The ECCO Report Series [1]

State Estimation In Modern Oceanographic Research

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Report Number **14**

November, 2001.

[1]The ECCO Project is a consortium of the Jet Propulsion Laboratory, The Massachusetts Institute of Technology and the Scripps Institution of Oceanography and is funded through a grant from the National Oceanographic Partnership Program (NOPP). Copies of this Report are available at www.ecco-group.org or from Detlef Stammer, Scripps Institution of Oceanography, La Jolla CA 92093-0230, ph.: (858) 822-3376; fax: (858) 534-4464; e-mail: dstammer@ucsd.edu.

The ocean is a major element in the climate system, being the dominant reservoir of fresh water, a primary mechanism of meridional heat transport, a major sink (and source) of carbon dioxide, and a focus of biological productivity among other roles. Ongoing and planned oceanic and climate research activities are intended to measure, understand, and eventually predict variations in the ocean and its interaction with the atmosphere, land and cryosphere. But because the ocean changes vigorously on all time and space scales, substantial problems exist for any system of observing and simulating the rapidly changing flow field and associated properties such as temperature, and, their consequences. Requisite observation systems are still under debate and development, but ocean observing systems are now in place as a legacy of programs such as the World Ocean Circulation Experiment (WOCE) and the Tropical Ocean Global Atmosphere Program (TOGA). Satellite altimetry and the ARGO floats (e.g., *Roemmich and Owens*, 2001) have been identified as the initial backbone of a global system.

Oceanic observations are likely to remain scarce and expensive relative to the full need. In addition, an extraordinary diversity of oceanic observations exist—varying from in situ data of all kinds, to ocean surface observations from space; these have spatial and temporal coverage differences ranging over many orders of magnitude. But combining these data into a dynamically self-consistent picture is far from straightforward. A second major source of information about the ocean lies with theory and models which are a concise statement of our understanding of the ocean circulation. Ocean state estimation ("data assimilation") has as its goal to obtain the best possible description of the changing ocean by combining, in some suitably optimum way, those two elements, i.e., knowledge from all types of observations with suitable models. If carried out properly, the result is a dynamically self-consistent estimate of the time-evolving ocean circulation in the past and present, which carry greater information and forecast skill than does either model or data alone.

An analogous, but significantly different problem, is well-known in numerical weather prediction (NWP). Major differences lie in the focus of NWP on short-term forecasting whilst optimal state estimation uses formally future, past and present data to estimate the state of the ocean over a period of time, from years to decades and beyond. The much longer time scales in the oceanic problem and the sometimes very different data types present challenges that are significantly different from atmospheric experience.

To the extent that rigorous state estimation can be accomplished, it has many diverse applications; among them are:

- The synthesis of all observations of the present oceanic state for climate forecast purposes.
- A foundation for hypothesis testing about the ocean, and for model improvements.
- A platform for assessment of the global observing system 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.).
- Understanding 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 cryospheric ones.

A schematic of an ocean observing and synthesis system is shown in Fig. 1 and Fig. 1
includes an observing system, a state-of-the-art OGCM and and assimilation/synthesis system. The main elements of a possible global ocean observing system are described in detail in *Smith and Koblinsky* (2001). The status of ocean modeling and anticipated improvements are addressed by *Griffies et al.* (2000). Here we will focus on issues and progress of the estimation side: the synthesis of all elements into one best estimate.

Ocean state estimation activities exist or are under development. A recent summary of ongoing international assimilation efforts in support of CLIVAR (http://www.clivar.org) and GODAE (http://www.bom.gov.au/GODAE) can be found by *Stammer et al.*

(2001d). Many of these efforts employ very approximate methodolgies, and restrict themselves to subsets of the data, to small regions, to short-term or seasonal/interannual forecasting, or all of these in concert.

The purpose of this note is to describe the problems being tackled by ocean state estimation and the rigorous methods being used. We summarize the current status of the efforts, and describe the first applications, including those outside physical oceanography. Finally, the future directions for this type of effort are discussed. Results presented are taken from the ECCO consortium of the National Oceanographic Partnership Program (see below), and are intended to provide an overview of general accomplishments achieved to date by the community. They will be used as a foundation for a more general discussion of what is feasible now and in the near future as applications in many, if not all, disciplined of oceanography.

