A Consortium for Ocean Circulation and Climate Estimation

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2 Abstract and Table of Partnership

Abstract
A consortium of scientists at the Massachusetts Institute of Technology, the Jet Propuslion Laboratory, the Scripps Institution of Oceanography and the Max-Planck Institut für Meteorologie of Hamburg proposes a five-year NOPP A2 (Phase B) "node" to bring ocean state estimation from its current experimental status to a practical and quasi-operational tool for studying large-scale ocean dynamics, designing observational strategies and examining the ocean's role in climate variability. Our central technical goal is a complete global-scale ocean state estimation over at least the 15 year period 1985-2000 at $1/4°$ resolution with a complete error description and regional refinements to support CLIVAR and GODAE needs. We will combine all available and anticipated large-scale data sets — including TOPEX/POSEIDON, TOGA-TAO, High-resolution VOS XBT/XCTD, profiling floats, and drifters — with the dynamics embodied in a general circulation model to estimate the time-evolving, three-dimensional physical state of the full oceanic circulation. Results will be evaluated by the consortium in collaboration with the community and made available to all, fostered through a strong educational and visitor program.

3 Response to NOPP Objectives

A consortium of scientists at the Massachusetts Institute of Technology (MIT), the Jet Propulsion Laboratory (JPL), the Scripps Institution of Oceanography (SIO) and the Max-Planck Institut für Meteorologie (MPI), proposes to bring global ocean state estimation from its current experimental status to a quasi-operational tool. The scientific goal is to describe and contribute to the understanding of the global general circulation of the oceans by combining modern large-scale data sets with a state-of-the-art general circulation model (GCM). It is proposed as a five-year NOPP A2 (Phase B) "node." The work would be carried out by a team with long experience in developing and using the tools of ocean observation, ocean modeling and state estimation.

The initial motivation for this work came from studies such as WOCE, TOGA and JGOFS where it was realized that understanding the ocean circulation, its interaction with the atmosphere and role, e.g., in climate and biogeochemical cycles, demands combining data with ocean models in a way similar to the meteorological practice of "assimilation". The need for global-scale synthesis is now widely perceived in many areas of oceanography including WOCE AIMS, CLIVAR, GLOBEC, GODAE and others (Powell, 1998; GODAE docs. etc). Realizing this goal has been elusive in oceanography, in part because of technical and scientific challenges, but also because of limited manpower and computational resources. We aim to overcome some of these obstacles through a collaborative effort focused on attaining the most comprehensive global synthesis possible and applying it to some specific science questions. We propose to:

- Apply and continue to develop the necessary tools to produce high quality state estimates of the global ocean and use them for science, both globally and regionally.
- Supplement the global state-estimates with high-resolution regional studies in support of CLIVAR's Basin-wide Extended Climate Studies (BECS) in the North Atlantic and the North Pacific.
- Evaluate global and regional results using available high-quality data sets and estimate covariance functions for processes and errors in data and models.
- Develop ocean models in support of state estimation.
- Collaborate with the wider community in the sharing and evaluation of the products and techniques.

The central goal of the consortium is to make ocean state estimation (data assimilation) a practical tool. We will work together to improve the ocean general circulation models upon which assimilation is based, evaluate and improve assimilation techniques, and confront the practical problems of marshalling large data sets — including TOPEX/POSEIDON, TAO, high-resolution VOS XBT/XCTD, profiling floats, and drifters — and carrying out routine assimilation runs. This is an ambitious goal and will require a concerted effort of all partners in the sharing of scientific, computational and technical skills and resources. If successful, the proposed activity will create a new 'tool' which, we believe, would become a central operational element in any future oceanography application, whether it be monitoring of coastal pollution, studies of small-scale physical-biological interactions, or global climate studies and prediction on seasonal to decadal time-scales and longer.

Data assimilation in to ocean models has long been a focus of theoreticians and modelers and we are very much aware of the tremendous efforts of the community that bring us to where we are now. There are on-going assimilation efforts, e.g., at NCEP, GSFC, and LDEO/SIO in support of ENSO prediction, at U. of Maryland, OSU (directed primarily at tidal problems), or at NRL in support of Navy needs see Malanotte-Rizzoli, 1996 for an overview of recent activities). But unlike all of the above efforts, our focus is on the state estimation of the global ocean in its entirety combining together into a coherent whole all suitable data sets. Our interest is to draw models and observations together over decades of time to arrive at a detailed synthesis describing the entire evolving ocean which can be used for science to elucidate mechanisms and rigorously quantify what is going on.

We will combine, and develop the methods to make it routine, the currently available and anticipated large-scale data sets with the dynamics embodied in a GCM to estimate the time-evolving, three-dimensional physical state of the full oceanic circulation. This yields a 'state estimate' that is consistent with observations and dynamics which can be used to diagnose phenomena, to initialize climate forecast models and provide the physical context for studying ocean biology, carbon transport or the design of improved observing arrays. The state estimation procedure also provides, through the comparison of model-data misfits and statistical estimates of observational noise, a powerful tool for testing and improving the dynamics in the underlying GCM. To motivate greater use of the results by the community we will compare them with observational descriptions of ocean phenomena developed in other ways. We will encourage community involvement and entrain new scientists in to the use and evaluation of assimilation results by making the results widely available, through visitor programs and through collaboration with other programs.

Our central technical goal is a complete global-scale ocean state estimation over the 15 year period 1985-2000 at the highest possible resolution along with a complete error description. To develop the technical understanding required to incorporate all available data types, develop associated error covariances, and to continue to improve models in support of the global estimate, we will begin with coarser-resolution global and basin-wide models. This will also allow us to develop a near-real time capabilities in support of community needs.

In addition to developing data assimilation models and routine tools, the consortium will provide a novel experiment in integrating the modeling and observational communities. Some of the investigators have their expertise primarily in modeling or assimilation while others have the somewhat more phenomenological perspectives of an observer or theoretician. An important goal of the partnership is to develop a common language and techniques for bringing all perspectives together to advance ocean science.

3.1 Broad Participation

Meeting our goal requires bringing together several major activities and skills: global-scale general circulation models; global-scale data sets (both spaceborne and *in situ*); optimization algorithms for combining the model with the data; and skillful use of available computational power. To match these needs the consortium brings together investigators with the diverse backgrounds required. The MIT (Stammer, Wunsch) and JPL (Fu, Fukumori, Menemenlis) groups, collaborating over the past 10 years, have learned how to combine large-scale global data sets with GCMs (Fu et al., 1993; Fu and Smith, 1996; Fukumori et al., 1993; Marotzke and Wunsch, 1993; ATOC Group, 1998, Stammer and Wunsch, 1996, Stammer et al., 1997). They also have long experience in testing and using the altimetric data which are a central focus of the proposed work (Wunsch and Stammer, 1998). Marshall and his group (MIT) developed the ocean model that is at the heart of our assimilation tool, and they will continue to improve it in an essential activity of the consortium. Niiler and Davis (SIO) have developed large-scale in situ data sets in TOGA and WOCE while Wunsch (MIT), Menemenlis (JPL) and Cornuelle (SIO) has developed assimilation methods for acoustic tomography. Stammer, after having collaborated with Wunsch at MIT for several years on analyzing ocean data and combining them with global ocean circulation models, will join the SIO faculty during the summer of 1999, thus strengthening the collaborative ties within the consortium.

