-2008	Data1.gfdl.noaa.gov/nomads/forms/assimilation.html
GODAS, NCEP/NOAA, USA	3D-VAR	SST, T profiles from XBT, CTD, Argo, TAO	1979-present	www.cpc.ncep.noaa.gov/products/ GODAS
SODA, USA	OI	Altimetry, Satellite and in-situ SST, T & S profiles from MBT, XBT, CTD, Argo and other float data, TAO and other buoys.	1958-2007	www.atmos.umd.edu/~ocean/data.h tml or soda.tamu.edu
ORA-S3 ECMWF, EU	3D OI with online bias correction	Altimeter (sea level anomalies and global trends), SST, T & S from XBT, CTD, Argo, TAO	1959-present	Graphical: www.ecmwf.int/products/forecasts/ d/charts/ocean/reanalysis Data: ensembles.ecmwf.int/thredds/ocean /ecmwf/catalog.html
MERCATOR, France	SEEK filter	Altimetry, SST, T & S from XBT, CTD, Argo, TAO	1980-present	www.mercator-ocean.fr
CERFACS, France	3D-VAR	SST, T & S profiles from EN3	1960-2006	http://www.ecmwf.int/research/EU_projects/ENSEMBLES/data/datadissemination.html

INGV, Italy	OI	SST, T & S profiles from XBT, CTD, Argo, TAO	1958-2006	www.bo.ingv.it/contents/Scientific- Research/Projects/oceans/enact1.ht ml
DePreSys, UK	OI	SST, T & S profiles from XBT, CTD, Argo, TAO	1950-2007	http://www.ecmwf.int/research/EU_projects/ENSEMBLES/data/index.html
Reading, UK	OI with S(T)	T & S profiles from EN3 and Argo	1960-2007 at 1° and 1987-2007 at 1/4°	www.resc.reading.ac.uk/godiva2
K-7, Japan	Adjoint	Altimetry, SST, T from XBT, CTD, Argo, TAO	1960-2006	www.jamstec.go.jp/frcgc/k-7-dbase2/
MOVE-G, Japan	3D-VAR	Altimetry, SST, T & S from XBT, CTD, Argo, TAO	1948-2007	www.mri-jma.go.jp/Dep/oc/oc.html

Table 1. Brief summary of ocean state estimation systems

Many data types are routinely synthesized to produce ocean state estimates. The type and volume of data vary systems. Previous studies have complementarity of different data types in improving ocean state estimates. For this reason, all systems use data from more than one observing system. Table 1 summarizes the observations synthesized by various systems. The most commonly used data are sea level anomaly from altimeters (e.g. TOPEX/Poseidon and JASON-1), in-situ temperature profiles (e.g. from XBT/CTD, TAO moorings, and Argo), and salinity profiles from Argo. The impact of the data constraint on the estimation can be seen from the reduction of modeldata misfit for the different observations as a result of the minimization procedure. Figure 1 is an example showing the reduction of model-data misfit as a result of the optimization of the ECCO-GODAE system. In this case, altimeter data, Argo T/S profiles, and SST data have relatively large impact on the estimation. Many of the ocean state estimation products are publically available through data servers (Table 1). A few recent studies have attempted to compare these products with a uniform set of observational data (e.g. Gemmell et al. 2009). In the future, it would be valuable to provide more misfit diagnostics (e.g. Fig. 1) for different synthesis products calculated in a uniform way against the same data. More details of the state estimation efforts can be found in CLIVAR GSOP web page http://www.clivar.org/organization/gsop/gsop.php.