A Consortium for State Estimation and Model Improvements

The effort required to carry out global ocean state estimation is formidable. To marshal adequate resources, a consortium has been formed called "Estimating the Circulation and Climate of the Ocean" (ECCO) with funding provided by the National Aeronautics and Space Administration (NASA), the National Science Foundation (NSF), and the Office of Naval Research (ONR) under the National Oceanic Partnership Program (NOPP). ECCO is one of several national and international ocean state estimation effort (see also *Stammer and Chassignet*, 2000). It builds on an effort that began at the Massachusetts Institute of Technology (MIT), but now also involving scientists at the Scripps Institution of Oceanography (SIO) and the Jet Propulsion Laboratory (JPL). ECCO intends to transform existing ocean state estimation efforts from their present experimental status into quasi-operational applications that can support scientific, societal and navy needs alike. ECCOs ambitious ultimate goal is to employ rigorous methods of ocean/data syntheses, to describe the ocean circulation anywhere on any time from a year to several decades, and to use data of any type.

ECCO activities are based on the MIT general circulation model (*Marshall, et al.*, 1997a,b), including a complete mixed layer model (*Large et al.*, 1994), and an eddy parameterization scheme (*Gent and McWilliams*, 1990). A first MIT ECCO model release with a full documentation of both forward and adjoint codes is available at http://mitgcm.org/sealion. The forward model code continues to evolve as part of the ECCO project and the community is strongly encouraged to use it. Results from all ECCO assimilation efforts can be accessed by the general community via the ECCO data server (Live Access Server at http://www.ecco-group.org/las). The server also carries the input observations and forcing fields as they were used during the various experiments for reference. See *Lee et al.*, (2002), *Fukumori et al.* (2002) and *Stammer et al.* (2002a,b,c) or http://www.ecco.ucsd.edu) for details.

Methodology

All data assimilation methods deal, in principle, with a vector $\mathbf{x}(t)$ representing a time-dependent model simulation of the state of the ocean. These state vectors include, typically on a grid, the values of temperature, salinity, pressure and velocity required by a general circulation model (GCM) to take one time-step into the future, if accompanied by appropriate boundary conditions. From the state vector, one can compute any derived quantity (e.g., potential vorticity flux, enstrophy, enthalpy flux, etc.) of interest. All oceanic measurements can be associated with its model equivalent through a functional relationship that can be written as,

$$\mathbf{E}(t)\,\mathbf{x}(t) + \mathbf{n}(t) = \mathbf{y}(t)\,, \tag{1}$$

where E is a matrix, n(t) is the error of this relationship including the inevitable observation noise, and y(t) is the vector of observations. A time-dependent estimated solution, $\tilde{\mathbf{x}}(t)$, is then sought, that minimizes in a least-squares sense the model-data misfits, which can be written as,

$$J = \sum_t (\mathbf{y}(t) - \mathbf{E}\mathbf{x}(t))^T \mathbf{R}(t)^{-1} (\mathbf{y}(t) - \mathbf{E}\mathbf{x}(t)), \tag{2}$$

subject to the model dynamics as constraints. Here $\mathbf{R}(t)$ is the observational error covariance.

Simplified methods (e.g., nudging, robust diagnostic, and objective mapping), intended to find approximations to the minimum of J subject to the model constraints, are easy to set up and are computationally inexpensive. The main issues are that information in the data and error fields is thereby arbitrarily suppressed, and the temporal and spatial evolution of the result is not dynamically consistent with the model. On the other hand, rigorous methods, as used by ECCO and described below, are computationally very expensive. But we note that they are the only approach that will produce dynamically self-consistent ocean estimates exploiting as much information as the data contain and that can be used for understanding the physics of the system. Detailed accounts of theoretically rigorous approaches to minimizing J subject to the model are described, e.g., by *Bennett* (1992), *Wunsch* (1996), *Malanotte-Rizzoli* (1996), *Fukumori* (2000).