We will collaborate with MPI (Latif, Hasselmann) with the goal of exchanging scientific understanding on ocean state estimation, coupled ocean-atmosphere models and climate predictability, particularly in the tropics. MPI has collaborated with key personnel at JPL, MIT and SIO in similar areas for many years. The only costs of this specific collaboration are travel.

Our activity will also be strengthened by the on-going assimilation project in the Consortium on the Ocean's Role in Climate (CORC) headed by Cornuelle. The goal of the CORC project overlaps the present one, but has a specific regional objective: to test and improve Pacific Ocean models and forcing fields by demanding consistency between model and observations. The comparison of results between the CORC and NOPP projects - using different models and methods (Oberhuber's isopycnal model and

Green's function techniques) - will allow differences between the models and techniques to be evaluated.

Ocean state estimation is urgently needed in a number of community projects including WOCE synthesis, analysis of TOPEX/POSEIDON and JASON-1/2 data, planning and carrying out GODAE and CLIVAR, and developing analysis tools for GRACE. Each activity is at the forefront of an important area of ocean science and at least one consortium investigator is deeply involved in each. These activities will be an important venue for the consortium to engage with the wider community.

We also plan to interact with other NOPP nodes (coastal ocean, marine biogeochemistry, physical-biological) and with groups involved in operational and research studies of seasonal to decadal climate variability. A global circulation estimate, with quantitative error bars, will immediately support initialization of coupled-model climate forecasts (see enclosed supporting letters by A. Leetmaa and T. Barnett). For example, NCEP intends to use our results to improve their routine ENSO predictions. Our regional foci in the North Atlantic and North Pacific (in both cases including the tropics) will provide the higher resolution fields needed to support studies of coupled physical-biological and geochemical cycles. They will also provide boundary conditions for coastal data assimilation modeling. A particular concern will be developing in these regional foci the high-resolution capabilities needed to support CLIVAR's Basin-wide Extended Climate Studies (P-BECS and ACVE discussed below).

In addition to the scientific and practical aspects of our work, there will be a significant educational component and community involvement within the consortium. Today there are few in the oceanographic community exploiting the combined use of observations and GCMs. MIT and SIO will host a visitor program to involve scientists in the evaluation of our state-estimates and to assist them in using the assimilation results. Moreover, SIO will host, in cooperation with the multi-institutional CORC, an annual meeting to compare our current state estimates with the observations and analyses being made by CORC or other scientists. To support this community involvement, the consortium will develop ways to make its models, its results, and the underlying statistical assumptions and all the public data used, readily available to all.

Finally, SIO and MIT have significant oceanographic educational programs and will fully involve both students and post-docs in understanding the techniques and challenges of ocean data assimilation. This will help to build the new oceanographic community required to exploit what we believe will in future be a central oceanographic methodology.

3.2 Commitment and Cost Sharing

The consortium members have a long-standing commitment to global ocean observations, ocean modeling and the sythesis of the two. Moreover they have considerable experience in working together. The participating institutions are also committed to success and will invest in the effort. SIO will contribute with salaries of academic personnel and will additionally contribute about $30,000.00 per year to the consortium effort.

4 General Plan

The efforts in modeling and data preparation required to meet our goals - production of global and regional state estimates and global and regional model evaluation and development - will be shared across the consortium. We begin by discussing the general work to be done. This is followed by a description of specific tasks of teams and institutions.

4.1 The Global Effort

The production and evaluation of continuing three-dimensional estimates of the global state of the ocean is our central goal and the foundation of everything else that is proposed here. While some climate processes are regional, the climate is fundamentally global and must be addressed from a global perspective. We do not adequately understand the physical processes linking the ocean with the changing atmosphere

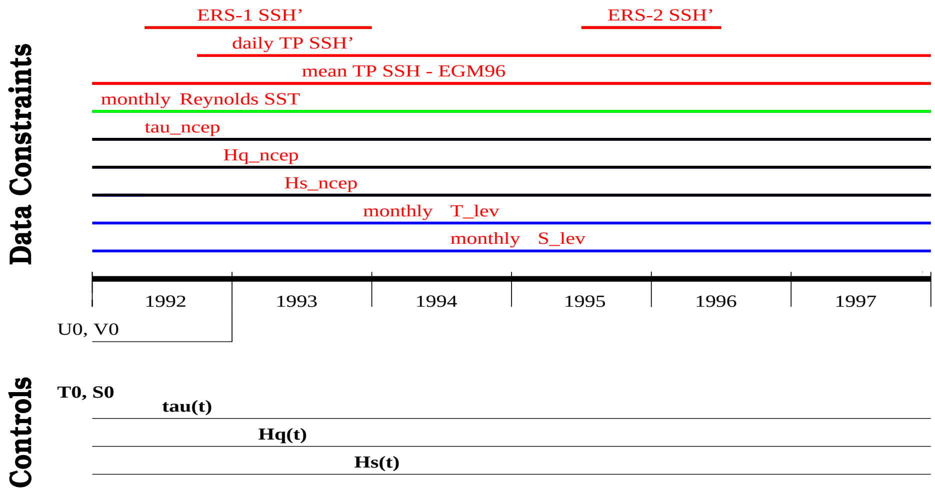

Figure 1: Schematic of the ongoing optimization. The upper part of the figures shows the data constraints and their distribution in time. The lower part shows the "control" parameters, which are the initial T and S fields, and the time-varying surface forcing (wind stress, heat and fresh water fluxes), which are adjusted to bring the model into consistency with the data.

or its role in global climate variability (e.g., What are the physics causing global and regional sea level rise? What is the role of the Southern Ocean and other critical regions in global balances?). These, and related questions in biogeochmical cycling, demand the best possible state estimate and understanding of the global ocean. The global state-estimation is therefore the common denominator for all the involved scientist and is a pre-requisite to be able to sensibly address our regional interests - it will be the responsibility of all four institutions, but led by Stammer.

The central task is to bring together a global GCM with existing global data streams — including TOPEX/POSEIDON altimeter observations and *in situ* hydrographic and current measurements — to obtain the best possible estimate of the time-evolving ocean circulation and related uncertainties. We choose to use the MIT GCM (Marshall et al; 1997a,b) and its adjoint model because, as builders of the model, we are intimate with it, because it is a modern code written for parallel computers in a manner which can easily exploit automatic adjoint compilers, and because it incorporates many of the best innovations - algorithmic, physical and numerical - of the wider community.

The anticipated data time period of our initial state-estimate will be 1985-2000. This encompasses the TOPEX period (launched in October 1992) and includes most of the WOCE and TOGA data. Although very demanding, this computation is already feasible, in principle, on existing computer resources, but will require the planned NOPP "hub" for continuation.[1]

With NASA and NSF support, we have already gained considerable experience in global and regional ocean state estimations. Stammer, et al., (1997) carried out a demonstration calculation with data restricted to one year, using the MIT GCM and its adjoint model. We have now switched to a full 6-year data span using a more complete representation of model physics. Improvements include an increased model resolution to 1°, an extended estimation period to 6 years (1992 through 1997), as well as more accurate representations of straits and sills in the topography. Equally important, a complete mixed layer model (Large et al., 1994) and an eddy parameterization (Gent and McWilliams, 1990) have been incorporated into the forward and adjoint model.