3. APPLICATIONS

Ocean state estimation products and tools have been applied to studies over a wide range of topics in physical oceanography, for instance, the nature of sea level variability (e.g. Carton et al. 2005, Wunsch et al. 2007, Fukumori et al. 2007, Köhl and Stammer 2008a), water-mass pathways (e.g. Fukumori et al. 2004, Wang et al. 2004, Masuda et al. 2006, Toyoda et al. 2009),

estimating surface fluxes and river runoff (e.g. Stammer et al. 2004, Romanova et al. 2009), and interannual and decadal variability of the upper-ocean and heat content (e.g. Masina et al. 2004, Capotondi et al. 2006, Köhl et al. 2007, Carton and Santorelli 2009). They have also been applied to research in other disciplines such as biogeochemistry (e.g. McKinley et al. 2000 and 2004, Dutkiewicz et al. 2001 and 2006) and geodesy (e.g. Ponte et al. 2001, Dickey et al. 2002 Chao et al. 2003, Gross et al. 2005). Due to limited space, here we only highlight a very limited number of examples for ocean circulation studies and discuss the implications for observing systems.

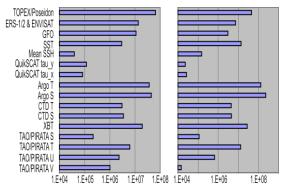


Figure 1. Non-dimensional model-data misfits (normalized by data error) in the ECCO-GODAE system after the optimization (left), and the reduction of the model-data misfits as a result of the optimization (right). The former is the components of the so-called cost function at the end of the optimization. The latter, describing the reduction of the cost function, reflects the impact of various data on obtaining the estimate. Courtesy of Patrick Heimbach of MIT and Ichiro Fukumori of JPL.

Ocean state estimation products have been widely used to study the meridional overturning circulations (MOCs) as well as heat and freshwater transports, which are quantities that are difficult to measure directly (e.g. Stammer et al. 2003, Lee and Fukumori 2003, Schoenefeldt and Schott 2006, Wunsch and Heimbach 2006, Balmaseda et al. 2007, Köhl and Stammer 2008b, Schott et al. 2007 and 2008, Cabanes et al. 2008, Rabe et al. 2008, Volkov et al. 2008). These analyses often have direct implications to the observing systems. For instance, Lee and Fukumori (2003) and Schott et al. (2007) identified the anti-correlated variability of meridional pycnocline transports in the western boundaries and the interior associated with interannualdecadal variation of the Pacific subtropical cells (STC). Therefore, the low-latitude western boundary currents (LLWBCs) and interior flow play opposite roles in regulating upper-ocean heat content in the Pacific (with the interior flow being more dominant). Such an anticorrelated variability is associated with the oscillations of the tropical horizontal gyres in the western-central Pacific Ocean in response to near-local Ekman pumping. The oscillations of the tropical gyres and their forcing have signatures in sea level anomaly as observed by altimeters and wind stress curl captured by scatterometers (see Fig. 2 for altimeter data examples).

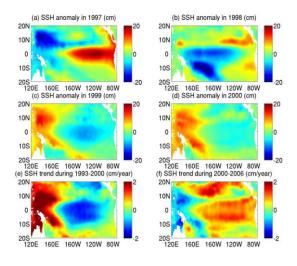


Figure 2. Interannual-to-decadal variability of SSH captured by TOPEX/Poseidon and JASON-1 altimeters imply oscillations of tropical gyres in the western tropical Pacific near 10°N and 10°S, which result in counteracting variations of pycnocline transports in the interior and near the western boundaries (with the interior being more dominant). These data, presented by Lee and Fukumori (2003) and Lee and McPhaden (2008), provide an effective constraint on the estimates of pycnocline flow variability in ocean state estimation, as discussed by Lee and Fukumori (2003) and Schott et al. (2007).

These signatures provide some constraint on the estimated partial compensation of the western-boundary and interior flows and thus tropical heat content. Nevertheless, the satellite data have footprints that are too coarse to resolve the sharp changes near the LLWBCs. Therefore, systematic measurements of the LLWBCs, which are not well resolved by existing insitu observing systems, would enhance the observational constraint on the state estimates.