Ongoing ECCO Activities

Initially, two methods for minimizing J subject to the model dynamics are being use by the ECCO consortium. One approach relies upon enforcing the model through what has come to be known as the "adjoint method". Details of how this has been done, choices for the elements of $\mathbf{R}(t)$, and the model error, as well as a full description of the model as run on a global 2° grid can be found in *Stammer et al.* (2002a). We refer to this calculation as the "preliminary WOCE synthesis." To bring the model into consistency with the observations, the initial-conditions for potential temperature and salinity fields are modified, as well as the surface forcing fields. Changes in those fields (often referred to as "control" terms) are determined as a best-fit, in a least-squares sense, of the model state to the observations and their uncertainties over the full data period. The "first guess" estimate of the surface forcing is provided by the daily time-varying National Center for Environmental Prediction (NCEP) reanalysis fluxes of momentum, and daily estimates of heat, and freshwater (*Kalnay et al.*, 1996). Scatterometer results are used to estimate wind stress errors; see the references for a more general discussion of error estimates.

In parallel with the global 2° WOCE synthesis, a second global estimate employing a combination of the adjoint method and a reduced-state Kalman filter/RTS smoother is being used on a telescoping grid with 1° resolution in latitude and longitude in mid and high latitudes, and a meridional resolution decreasing to 1/3° near the equator. This latter approach is intended to test the merits of the alternative minimization algorithm while focusing the science on the seasonal-to-interannual variability of the Pacific Ocean. Thus far, TOPEX/POSEIDON sea level anomalies, climatological mean temperature and salinity, and surface flux data from 1993 to present are being used. Results are described in detail by *Lee et al.* (2002), *Fukumori* (2001), *Fukumori et al.* (2002).

In addition to the global state estimates, 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, we model the North Atlantic and the tropical Pacific at 1/6° horizontal resolution or higher. Both open and closed boundary conditions are used.

Ongoing efforts of the ECCO Consortium are now aiming to produce two major, sustained analysis products: (1) A full global synthesis of all available data, done to the highest resolution and with the nearest to optimal estimation method that are feasible. (2) A near-real time product, whose time delay is to be no longer than about two weeks, using most of the available continuing data, and an estimation method sensibly compromising the need for optimality with that for computational efficiency. Both products will be routinely distributed through the projects data server (http://www.ecco-group.org/las).

First Science Applications

Both global state estimation efforts have successfully reduced J to levels that they are sufficiently acceptable to provide a basis for exploring how such solutions can be used scientifically. These three-dimensional, time-evolving oceanic state estimates with known dynamics have a wide range of uses and the calculated fields are now being analyzed. Here we can only provide a few examples of what is expected to emerge over the next months and years in many fields of oceanographic research.

Within ECCO, a particular science focus is the determination of transports and the budgets of mass, heat, freshwater, and energy across various regions of the global domain. The state estimates are also being examined to assess the accuracies 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. Beyond the traditional realm of physical oceanography, output from the optimizations are also being used in studies such as the Earth's angular momentum budget (*Ponte et al.*, 2001) and simulations of bio-geochemical tracer transport and distribution.

Fig. 1 in its right panel shows the mean flow field at 27m and 1975 m depth from the 2° WOCE synthesis calculation, together with the mean sea surface height and the temperature field at 1975 m. All major circulation structures are simulated, but are overly smooth due to the present low model resolution. The mean net surface heat flux field resulting from the the optimization is displayed in the upper panel of Fig.2. The Fig.2 adjustment relative to the prior NCEP estimate is also shown and is required to bring the model state into consistency with the ocean data. Modifications of the net NCEP heat fluxes are of the order of ± 20 W m^{-2} over large parts of the interior oceans. Maximum changes occur along the boundary currents in the Northern Hemisphere where shifts of up to ± 80 W m^{-2} can be found. Most of the eastern boundary currents now show a significant heat uptake. The same is true in the Arabian Sea, where similarly, the off-shore Ekman transport brings up cold water, and which is being heated by the atmosphere. Strong warming occurs over Flemish Cap, in the North Pacific, and along most of the Antarctic Circumpolar Current. Note that the optimization also removes some of the small-scale Gibbs effects known to be present in the initial NCEP estimates of buoyancy flux fields as a result of numerical treatment of mountain ranges such as the Andes, visible in the eastern Pacific. *Stammer et al.* (2002c) demonstrate considerable skill in the ECCO-estimated momentum, heat and fresh water fluxes, comparable in quality to independent estimates obtained from satellite data and regional bulk formula estimates. Combined ocean observations and dynamics thus do appear to be a route to improving air-sea flux measurements that is complementary to estimates from atmospheric models or direct observational and analysis campaigns.

