DATA ASSIMILATION IN MODELS

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Introduction

Data assimilation is a novel, versatile methodology for estimating oceanic variables. The estimation of a quantity of interest via data assimilation involves the combination of observational data with the underlying dynamical principles governing the system under observation. The melding of data and dynamics is a powerful methodology which makes possible efficient, accurate, and realistic estimations otherwise not feasible. It is providing rapid advances in important aspects of both basic ocean science and applied marine technology and operations.

The following sections introduce concepts, describe purposes, present applications to regional dynamics and forecasting, overview formalism and methods, and provide a selected range of examples.

Field and Parameter Estimation

Ocean science, and marine technology and operations, require a knowledge of the distribution and evolution in space and time of the properties of the sea. The functions of space and time, or state variables, which characterize the state of the sea under observation are classically designated as fields. The determination of state variables poses problems of state estimation or field estimation in three or four dimensions. The fundamental problem of ocean science may be simply stated as follows: given the state of the ocean at one time, what is the state of the ocean at a later time? It is the dynamics, i.e., the basic laws and principles of oceanic physics, biology, and chemistry, that evolve the state variables forward in time. Thus, predicting the present and future state of oceanic variables for practical applications is intimately linked to fundamental ocean science.

A dynamical model to approximate nature consists of a set of coupled nonlinear prognostic field equations for each state variable of interest. The fundamental properties of the system appear in the field equations as parameters (e.g., viscosities, diffusivities, representations of body forces, rates of earth rotation, grazing, mortality, etc.). The initial and boundary conditions necessary for integration of the equations may also be regarded as parameters by data assimilation methods. In principle the parameters of the system can be estimated directly from measurements. In practice, directly measuring the parameters of the interdisciplinary (physical-acoustical-optical-biological-chemical-sedimentological) ocean system is difficult because of sampling, technical, and resource requirements. However, data assimilation provides a powerful methodology for parameter estimation via the melding of data and dynamics.

The physical state variables are usually the velocity components, pressure, density, temperature, and salinity. Examples of biological and chemical state variables are concentration fields of nutrients, plankton, dissolved and particulate matter, etc. Important complexities are associated with the vast range of phenomena, the multitude of concurrent and interactive scales in space and time, and the very large number of possible biological state variables. This complexity has two essential consequences. First, state variable definitions relevant to phenomena and scales of interest need to be developed from the basic definitions. Second, approximate dynamics which govern the evolution of the scale-restricted state variables, and their interaction with other scales, must be developed from the basic dynamical model equations. A familiar example consists of decomposing the basic ocean fields into slower and faster time scales, and shorter and longer space scales, and averaging over the faster and shorter scales. The resulting equations can be adapted to govern synoptic/mesoscale resolution state variables over a large-scale oceanic domain, with faster and smaller scale phenomena represented as parameterized fluctuation correlations (Reynolds stresses). There is, of course, a great variety of other scale-restricted state variables and approximate dynamics of vital interest in ocean science. We refer to scale-restricted state variables and approximate dynamics simply as 'state variables' and 'dynamics'.

The use of dynamics is of fundamental importance for efficient and accurate field and parameter estimation. Today and in the foreseeable future, data acquisition in the ocean is sufficiently difficult and costly so as to make field and parameter estimates by direct measurements, on a substantial and sustained basis, essentially prohibitive. However, data acquisition for field and parameter estimates



- IIIII Dynamical linkages

Figure 1 Data assimilation system schematic. Arrows represent the most common direction for the flows of information. The arrows between the measurement models and dynamical models are double because measurement models can include operators that map state variables and parameters to the sensor data (e.g. interpolations, derivatives or integrals of state variables/parameters) and operators that transform sensor data into data appropriate for the model scales and processes (e.g. filtering, extrapolations or integrals of sensor data). The legend at the bottom explains abbreviations.

via data assimilation is feasible, but substantial resources must be applied to obtain adequate observations.

The general process of state and parameter estimation is schematized in Figure 1. Measurement models link the state variables of the dynamical model to the sensor data. Dynamics interpolates and extrapolates the data. Dynamical linkages among state variables and parameters allow all of them to be estimated from measurements of some of them, i.e., those more accessible to existing techniques and prevailing conditions. Error estimation and error models play a crucial role. The data and dynamics are melded with weights inversely related to their relative errors. The final estimates should agree with the observations and measurements within data error bounds and should satisfy the dynamical model within model error bounds. Thus the melded estimate does not degrade the reliable information of the observational data, but rather enhances that information content. There are many important feedbacks in the generally nonlinear data assimilation system or ocean observing and prediction system (OOPS) schematized in Figure 1, which illustrates the system concept and two feedbacks. Prediction provides the opportunity for efficient sampling adapted to real time structures, events, and errors. Data collected for assimilation also used for ongoing verification can identify model deficiencies and lead to model improvements.