The data which are being used to constrain the model (see Fig. 1) include the absolute and time-varying T/P data (relative to the EGM-96 geoid model; see *Lemoine et al.*, [1997]) from October 1992 through December 1997, SSH anomalies from the ERS-1 and ERS-2 satellites, monthly mean SST data (Reynolds and Smith, 1994), and the twice-daily time-varying NCEP Re-Analysis fluxes of momentum,

[1] We estimate that a 40-iteration minimization experiment over this period would require about 15 months of continuous run time using 64 of the 256 processors on the HP exemplar at CalTech. The upcoming NPACI/SDSC facilities, slated to become operational in the spring of 1999, would shorten this time considerably.

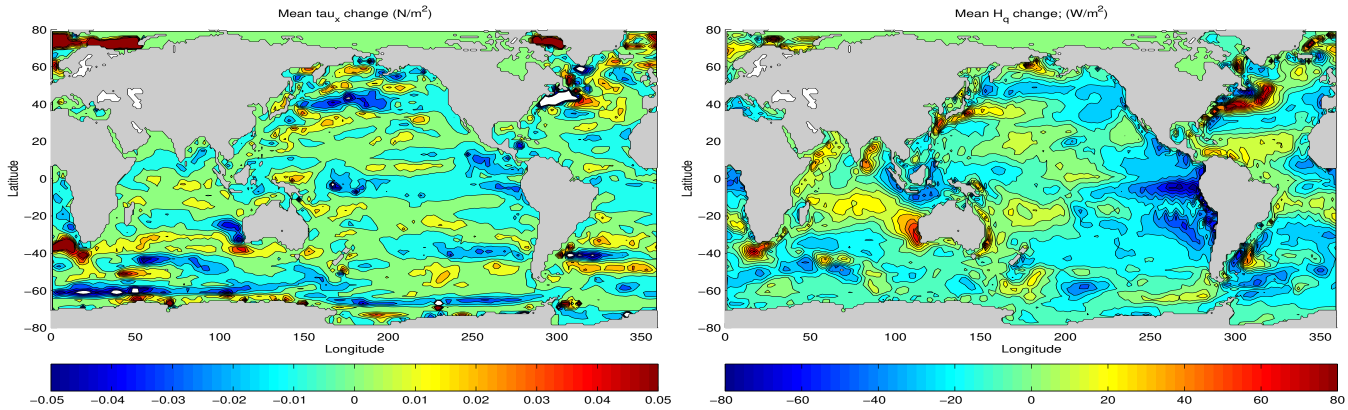

Figure 2: Changes to the time-mean zonal windstress τ_x and surface heat flux H_q required to minimize model-data differences over the 6-year long assimilation period, after 28 iterations (the same for all following figures). These and similar changes in meridional wind stress and and freshwater flux will be used to understand and improve uncertainties in meteorological forcing fields after a fully optimized solution has been obtained.

heat and freshwater. In addition, monthly means of the model state are required to remain within assigned bounds of the monthly-mean Levitus et al. (1994) climatology, and NSCAT estimates of wind stress errors (*D. Chelton*, pers. communication, 1997) are being employed. At the moment, all error covariance matrices $\mathbf{W}_j$ are diagonal with the important exception of the $\mathbf{W}_{EGM96}$ matrix for the mean sea surface height which is fully non-diagonal and dense and is identical to the EGM96 error covariance matrix to degree and order 70.

This global adjoint estimation is now under way and will serve as a starting point for the proposed NOPP work. Although still preliminary, it already shows that the envisioned synthesis can be fully realized. Many of the results from the ongoing computation can be seen on the Website http://puddle.mit.edu/˜detlef/OSE/global.html. To give a feeling for what can be done now, Figs. 2 through 5 (and legends) show selected results after a considerable reduction in the model-data misfit, but before reaching a fully optimized state (the calculation is still progressing).

If such calculations could be routinely made and continually improved (as numerical weather analyses have improved over time), many facets of oceanography - regional and coastal applications, physical-biological and bio-geochemical modeling, air-sea interaction, theory and models of the general circulation of the ocean - and indeed fields outside of oceanography, such as geodesy, are expected to come to rely upon the resulting products. An example of a specifically oceanographic application is the off-line use (M. Follows, personal communication, 1998) in transient tracer and biogeochemical (oxygen, carbon) models. A quite different application somewhat outside the realm of oceanography, is understanding the changes in earth's rotation and polar motion owing to fluctuations in ocean circulation (Ponte et al., 1998; Ponte and Stammer, 1999). It has already been demonstrated that our present estimate of ocean topography, if used to compute a marine geoid by subtracting it as the ocean component from mean altimetric sea surface height observations, often improves computed satellite orbits relative to those obtained with conventional geoid models (N. Pavlis, personal communication, 1998).

It should also be noted that in many regional applications, a global model is required to supply lateral boundary conditions and to understand large-scale adjustment processes, such as the response of the ocean to variable wind and pressure forcing.

4.2 Methodology

Over the last decade ocean models have evolved and improved in numerous ways (e.g., Semtner and Chervin, 1992; Marshall et al., 1997a,b; Smith et al., 1992) so that now global GCMs of much realism

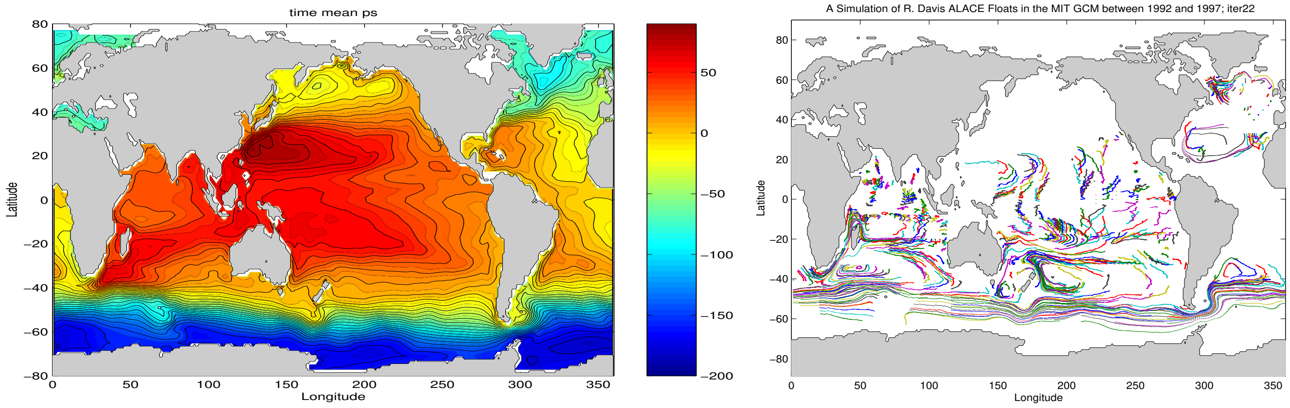

Figure 3: (left) Mean sea surface height (in cm) of the constrained model. (right) Float trajectories simulated by the constrained model over the 6-year period. They are now being compared with WOCE PALACE trajectories prior to their use in the state estimation (e.g., Davis, 1998).