An example of the use of rigorous estimation approaches for inferring physical processes in the ocean is given in Fig. 3. In its top panel the figure shows a temperature timeseries Fig. 3 at 100m depth of the constrained model and compares it with observations from one of the TOGA TAO buoys at that location (*McPhaden et al.*, 1998), as well as with a similar timeseries, but from the unconstrained model. In contrast to the unconstrained run, the constrained results (taken here from *Fukumori et al.*, 2002 with up to 1/3°resolution near the equator) simulate the temperature observations quite closely without actually assimilating them. Taking the figure as an indication of the constrained models skill in simulating the observed flow, temperature and salt fields, one can than start using the model output to compute unobserved quantities, such as ocean transports or heat storage. In the lower two panels the figure is showing a related diagnosis of the models mixed-layer temperature evolution in the eastern equatorial Pacific (Ñino-3: 5S-5N, 150W-90W) during 1997-2000. The tendency of advection and horizontal diffusion to warm the mixed layer during 1997-2000, is counterbalanced by a loss of heat to the atmosphere. Vertical advection, which is one of the dominant agents in regulating mixed-layer temperature here, changes its sign in 1999 as El Nino switches to La Nina (see *Lee et al.*, 2002) for details). The examples illustrate what can be accomplished by rigorous state estimation. Inference is being provided about unobserved quantities from sparse observations. Furthermore, the estimated state evolution is dynamically consistent in the sense that changes can be attributed to a sum of explicit physical processes. Less rigorous estimation in general cannot close the budget in such manner.

On a global scale, meridional heat fluxes integrated across basins equal the air-sea heat divergence over the respective basins (see *Stammer et al.*, 2002b). Such meridional transport for the Atlantic and Indo-Pacific Oceans, show good agreement (within error bars) with the wholly independent estimates of *Ganachaud and Wunsch* (2000) from a global hydrographic inversion. Significant discrepancies do exist over the North Atlantic where the present result is only 50% of their amplitude at mid-latitudes. This result is unsurprising in a relatively viscous model with 2° lateral resolution, in which the boundary currents (Gulf Stream and deep western boundary current) are sluggish and diffuse.

A demonstration of the skill of a global circulation model is the simulation of observed tracer distributions (*Follows et al.*, 1999; *Walker et al.*, 2002). Work is underway to understand how best to directly assimilate tracer data so as to further constrain the physical flow field of the ocean. An ultimate application then will be to investigate and understand the uptake and redistribution of carbon in the ocean based on our best possible flow estimates.

Applications beyond the traditional oceanographic realm include ocean angular momentum (OAM) calculations. *Ponte et al.* (1998), using forward model runs without any data constraints, revealed recently the effects of OAM variability on the Earth's rotation. *Ponte et al.* (2001), using the ECCO results, show that the optimization procedure yields substantial improvements in OAM estimates, related to adjustments in both motion and mass fields, as well as in the wind stress torques acting on the ocean. The assimilated model produces significant improvements in coherence (not shown) between the ocean estimates and the observed OAM. This comparison with Earth rotation measurements provides a stringent independent consistency check on the estimated ocean state and underlines the importance of ocean state estimation for quantitative studies of the variable large-scale oceanic mass and circulation fields. Ultimately those fields will be used to constrain the ocean flow field as will modern measurements of gravity fluctuations and respective changes in the ocean mass field obtained from the upcoming GRACE gravity mission (http://www.csr.utexas.edu/grace/).