Another example of the feedback between state estimation and observing system is the study of decadal variability of the North Atlantic MOC by Wunsch and Heimbach (2006), Balmaseda et al. (2007), Köhl et al., (2007), and Köhl and Stammer (2008). These studies discussed the complex structure of the estimated decadal variability in the MOC in depth and latitude. In the ECCO-GODAE estimate (Wunsch and Heimbach 2006), for instance, the decadal weakening of the upper meridional circulation (associated with reduced northward transport above 1200 m) at 26°N is accompanied by a strengthening deep meridional circulation (i.e. the southward outflow of North Atlantic Deep Water and northward inflow of abyssal water) in the ECCO-GODAE estimate (Fig. 3). In the ECMWF operational analysis product (ORA-S3), there is a weakening northward flow (Balmaseda et al. 2007) at most latitudes of the North Atlantic basin.

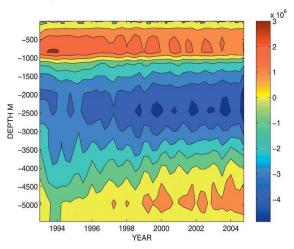


Figure 3. Seasonal averages (3 months) of volume transport contours (m³ s⁻¹) through time as a function of depth estimated by the ECCO-GODAE system. The weakening of the upper part of the meridional circulation (associated with the reduced Northward transport) is accompanied by a strengthening of the deeper meridional circulations (i.e., the southward outflow of North Atlantic Deep Water and northward inflow of abyssal water). After Wunsch and Heimbach (2006).

At 50°N, the northward transport is well correlated with the intensity of the subpolar gyre (which can be derived from altimeter data) at interannual-decadal time scales, but the trends are opposite. Data assimilation substantially improves the estimated time-mean strength of the MOC (Fig. 4). There is apparent agreement between the ECMWF analysis with the estimates by Bryden et al. (2005) based on synoptic hydrographic sections in the 1980s and 1990s. However, both Wunsch and Heimbach (2006) and Balmaseda et al. (2007) discussed the large month-to-month fluctuations in the MOC estimate, which could cause aliasing if sampled infrequently. Both studies showed that the trend in the meridional heat transport was smaller than that of the MOC strength because surface warming partially counteracted the weakening (upper) MOC. Therefore, an observing system that is capable of inferring changes in the volume transport may not be alone adequate to monitor the heat transport. These findings suggest that a systematic measurement network for the Atlantic MOC and heat transport at different latitudes (and different depths) beyond the traditional synoptic hydrographic survey are needed. The extension of such a system as the RAPID array is a step towards that direction (please refer to the white paper by Cunningham et al. (2007) on Atlantic MOC monitoring system). However, much of the ocean is still vastly under-sampled. The studies on decadal variation of the MOC re-emphasize the importance of having systematic, sustained, and consistent measurements of the global ocean circulation in general.

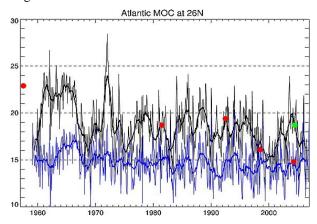


Figure 4. Meridional overturning circulation (MOC) variability at 26°N (in Sv). The time evolution of the MOC for ECMWF's ocean reanalysis (black) and for the no-assimilation run (blue) is shown using monthly values (thin lines) and annual means (thick lines). Overplotted are the annual-mean MOC values from Bryden et al. (2005) based on synoptic hydrographic sections and Cunningham et al. (2007) based on RAPID mooring data (green circle). After Balmaseda et al. (2007).