A data assimilation system consists of three components: a set of observations, a dynamical model, and a data assimilation scheme or melding scheme. Modern interdisciplinary OOPS generally have compatible nested grids for both models and sampling. An efficient mix of platforms and sensors is selected for specific purposes.

Central to the concept of data assimilation is the concept of errors, error estimation, and error modeling. The observations have errors arising from various sources: e.g., instrumental noise, environmental noise, sampling, and the interpretation of sensor measurements. All oceanic dynamical models are imperfect, with errors arising from the approximate explicit and parameterized dynamics and the discretization of continuum dynamics into a computational model.

A rigorous quantitative establishment of the accuracy of the melded field and parameter estimates, or verification, is highly desirable but may be difficult to achieve because of the quantity and quality of the data required. Such verification involves all subcomponents: the dynamical model, the observational network, the associated error models, and the melding scheme. The concept of validation is the establishment of the general adequacy of the system and its components to deal with the phenomena of interest. As simple examples, a barotropic model should not be used to describe baroclinic phenomena, and data from an instrument whose threshold is higher than the accuracy of the required measurement are not suitable. In reality, validation issues can be much more subtle. Calibration involves the tuning of system parameters to the phenomena and regional characteristics of interest. Final verification requires dedicated experiments with oversampling.

At this point it is useful to classify types of estimates with respect to the time interval of the data input to the estimate for time t. If only past and present data are utilized, the estimation is a filtering process. After the entire time series of data is available for (0,T), the estimate for any time $0 \le t \le T$ is best based on the whole data set and the estimation is a smoothing process.

Goals and Purposes

The specific uses of data assimilation depend upon the relative quality of data sets and models, and the desired purposes of the field and parameter estimates. These uses include the control of errors for state estimates, the estimation of parameters, the elucidation of real ocean dynamical processes, the design of experimental networks, and ocean monitoring and prediction.

First consider ocean prediction for scientific and practical purposes, which is the analog of numerical weather prediction. In the best case scenario, the dynamical model correctly represents both the internal dynamical processes and the responses to external forcings. Also, the observational network provides initialization data of desired accuracy. The phenomenon of loss of predictability nonetheless inhibits accurate forecasts beyond the predictability limit for the region and system. This limit for the global atmosphere is 1-2 weeks and for the midocean eddy field of the north-west Atlantic on the order of weeks to months. The phenomenon is associated with the nonlinear scale transfer and growth of initial errors. The early forecasts will accurately track the state of the real ocean, but longer forecasts, although representing plausible and realistic synoptical dynamical events, will not agree with contemporary nature. However, this predictability error can be controlled by the continual assimilation of data, and this is a major use of data assimilation today.

Next, consider the case of a field estimate with adequate data but a somewhat deficient dynamical model. Assimilated data can compensate for the imperfect physics so as to provide estimates in agreement with nature. This is possible if dynamical model errors are treated adequately. For instance, if a barotropic model is considered perfect, and baroclinic real ocean data are assimilated, the field estimate will remain barotropic. Even though melded estimates with deficient models can be useful, it is of course important to attempt to correct the model dynamics.

Parameter estimation via data assimilation is making an increasingly significant impact on ocean science via the determination of both internal and external parameter values. Regional field estimates can be substantially improved by boundary condition estimation. Biological modelers have been hampered by the inability to directly measure *in situ* rates, e.g., grazing and mortality. Thus, for interdisciplinary studies, internal parameter estimation is particularly promising. For example, measurements of concentration fields of plankton together with a realistic interdisciplinary model can be used for *in situ* rate estimation.