A by-product of the adjoint method is the estimate of the adjoint solution. This solution exists in a space dual to that of the forward model (e.g., *Wunsch,* 1996), and represents a nearly complete description of estimate sensitivity to data, and of the flow of information in the model. Use of this solution, to examine the controlling factors on oceanic meridional heat flux, was described by *Marotzke et al.* (1999).

Outlook

Physical oceanography is entering a new era in which there will be a far greater reliance on global observations and ocean state estimation as a synthesis tool to provide the community with estimates of the time-evolving ocean and climate state. The preliminary results reported here show that the existing data-base and the available modeling and computing capability have advanced to the point where true three dimensional, skillful estimates of the global time-evolving general circulation are practical. To a large extent, this statement is a vindication of the vision which drove the World Ocean Circulation Experiment—that such estimates could become possible by the year 2000, and that they would be necessary for the advancement of the science. Both CLIVAR and GODAE programs are built to a great extent upon the assumed availability of routine state estimates. We show here the first of those results anticipated to emerge through GODAE.

However, we strongly emphasize that we are at the very beginnings of what will be a long process of improvements and enlargement of the scope of oceanic state estimation somewhat like efforts going on in weather analyses over the last decades. With expected advances in computer power and numerical algorithms, models with greatly increased spatial resolution, and more sophisticated and complete physical parameterizations will come. Regional estimates at extremely high resolution with open boundaries are already underway. Global estimates at $1/4°$ are envisioned as being feasible in two-to-three years. A much fuller exploration of the control vector space will be undertaken, including adjustments to internal parameters such as diffusion and viscosity coefficients, and external parameters such as the bottom topography and sidewall boundary condition relationships. The information contained in adjoint solutions remains to be more fully exploited. Many, if not all, of these results should be available with little or no delay as the need arises.

Looking further into the future, one can envision ongoing global estimates of coupled ocean/atmosphere/cryosphere models with sufficient skill that true climate forecasting (that is, with skill estimates) will be possible. At the same time we envision a vigorous interaction between estimation activities and bio-geochemical efforts spinning up. It is generally accepted that the most important element for enhanced understanding of biological processes in the ocean is a realistic flow fields available from ocean state estimates. Yet, the greatest challenge of all may be to find a way to sustain the effort needed to produce the benefits of such an approach to oceanography, which involves longterm observing systems and synthesis activities alike.

Acknowledgments The authors acknowledge support of the ECCO project through the National Oceanographic Partnership Program, with funding from NASA, NSF and ONR. The ECCO consortium also acknowledges computational support through NSF (NPACI, NCAR), ONR and NASA.