With their near continuous measurements at fixed locations, mooring observations have provided a valuable source of data to constrain and evaluate state estimation products (see the white paper by McPhaden et al. (2010) for the global tropical buoy array). These data also allow local heat budget analyses near mooring sites (e.g. Wang and McPhaden 2000, McPhaden (2002)). Although not all the budget terms can be measured directly, the analysis are helpful for evaluating the budget of state estimation products, and they give better confidence for using these products to study the budget on larger scales, which are difficult to capture completely with mooring systems. The studies of mixed-layer temperature balance by Kim et al. (2004, 2007), Du et al. (2008), and Halkides and Lee (2009) are examples of the application of state estimation products for heat budget analysis. In particular, the dynamical consistency of ECCO estimates allows the heat budget to be closed because there are no internal sources or sink of heat being produced by the assimilation procedure.

Apart from the studies of ocean circulation, state estimation products and tools have also many other applications. For example, the estimation systems can be used to evaluate the impact of existing observations or the design of future observational systems (e.g. Oke and Schiller 2007). The use of ocean state estimation products to initialize seasonal climate forecasts has become an important routine practice in operational and experimental prediction centers. This subject is reviewed by the white paper by Balmaseda et al. As part of the CLIVAR/GODAE global ocean reanalysis evaluation efforts, many assimilation groups in the US, Europe, and Japan have participated in an effort to compare a suite of derived diagnostic quantities among different products and with observations. Among other goals, the ENSEMBLE analysis helps identify the minimum accuracy of observation that can distinguish the products or to constrain the estimation effectively. Stammer et al. (2010) is related to the intercomparison of various estimation products. Additional feedbacks of state estimation to observational requirements are addressed by Heimbach et al. (2010).

4. CHALLENGES

Despite significant advances in ocean state estimation, many challenges remain. 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 the observationalists to obtain robust estimates of data errors (including biases), an important issue that is often left to the hands of assimilation groups. A close collaboration with the modeling community is also needed to better understand model errors. The quantification of model errors is only one aspect. The

identification of model error sources is critical to the 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. Moreover, assimilation groups need to work closely with the modeling community to improve model physics, especially those associated with the bias in the mean state.

The estimation of decadal and longer-term variability remains a challenge due to the lack of observations on these time scales in the ocean and for the forcing fields and the insufficient understanding of the errors associated with these observations. This is compounded by the limitation in model physics. Sustained observations of the ocean and its forcing are therefore critical to the improvement of decadal and longer-term ocean state estimation.

Many of the state estimation products 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, to more fully utilize the existing observations that capture eddy variability (e.g. the multi-altimeter system), and to develop the capability to synthesize future observations such as those from the Surface Water Ocean Topography (SWOT) mission. Computational resources remain a critical issue for estimation efforts that are based on ENSEMBLE or adjoint methods because they limit the ENSEMBLE size and model resolution that one can afford. Finally, the coupled nature of the climate system prompts for a coupled approach for state estimation that includes different components of the climate system (such as the atmosphere, land, cryosphere, biogeochemistry) in order to properly account for the potential feedback among different components. Currently, coupled ocean-atmosphere, ocean-ice, and ocean physics-biogeochemistry state estimations are still in their infancy. Examples of emerging efforts include (NOAA) GFDL's use of ENSEMBLE Kalman filter (Zhang et al. 2007) and (Japan) K-7's use of adjoint method (Sugiura et al. 2008) to perform estimation using coupled ocean-atmosphere models. Coupled estimation efforts are expected to pick up momentum in the coming decade.

5. SUMMARY

Aided by the development of global ocean observing systems, significant accomplishments have been achieved in global ocean state estimation efforts that are

aiming towards climate applications. A suite of global ocean state estimation products have been produced to describe the time evolving three-dimensional ocean circulation. There have been an ever increasing number of applications of these products for oceanographic and climate-related studies over a wide range of topics in physical oceanography and other disciplines. These studies provide important feedback to the requirement and design of the observing systems. The estimation systems need further improvement through a better understanding and quantification of model, data, and forcing errors, improved model physics and resolution, and the inclusion of other components of the climate system as part of the estimation. Despite these challenges, ocean state estimation remain a pivotal approach to understanding the climate system, and will be ever even more so in the future as we aim to quantify the feedbacks in the system and investigate longer time

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