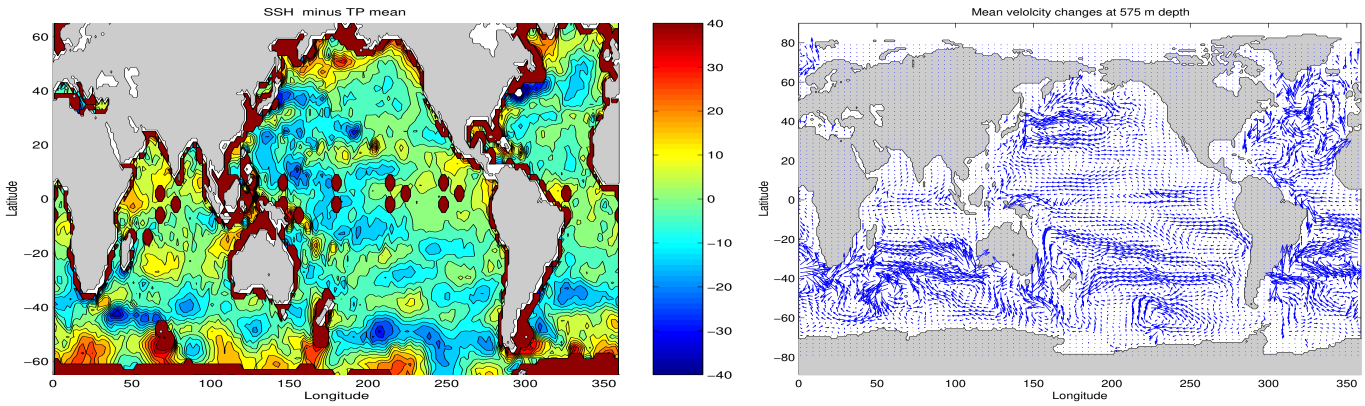

Figure 4: (left) The model-data misfit of absolute sea surface height (in cm). There is a close correlation of the residuals with independent information about the error of the EGM96 geoid model. (right) The difference between the first-guess mean flow field at 575 m depth and that obtained from the constrained model. Maximum amplitudes are about 1.2 cm/s, or a full 30% of the mean.

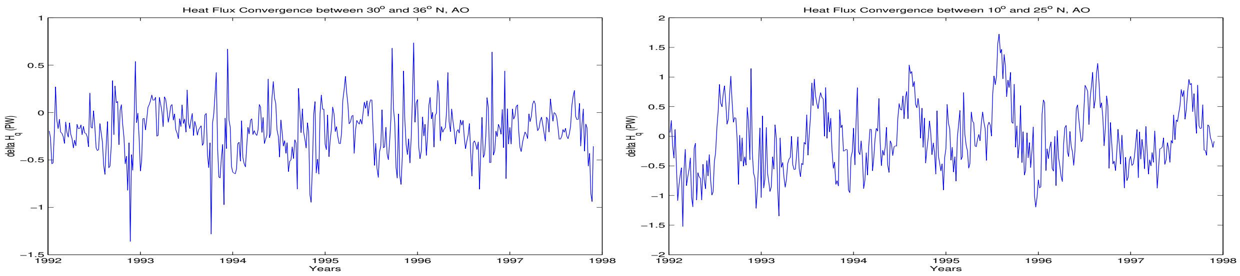

Figure 5: The convergence of zonally integrated heat transports in the North Atlantic. The left panel shows the convergence between 36° and 30°N; the same field, but between 25° and 10°N is shown on the right side. There is a significant amount of high-frequency variations superimposed on seasonal and interannual variability. This needs to be analysed in terms of its relation to (local and remote) air-sea interactions, heat storage and, ultimately, its climate implications.

exist with resolution better than $1/6°$, and regional versions at even higher resolution. We also have global data sets and technologies that will provide autonomous observations of the interior of the ocean. Finally, enough has also been learned about the estimation procedures (books by Bennett, 1992 and Wunsch, 1996 were produced, in addition to innumerable papers and reviews in both the oceanic and atmospheric literatures; for the latter see Daley, 1991) so that the models and observations can be brought together to give us a description of the ocean that is better than either alone.

The central methodology for the proposed state estimation will be the "adjoint method", known in control theory as the "Pontryagin Principle". This method has been much discussed in the oceanographic literature in the past 10 years (Thacker and Long, 1988; Tziperman and Thacker, 1989; Wunsch, 1988; Marotzke and Wunsch (1993); Sirkes and Tziperman, 1997) and a large literature also exists in meteorology (e.g., Errico 1997). We will only very briefly summarize the elements which are required here. A full account on ocean state estimation, including the adjoint method, can be found in Wunsch (1996).

Let us write the GCM in greatly condensed fashion as a time-stepping rule:

$$\tilde{\mathbf{x}}(t+1) = \mathcal{L}(\tilde{\mathbf{x}}(t), \boldsymbol{\tau}, ..., \boldsymbol{\epsilon}) \tag{1}$$

where $\tilde{\mathbf{x}}(t)$ is the model "state vector" (velocity, temperature, salinity, pressure,...) at all model grid points at model time t. $\boldsymbol{\tau}, ...$ is the wind field and other boundary conditions, and $\boldsymbol{\epsilon}$ represents model errors of all kinds. If run forward in time, we can compute from $\tilde{\mathbf{x}}(t)$ the values of quantities we also observe. These observations can be written, generically (assumed linear, however), as

$$\mathbf{y}(t) = \mathbf{E}(t)\,\mathbf{x}(t) + \mathbf{n}(t) \tag{2}$$

where $\mathbf{x}$ now represents the true ocean state, $\mathbf{E}(t)$ is the observation response matrix and $\mathbf{n}(t)$ is the inevitable observation noise (notation is from Wunsch, 1996).

Most assimilation methods, including the ones we mainly use, are equivalent to finding the least-squares value of a measure of the misfit between observations and the model,

$$J = \sum_t (\mathbf{y}(t) - \mathbf{E}(t)\,\tilde{\mathbf{x}}(t))^T\, \mathbf{W}(t)\, (\mathbf{y}(t) - \mathbf{E}(t)\,\tilde{\mathbf{x}}(t)) \tag{3}$$

where $\mathbf{W}$ is a weight matrix, often chosen to be the inverse covariance of $\mathbf{n}(t)$. In general terms, the assimilation problem is to minimize J subject to Eq. (**??**) by adjusting model parameters including initial and boundary conditions, mixing coefficients etc. Here the "adjoint method" has proven to be very efficient in providing a vehicle to iteratively solve the above minimization problem. In practice it is a problem of huge dimension and intrinsically non-linear.[2] The solution of the adjoint model, however, provides more than just a minimization procedure, for the adjoint variables themselves carry important information about dynamics related, for example, to the adjustment of the ocean to changing atmospheric boundary conditions.

The adjoint problem has been made practical through the availability of a remarkable compiler written by R. Giering (Giering and Kaminski, 1998; Marotzke et al., 1999) which permits generation of the adjoint model code directly from the source code of the forward model (**??**). Moreover, the coding of the MIT model was masterminded by Chris Hill of MIT (in close consultation with Giering), so that it would interface tightly with Giering's compiler and yet not compromise our ability to efficiently target a wide variety of parallel computers. The resulting forward-adjoint software tool is now remarkably versatile and runs efficiently across a wide range of modern computer architectures, something that would not have been possible if we had started with 'legacy' code.

The "adjoint" assimilation will be complemented by analyses based on approximate Kalman filters and smoothers (e.g., Fukumori and Malanotte-Rizzoli, 1995; Fukumori, 1995). This secondary approach serves three purposes; (i) estimation of optimal weights, W etc in Eqs (**??**), (ii) exploration of higher resolution models than used by the "adjoint", (iii) applications to real time analyses.