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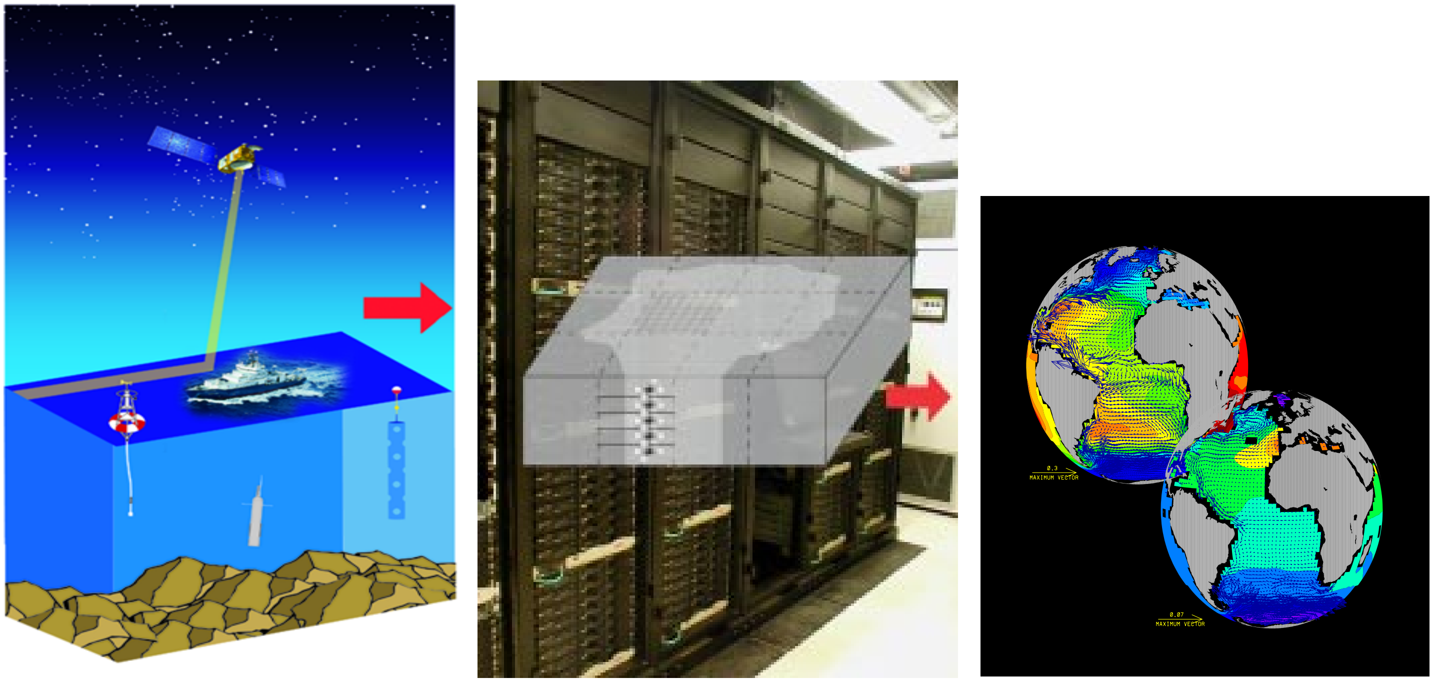

Figure 1: Schematic of ocean observing and assimilation system. The observing system on the left is providing near-realtime ocean observations. Combined with dynamics embedded in state-of-the-art circulation models that are run on super-computers (middle panel) ocean syntheses are obtained that form the basis for studies of the ocean circulation. Shown are here in the right panel is example of the ongoing state estimation for the near surface and the deep circulation.