[2] In the global oceanic case (at $1°$ horizontal resolution, 20 vertical levels, and 6 state variables at each grid point) the state vector has about 3×10^6 elements at each time step. There are about 3×10^5 control variables to be optimally chosen.

Because of the very large number of degrees of freedom in the global adjoint computation, and because of the comparatively small number of measurements, the skill of the estimates for unobserved variables resides to a large extent in the *a priori* information, that is, in the form of the cost function (the weights in (**??**) and in the GCM itself (**??**)). The approximate Kalman filter and its extensions are the most fully tested methods for estimating both *a priori* and *a posteriori* uncertainties (Fu et al., 1993; Menemenlis and Chechelnitsky, 1999). The approximate Kalman filter permits the forward model to be integrated at arbitrarily higher resolution than that at which the Riccati equation for the model error is solved, with little additional computing overhead beyond that of the forward model. Given finite computer resources, the approximate Kalman filter can therefore afford a much higher resolution for the forward GCM integration than that of the adjoint, thereby minimizing model representation errors in the final estimates.

The Kalman filtering approach is also particularly suited for regular, real-time, analyses (cf section 5.2). Optimal restarts are possible without reanalyses from the past, because full error information is carried along with the model state estimates.

4.3 Regional Foci

Embedded within our overall global effort, there are two major regional foci to support CLIVAR Basin-wide Extended Climate Studies (BECS) in the Atlantic (ACVE) and in the Pacific (P-BECS). CLIVAR (CLIVAR, 1998) is concerned with seasonal to decadal phenomena like ENSO, the Pacific Decadal Oscillation, the North Atlantic Oscillation, the Atlantic tropical dipole of SST and its associated atmospheric pattern. These are large-scale, recurrent patterns of variability that involve the ocean and influence continental climate. The BECS concept derives from a meeting of the oceanographic community in San Antonio (Davis, 1996) where it became clear that understanding these climate phenomena would require studying the large-scale ocean employing a process oriented approach usually reserved for small-scale studies. The meeting recognized that the emerging ability of assimilating modeling and low cost observations made it feasible to diagnose processes inside a dynamical model that was constrained by feasible large-scale observations. An experiment to exploit this concept was dubbed a BECS and the community has begun to plan a BECS for the North Atlantic and Pacifc.

The consortium plans to develop the modeling and state estimation capabilities required for the upcoming BECSs to reach their goals. This demands the use of higher resolution than is feasible with a global model. The many scientific and practical commonalities between global and regional assimilation studies, and between the Atlantic and Pacific BECS themselves, make it desirable to approach their more operational and technical aspects together. Commonalities include scientific questions (e.g., tropical-subtropical interaction through shallow overturning circulations, variations in upper ocean mixing and entrainment, variations of boundary current transports and locations), observing networks and data links, model improvements, as well as many questions related to state estimation.

Our strategy for the regional foci is to embed the models of the Atlantic and the Pacific in to the global, but coarser-resolution, ocean state estimate, thus allowing the information of the global data sets to propagate into the limited-domain set-ups. This will be accomplished by prescribing from the global solution the boundary conditions which subsequently will be further modified as part of the regional optimization. As described below, the resolution in the regional approaches will be increased towards the equator and possibly towards the eastern and western boundaries. At the same time the resolution will also be enhanced in the vertical, e.g., to allow a more appropriate estimate of shallow ocean phenomena involved in the tropical-subtropical interaction in low latitudes.

Clearly, the regional studies will benefit from the global state estimate. At the same time, they will benefit the global effort. The cost of global estimates suggests that technical aspects of the global estimation procedure should be first tested in a limited-area context. The regional approaches with varying horizontal resolution can serve as testbeds for dealing with new data types and error covariance functions. Similarly, the ultimate goal of the global work is ocean state estimation with at least eddy-permitting resolution. Our experience with eddy-resolving state estimation is rudimentary and we propose to gain insight into this first on a regional scale in the Atlantic and Pacific areas. Experience from those regional approaches will subsequently be built into the global estimation.

5 Consortium Tasks

5.1 The Global Effort

Many of the model subcomponents, the inverse error covariance estimates $\mathbf{W}$, and optimization methods are regarded as preliminary and part of the proposed work is to bring all of them onto a more operational level. *A posteriori* errors will be used to evaluate and possibly revise *a priori* data and model error covariances used in the estimation procedure.

Observations:
Although we have experience in the assimilation of a wide variety of data types (see listing above), a goal is to accommodate the entirety of the oceanic observation set including the suit of *in situ* hydrographic and current observations, to the extent that observations are (a) overlapping with our estimation period, and (b) more than purely regional. Bringing in a new data type is a two-step process: first one simply compares the existing state estimates with the new data (this is essentially a comparison of $\mathbf{y}(t)$ in (**??**) with $\mathbf{E}(t)\,\tilde{\mathbf{x}}(t)$ where $\tilde{\mathbf{x}}(t)$ is the *estimated* (modeled) ocean state (as distinguished from the real one). Given some understanding of the uncertainty of $\tilde{\mathbf{x}}(t)$ (see below), and of the noise in $\mathbf{y}(t)$ (specified by a covariance for the noise, $\mathbf{n}(t)$) one must decide if there is a basic consistency between the model and data already being used, and the new data. Assuming statistical consistency has been found, one can turn to using the new observations to make an improved estimate.

The data to be dealt with next include (not in priority order) autonomous float velocity and profile data (becoming ARGO; see Roemmich, 1998); the WOCE hydrographic lines (not as climatologies); current meter data (especially the TAO array); XBTs; satellite sea surface temperature; and the forthcoming GRACE mission time-dependent gravity data. Note that tomographic data have already been used (Menemenlis, et al., 199x; The ATOC Consortium, 1998) in regional assimilations. An example of a first comparison is illustrated in Fig. 4b, which shows the computed float trajectories for comparison with the WOCE results (e.g., Davis, 1998).

Some of these new data types should be comparatively straightforward to use, being just variations on data already in-hand (e.g., the GRACE data, the floats if used as Eulerian values, etc.). Others raise potential difficulties (the floats if used in trajectory form; the hydrography because of the very long baroclinic and mixing adjustment times of the ocean). Some thought has been given to these latter problems. For example, for the hydrography large-scale baroclinic adjustment EOFs or equivalent long range covariances, can be used to "short-circuit" the long adjustment times. To fully understand the hydrographic adjustment problem, we propose to use the fully implicit LSG model (MPI) which allows 500 to 1000 year runs by using a one-month time step to understand the long adjustment processes of the ocean interior to varying surface forcing. This work will reside primarily with our MPI partners. Estimated space and time scales of the variations in T and S can be used subsequently as hydrographic weighting factors in the global assimilation.

Model Configuration
Our final goal is a global ocean state estimation with a resolution of about $1/4^\circ$, horizontally. However, the first step is to increase our current resolution, to span a longer time period and to encompass the data types outlined above. For that purpose we propose to carry out the global estimation on a grid with 1° nominal spacing between $\pm\ 22^\circ$ and $\pm\ 80^\circ$ in latitude, telescoping down to 0.3° meridionally near the equator. The forward model has already been set up at JPL and integrated forward in this configuration, including high-end physical parameterizations of the mixed-layer and subgrid-scale eddy processes. This resolution and model domain are believed to be a minimum required to address many of our scientific objectives. Higher-resolution regional experiments will be carried out to gain experience

with eddy-permitting resolution in support of regional studies. Regional approaches are also required with varying spatial resolution for many practical purposes, e.g., to test new data types, *a priori* statistical assumptions or new model components.