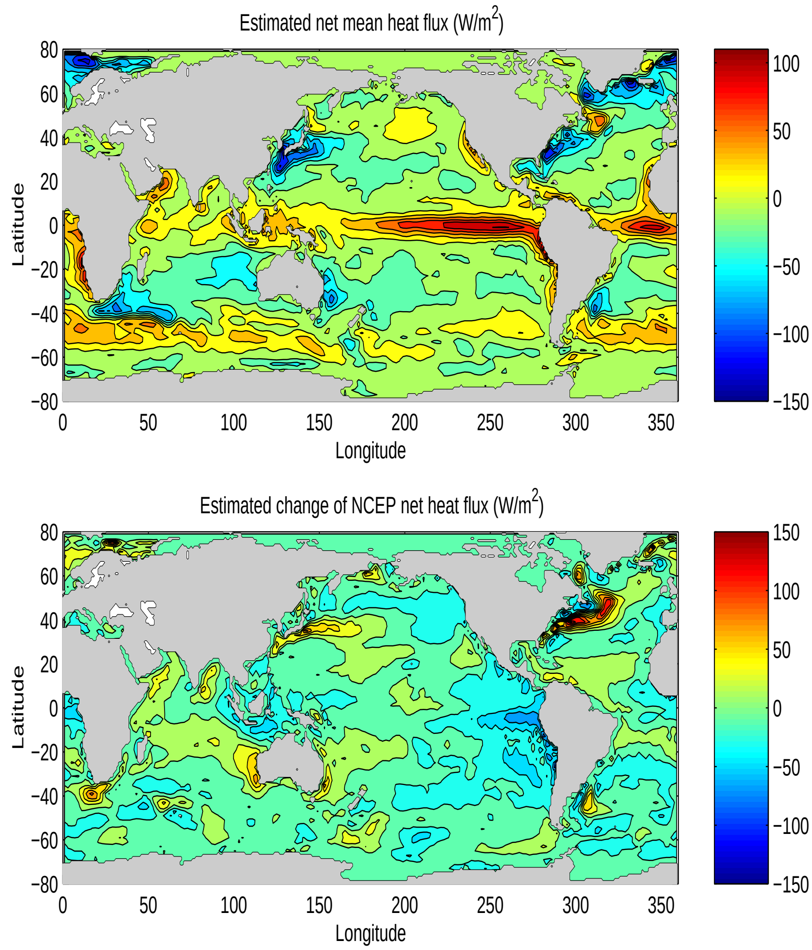

Figure 2: (upper panel) Mean estimated net surface heat flux required to bring the model into consistency with data (in Watts/m^2). (lower panel) Mean estimated adjustment of the National Center for Environmental Prediction (NCEP) net surface heat flux required to bring the model into consistency with data (in Watts/m^2). See *Stammer et al.* (2002a,c) for details.

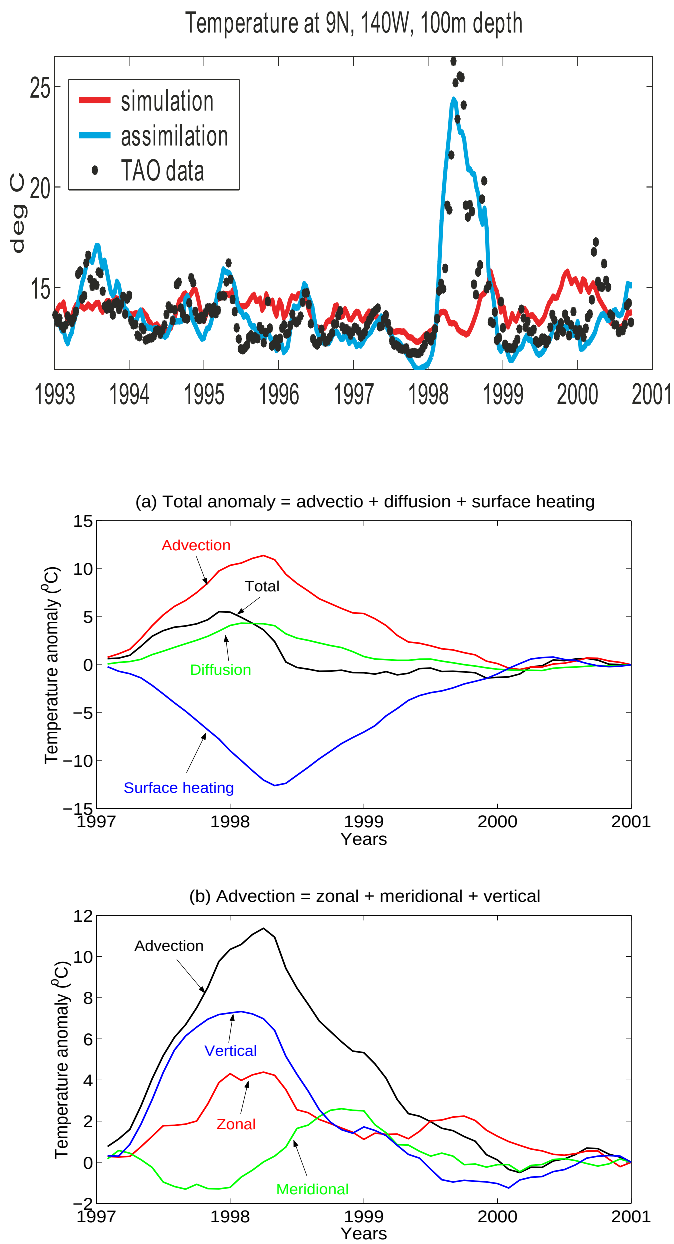

Figure 3: top: (top): Temperature time series at 9°N, 140°W at 100 m depth. Show are results from the constrained run discussed by *Fukumori et al.* (2002) in blue and from an unconstrained run in red. Observations from a TOGAR TOA buo at the same location are shown as bold dots. (Middle and bottom panels): Contributions of various terms to the tendency of the mixed layer temperature heat balances in the eastern tropical Pacific as described by *Lee et al.* (2002). Individual terms are specified in the panels.