Phenomenological Studies Using Global State-Estimates
Many of our global science foci are related to ocean variability, and associated interaction of the ocean with the atmosphere. Accordingly phenomenological studies on basin to global scale will include the calculation of meridional fluxes and flux divergences of heat, fresh water, carbon and nutrients so as to determine the basic oceanic climate state and its interaction with the atmosphere. Key elements here are:
(1) Heat and freshwater balance in the upper tropical and sub-tropical Pacific and Atlantic Oceans including the relative contributions of upwelling and subduction, horizontal advection, mixing, air-sea exchange and local storage;
(2) Tropical-subtropical exchange and mid-latitude subduction including temporal variability and north/south asymmetry of the western boundary current, how water is subducted in the subtropical oceans, its subsequent path and how its properties are changed;
(3) Decadal variability throughout the tropical and higher-latitude oceans, including circulation in the subtropical gyre, Ekman pumping, mixed layer processes and Ekman transport.

Our estimated state is constrained by ocean observations; however this does not guarantee that the state estimate will agree or be fully consistent with the observed ocean state. Disagreements may indicate model errors, inappropriate *a priori* assumptions about error covariance matrices or mistaken interpretations of the data. Reconciliation of the estimated state with observational descriptions is therefore an important element in the estimation procedure and a pre-requisite to the full community involvement. We will therefore carry out careful comparisons of the state estimates with data selected data sets, which will include:
- Temperature and velocity data from the TAO moorings;
- Repeated CalCOFI hydrographic surveys of the California Current;
- Global surface circulation derived from drifters and altimetry;
- Mid-depth circulation in the South Pacific measured by ALACE floats;
- Mixed-layer evolution observed from various well instrumented surface.

Comparisons of model and data will be both statistical (i.e. rms misfits of dynamically significant variables, and associated spectra) descriptive and phenomenological. The task of comparing data to the initial global (and regional) assimilation results will be shared among the three institutions, depending upon where the specific data expertise lies.

Computational Efficiency and Resources
Limited computer power is a major obstacle to routine production of (say) daily estimates of the three-dimensional flow field consistent with all of the above observations. An ocean modeling hub was called for in Powell (1998) and is envisioned in the NOPP announcement. In the meantime, until an adequate NOPP "hub" is in place, we will require all of the computational resources available to us at SDSC, JPL and anywhere else; and we will also help to bring a hub into being. At the present time, the global calculation is running on the NPACI CRAY T90 computer, located at the San Diego Supercomputer Center adjacent to SIO. The same model is now also being run by our JPL partner on the CalTech HP Exemplar computer (also an NPACI partner) located at JPL. It is our intention to run the system at both institutions (i.e., JPL and SIO/SDSC), swapping state estimates and model changes back and forth to take maximum advantage of existing computer resources and manpower at both locations. Fukumori will be the responsible individual at JPL for this purpose and Stammer at SIO.

The optimization procedure at the heart of the assimilation method consumes most of the computer resources. Improving the efficiency of the algorithms will, therefore, be a major priority. Our primary experience has been with two well-understood algorithms, including the adjoint method, which is iterative, and does not require the computation of the error covariances necessary to the use of filter/smoother algorithms. But the interpretation of the estimated states still requires the knowledge of its error covariance matrix, which at this point is most likely to be obtained from approximate (e.g., reduced-state) versions of the filter/smoother algorithms (and which for linearized systems can be computed "off-line"; e.g., see Fukumori and Malanotte-Rizzoli, 1995; Fukumori, 1995). The JPL group will have primary responsibility for continued development of the filter/smoother methodologies which in the future might become a practical alternative for near-real time ocean estimates in support of operational applications.

5.2 Data Flow

Scripps, MIT and JPL are all foci of major efforts working with global and near-global data sets. Scripps and MIT scientists in the consortium have long experience with the conventional *in situ* data, particularly hydrography, floats, drifters, current meters and tracers. The continuing ATOC tomographic data sets are dealt with at MIT (Wunsch), SIO (Cornuelle), and JPL (Menemenlis). The various data sets are already being swapped between the institutions—primarily by electronic means. Assuming that funding will continue at all three institutions for existing analysis and use of the various data sets, we anticipate being able to continue acquiring, archiving and redistributing to the community all of the fundamental data sets without major additional efforts. JPL's PO-DAAC will assure close connection to a broad satellite data base whereas SIO holdings of hydrographic, float and drifter data will provide key *in situ* data sets.

5.3 Model Development

GCMs continue to evolve and we will continue to make improvements to ours, particularly insofar as serious model/data combinations always turn up model problems, which become more subtle as time goes on. Responsibility for the model will remain with Marshall's group at MIT.

The MIT model, as a new code, has several features of particular interest to us:

1) The kernel algorithm and code was designed to exploit parallel computing technologies (Hill and Shaw, 1995; Shaw et al.; 1998).
2) It is algorithmically advanced, incorporating innovations from the wider ocean modeling community, such as an implicit free-surface methods (Dukovicz et al., 1994) and efficient preconditioners (Dukowicz et al., 1993), a mixed layer formulation KPP (Large et al., 1994) and interior mixing algorithms GM (Gent and McWilliams, 1990). Local innovations include finite-volume and shaved-cell representations of topography (Adcroft et al, 1998); a new treatment of the Coriolis force on the staggered grid (Adcroft et al., 1999); spatially variable eddy-transfer coefficients (Visbeck et al., 1997); parametric representations of convection (Marshall and Schott, 1999); and a non-hydrostatic capability is available.
3) The code is written to interface closely with the adjoint compiler (Giering and Kaminski, 1998; Marotzke et al. 1999).
4) It relaxes some conventional assumptions made in the hydrostatic primitive equations: hydrostatic, quasi-hydrostatic and non-hydrostatic versions are available, allowing it to be applied to coastal and small-scale process studies (Marshall et al., 1998).

Our initial emphasis on improvements will be in accord with the emerging views of the community, as expressed, for example, in Gent (1998) and Stammer et al. (1998):
(a) Allowing background eddy-transfer coefficients to be functions of space to capture stirring by spatially non-uniform geostrophic eddies—simple ideas have been put forward and implemented by our group in (Visbeck et al., 1997). But their performance needs to be evaluated against global data sets in the context of the model-data synthesis.
(b) Evaluation, in the light of the observations, of the KPP upper boundary layer mixing scheme and its interaction with ice models, eddy-parameterization schemes and performance in key regions of deep convection and water-mass transformation.
(c) Improvements of the bottom boundary layer of the code - e.g. Beckman and Döscher (1997) - ex-

ploiting our partial bottom cell scheme Adcroft et al. (1997), to permit conservation of T/S properties of water masses flowing over topography.
(d) Improved resolution, either through spatially-non-uniform gridding methods or increased computational power.
(e) Use of a generalized vertical coordinate to exploit the best properties of height-coordinates (near the surface), isentropic coordinates (in the interior) and sigma coordinates (near the bottom).

5.4 Becoming Operational

One of our major practical goals is to bring ocean state estimation from its present experimental stage to quasi-operational applications. The skill of such estimates can be expected to improve over time as general scientific understanding improves, and as the models and methods are refined.

An immediate need for operational estimates of the ocean state is now increasingly recognized and is described in various WMO/GOOS/GCOS/GODAE documents (see also Powell, 1998). In particular, recent studies at both MIT and JPL have shown that the ocean responds very rapidly to large-scale wind bursts on time scales of hours to days and on space scales of hundreds to thousands of kilometers (basin to global scale). These motions represent a signal which is important for coastal and other applications. But there is also an immediate practical issue: they are/will be aliased by the present sampling of the ocean by TOPEX/POSEIDON and successors, and particularly by the proposed GRACE time-varying gravity mission (GRACE, 1998). Preliminary studies suggest (e.g., Fu and Smith, 1996) that OGCMs have sufficient skill in simulating the fast barotropic fluctuation of the ocean and that much of this aliasing can be reduced by calculating the high frequency response of the ocean to the time-varying wind (and atmospheric pressure) fields. Subtracting it from the observed signals is likely to significantly improve our observational data base.[3]

We intend to gain experience with operational ocean modeling, by setting up the infrastructure and data links (i.e., links to meteorological centers providing forcing fields), to provide "forecasts" (simulations) of the high-frequency barotropic large-scale variability of the ocean. This work is expected to teach us a great deal about the practical aspects of maintaining a continuing estimation stream for the full global model over all accessible time scales. Here JPL will undertake, using the MIT model in either barotropic or full baroclinic mode, which ever is chosen, operational simulations of the ocean circulation by the time of launch of JASON-1 (2000) and GRACE, (2001).

Because data reduction will run approximately two weeks to one month behind real-time, it should be possible using the existing optimization formalism to use data formally future to the date of observation to increase the skill of the model estimate. Analysis of the results will be shared between JPL and MIT (Wunsch and V. Zlotnicki of JPL are members of the GRACE Science Team.)

5.5 Regional Foci

The Atlantic
Climate Variability of the Atlantic sector comprises three primary phenomena: Tropical Atlantic Variability (TAV), The North Atlantic Oscillation (NAO) and Atlantic Meridional Overturning Circulation (MOC). A sustained, Atlantic-wide observing system is being planned - The Atlantic Climate Variability Experiment (ACVE) - to provide the data necessary to test proposed hypotheses and to test models in the framework of CLIVAR[4]

The existing and planned programs in the Atlantic basin: the PIRATA (Pilot Research Moored Array in the Tropical Atlantic) program, the PALACE float and XBT arrays, tide gauges, surface drifters (as part of WOCE) and atmospheric soundings provide the context for our state estimation efforts in the Atlantic. A number of consortia PI's have been deeply involved in the planning of ACVE and the

[3]Experiments are continuing on understanding the skill of simpler barotropic models relative to those of the full baroclinic one (a conference on time- dependent mass and gravity variations over the ocean will take place in April in the UK).
[4]See http://www.ldeo.columbia.edu/~visbeck/acve/.

execution of recent major sea-going experiments in the Atlantic - ACCE and the Labrador Sea Deep Convection Experiment (Lab Sea Group, 1998). These experiments have already provided a wealth of observations of the North Atlantic Ocean and a detailed description of the watermass transformation process in the Labrador Sea along with contemporaneous air-sea flux measurements.

The objective of our state estimate will be (1) to arrive at the best possible description of the evolving Atlantic Ocean during the WOCE period, augmented by data from regional process studies such as the Lab Sea Experiment (2) evaluate it against available surface and subsurface observations, with particular attention to poorly understood phenomena such as the development, propagation and decay of heat content and salinity anomalies, subtropical-tropical interaction, and to basic features such as the distribution of principle water masses (3) to interpret it in terms of theories of subduction, convection and thermocline ventilation (4) use it as a vehicle for planning and refining ACVE.

To make a start on the problem the MIT forward/adjoint model has already been configured in the Atlantic by post-doc Nadia Ayoub, extending from 35°S to 80°N. This model has a resolution of 1° decreasing to 1/3° in the tropical band (exploiting the easy ability within the global model code for graded grids). The necessary open ocean boundary conditions at the southern and northeastern boundaries have been implemented as described by Zhang and Marotzke (1999) with the initial estimate of the values taken from the global model estimates and then refined as part of the optimization procedure. This code is prototypical of the regional model in the Pacific that will also be embedded in the global estimates. We plan to push the resolution down to 1/6° as soon as is practical.

As mentioned above, the adjoint model can also be used to calculate the sensitivities of key dynamical or climate variables (e.g., meridional overturning strength at certain locations, maximum meridional heat transport, SST, stratification), to the forcing or to quantities that are more readily observable. For example, Marotzke et al. (1999) calculated the sensitivity of 1993 annual-mean Atlantic heat transport at 29°N to variations in the hydrographic conditions on 1 January 1993 and to variations in wind stress. This computation must be considered highly preliminary since it is based on the relatively crude global assimilation solution of Stammer et al. (1997), but it demonstrates the potential of adjoint sensitivity calculations to elucidate dynamical pathways and to determine where and which specific type of observations are mostly needed to constrain climatically important estimates.

The MIT group (Marshall, Marotzke, Wunsch) will be primarily responsible for this effort, with an initial focus on the dynamics and potential monitoring of Atlantic meridional transports of mass, heat, and properties. The work will be carried out on local computers operated in conjunction with the MIT Laboratory for Computer Sciences, thus avoiding a competition for computer resources with the global effort.

The Pacific:
The other planned CLIVAR BECS in the Pacific is described in Lukas et al. (1998)[5]. A central focus will be on El Niño/Southern Oscillation (ENSO), its decadal modulation and decadal variability such as the Pacific Decadal Oscillation (PDO). ENSO is the strongest seasonal-to-interannual variability signal and affects many regions around the globe. ENSO theories which invoke adiabatic oceanic wave propagation along the equatorial wave guide are helpful in understanding the dominant characteristics of ENSO but do not provide a complete picture of how ENSO develops. Even in wave-like models, parameterized diabatic processes are central to formation of the ocean thermal anomalies involved in the ENSO cycle. Diabatic processes involved in the exchange of subtropical and tropical thermocline waters are also suspected of modulating, on decadal time scales, the evolution and predictability of ENSO cycle. Diabatic processes appear also to be at the heart of the air-sea coupling associated with the PDO. The several suggested mechanisms of PDO include ocean processes like variation of circulation in the subtropical gyre, trans-basin Rossby waves, wind-driven mixed layer entrainment and the same kinds of subtropical-tropical interactions that may affect ENSO.

The Pacific BECS is intended to add to the Pacific observational network enough data that an ocean

[5] See also http://www.soest.hawaii.edu/~rlukas/PBECS/pbecs.html.

model can indeed be constrained and the questions of mechanism in ENSO, decadal modulation of ENSO and in the PDO can be explored inside the estimated state.

There are ongoing efforts at both Scripps and JPL to model the Pacific Basin, while working with all of the available data types. This work will be a shared responsibility of the Scripps (Stammer, Davis, Niiler, Cornuelle) and JPL (Fukumori, Menemenlis, Lee) scientists with explicit collaboration with the MPI group (Latif, Hasselmann). As in the Atlantic, adjoint solutions will also be employed in the Pacific to determine the sensitivity of stratification in the equatorial Pacific to both local and remote subtropical forcing. In particular, dynamical and advective pathways can be determined, thus addressing the question of whether the equatorial Pacific stratification is more strongly influenced by the North Pacific or the South Pacific. Interaction with the many other groups studying ENSO and related phenomena is expected here, and would occur primarily through the MPI and SIO links already in place.

Many U.S. groups are actively exploring the use of coupled models to forecast both ENSO and decadal climate variability. Because initialization of the ocean is essential to predicting coupled evolution there is interest in our project for that purpose. NCEP (D. Beringer and Ming Ji) has requested our Pacific results to initialize their ENSO forecasts while T. Barnett has asked to do the same with his attempts to predict decadal variability. This opens the possibility of a practical benefit of our state estimates but forecast skill provides an important independent way of testing the validity of these estimates.

6 Anticipated Results

We anticipate a variety of results evolving through this NOPP activity, ranging from maintenance of data and model output for outside users, to operational products of the ocean state, to best possible estimates of climate-related heat and freshwater flux, as well as carbon budgets. Specifically we will provide during the funding period:
- Near real-time estimates of the time-evolution of the full 3-D ocean state.
- Estimates of ocean transports and budgets on an (approximately) weekly basis.
- Improved understanding of data and model errors.
- Improved model components.
- Improved understanding of climate observing system design
- Improved ocean state estimation methodology with near-eddy resolution.

Together with other NOPP "nodes", we will use our experience in performing the ocean state estimates and in interacting with the wider community to design the anticipated NOPP "hub". At the end of the NOPP funding period, parts of the estimation work are anticipated to migrate into center-like facilities for routine oceanographic applications. The work in the academic community will continue on inevitable new questions and problems. Related work in the meteorological community lasted over 30+ years and is still not finished. A similar development can be anticipated for the oceanographic community, which will require long-term funding beyond the NOPP A2 funding perspectives.

7 Summary of Institutional Responsibilities

The anticipated work is divided into various responsibilities as outlined in Table 1, with results freely available to all partners for joint scientific evaluation. Note that almost all of the sub-elements listed here involve collaborations with other individuals at the same or different institutions. Scientific and technical aspects of the ongoing work will be reviewed during regular working meetings of the full group. Working meetings between SIO and JPL will be more frequent. This consortium proposes to exploit modern electronic communications as well as distributed computing capabilities to fully share responsibility for the entirety of the work.

The Principal Investigator will be Detlef Stammer (SIO). The two US Co-Principal Investigators, Ichiro Fukumori (JPL) and John Marshall (MIT) will function with the PI as an executive committee for the effort. Together with Mojib Latif (MPI), they will perform the day-to-day management collectively, and as leaders within their own institutions.

Table 1: Institutional Responsibilities

Institution	Personnel	Task
Scripps	Stammer & post-doc	Global optimization computation; implementation of model and algorithmic developments into optimization.
	Stammer & post-doc	Use of the global results for studies of oceanic variability, global observation system design.
	Davis, Niiler, Stammer	Upper-ocean model-data comparison; estimation of data and error covariances.
	Davis, Niiler, Cornuelle, Stammer	Pacific BECS model.
JPL	Giering, Lee, joint with SIO	Global optimization computation.
	Menemenlis, Fukumori, Fu	Reduced Kalman filter/smoother.
	Lee, Giering	Pacific BECS model and regional optimization.
	Fukumori, Zlotnicki, Fu	Operational products; maintenance of data and model output flow both internally and to outside users.
MIT	Marshall & post-doc	Model improvement/development.
	Wunsch in collaboration with SIO and JPL	Use of global model for study of heat, salt, carbon budgets.
	Marshall, Marotzke, Wunsch, Ayoub	Atlantic BECS model.
	Marotzke & post-doc	Global and Atlantic adjoint model sensitivities.
MPI	Latif, Hasselmann	Biogeochemical cycling; marine geoid determination.
	Latif	ENSO dynamics and predictability; impact of improved initialization.

8 Qualification of Personnel

The proposed consortium brings together teams with first hand experience spanning all the problem areas involved in ocean state estimation, with the capability of exploiting newly arriving computer architectures, data types, algorithms, and with experience in working together.

Key personnel of this proposal are directly involved in WOCE AIMS, CLIVAR, GODAE and GRACE activities, among others, and will assure maximum communication and flexibility between scientific and technical requirements in those areas and activities within the proposed “node”.

9 Institutional Computational Capabilities

SIO: The institution has a close connection to the San Diego Supercomputer Center (SDSC) (T90, T3E; IMB SP) where the proposed ocean state estimation is already supported as part of the NPACI ESSP (PI: Carl Wunsch, Co-PI: D. Stammer). To build up local computing facilities we request as part of this proposal 2 high-end and two low-end workstations , as well as disc drives, a printer and later up-grade support.

SIO will submit a proposal to NSF's Major Research Instrumentation (MRI) program, asking for the acquisition of an intermediate size SGI Origin 2000 computer in support of growing modeling activities at SIO, as well as teaching needs.

JPL: JPL has an existing local computer cluster. It also has access to CalTech's HP Examplar supercomputer, which is also part of NPACI.

MIT: Local workstations exist, with sufficient disc and tape drive facilities to allow extensive local computing and analysis. The group is also collaborating with MIT's LCS where a cluster of SUN SMP's is available for our use (Xolas). Carl Wunsch is also a PI in NPACI's ESSP.

MPI: The MPI in Hamburg is fully equipped with local workstion environment as well as high-level supercomputing power which is sufficient to fully support its role in this partnership effort.

10 Community Interaction and Other Collaborations

The consortium will need to rely on wider community interactions in most of its activities. Not only will we depend upon the oceanographic and space observation communities at large for data access, and expertise in its use, but model innovations made elsewhere will be incorporated into our own computations. The products both of the consortium's own model improvements, and of the entire assimilation product should be of use to a very wide community (noted above as including coastal, biological, carbon cycle, tropical forecasts, etc.).

Because the consortium efforts will benefit from user feedback, our goal is to make our collaboration as open as possible. As envisioned this means redistributing data (where permitted), assimilation products, computational algorithms (model) etc. to anyone who is interested. Various mechanisms exist in the community facilitating such collaborations. These range from "user" meetings, to summer schools, visitor programs, public data bases, etc. As the NOPP process moves to establish other nodes, e.g. in the coastal area, and a hub, these other groupings would provide a natural mechanism for some of the requisite interaction.

To facilitate an easy interaction with the community we will also maintaine a data and model output flow both for internal use and to outside users. This work will primarily reside with our JPL partner who will make results available via the internet and build the required user and outreach Web page (JPL has already considerable experience in this work from ongoing T/P and JASON activities).

We have reserved a fraction of the funding in the US institutions for teaching activity and a visitor program. Given the potential for outside collaboration, however, it is unlikely that these resources will be adequate to have such a program in all the partner institutions. At MIT and SIO there will be a visitor program, which in the latter case will additionally be supported by matching institutional funds (see supporting letter). This program will enable users from within the general community to come and work with us for some time, with the goal to enable them to use our products, to gain insight into ocean modeling and ocean state estimation, and to help us improve models as well as the ocean estimates. We expect to seek additional funding both within the NOPP framework and outside, so as to expand the visitor program and to be able to fully respond to any sensible request for interaction.

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