Data-driven simulations can provide four-dimensional time series of dynamically adjusted fields which are realistic. These fields, regarded as (numerical) experimental data, can thus serve as high resolution and complete data sets for dynamical studies. Balance of terms in dynamical equations and overall budgets can be carried out to determine fluxes and rates for energy, vorticity, productivity, grazing, carbon flux, etc. Case studies can be carried out, and statistics and general processes can be inferred for simulations of sufficient duration. Of particular importance are observation system simulation experiments (OSSEs), which first entered meteorology almost 30 years ago. By subsampling the simulated 'true' ocean, future experimental networks and monitoring arrays can be designed to provide efficient field estimates of requisite accuracies. Data assimilation and OSSEs develop the concepts of data, theory, and their relationship beyond those of the classical scientific methodology. For a period of almost 300 years, scientific methodology was powerfully established on the basis of two essential elements: experiments/observations and theory/models. Today, due to powerful computers, science is based on three fundamental concepts: experiment, theory, and simulation. Since our best field and parameter estimates today are based on data assimilation, our very perception and conceptions of nature and reality require philosophical development.

It is apparent from the above discussion that marine operations and ocean management must depend on data assimilation methods. Data-driven simulations should be coupled to multipurpose management models for risk assessments and for the design of operational procedures. Regional multiscale ocean prediction and monitoring systems, designed by OSSEs, are being established to provide ongoing nowcasts and forecasts with predictability error controlled by updating. Both simple and sophisticated versions of such systems are possible and relevant.

Regional Forecasting and Dynamics

In this section, the issues and concepts introduced in the preceding sections are illustrated in the context of real-time predictions carried out in 1996 for

NATO naval operations in the Strait of Sicily and for interdisciplinary multiscale research in 1998 in Massachusetts Bay. The Harvard Ocean Prediction System (HOPS) with its primitive equation dynamical model was utilized in both cases. In the Strait of Sicily (Figure 2), the observational network with platforms consisting of satellites, ships, aircraft, and Lagrangian drifters, was managed by the NATO SACLANT Undersea Research Centre. In Massachusetts Bay (Figure 3), the observational network with platforms consisting of ships, satellites, and autonomous underwater vehicles, was provided by the Littoral Ocean Observing and Prediction System (LOOPS) project within the US National Ocean Partnership Program. The data assimilation methods used in both cases were the HOPS OI and ESSE schemes (see Estimation Theory below). In both cases the purposes of data assimilation were to provide a predictive capability, to control loss of predictability, and to infer basic underlying dynamical processes.

The dominant regional variabilities determined from these exercises and studies are schematized in Figures 2A and 3A. The dominant near surface flow in the strait is the Atlantic Ionian Stream, AIS (black lines for the stream; smooth and meandering dashed lines for the common locations of fronts and wave patterns, respectively) and dominant variabilities include the location and shapes of the Adventure Bank Vortex (ABV), Maltese Channel Crest (MCC), Ionian Shelfbreak Vortex (ISV), and Messian Rise Vortex (MRV), with shifts and deformations 0(10-100 km) occurring in 0(3-5 days). The variability of the Massachusetts Bay circulation is more dramatic. The buoyancy flow-through current which enters the Bay in the north from the Gulf of Maine may have one, two or three branches, and together with associated vortices (which may or may not be present), can reverse directions within the bay. Storm events shift the pattern of the features which persist inertially between storms. Actual real-time forecast fields are depicted in Figures 2B and 3B.

The existence of forecasts allows adaptive sampling, i.e., sampling efficiently related to existing structures and events. Adaptive sampling can be determined subjectively by experience or objectively by a quantitative metric. The sampling pattern associated with the temperature objective analysis error map (Figure 2C) reflects the flight pattern of an aircraft dropping subsurface temperature probes (AXBTs). The data were assimilated into a forecast in support of naval operations centered near the ISV (Figure 2A). The sampling extends to the surrounding meanders of the AIS, which will affect the current's thermal front in the operational region.

The multiscale sampling of the Massachusetts Bay experiment is exemplified in Figure 3C, D by ship tracks adapted to the interactive submesoscales, mesoscales, bay scales, and large-scales. Note that the tracks of Figure 3D are superimposed on a forecast of the total temperature forecast error standard deviation. The shorter track is objectively located around an error maximum. The longer track is for reduction of velocity error (not shown). Eigendecomposition of variability fields helps dynamical interpretations. This eigen-decomposition estimates and orders the directions of largest variability variance (eigenmodes) and the corresponding amplitudes (eigenvalues). The first temperature variability eigenmodes for the strait and the bay are depicted in Figures 2D and 3E respectively. The former is associated with the dominant ABV variability and the latter with the location, direction, and strength of the inflow to the bay of the buoyancy current from the Gulf of Maine.

A qualitative skill score for the prediction of dominant variations of the ABV, MCC, and ISV indicated correct 2- to 3-day predictions of surface temperature 75% of the time. The scores were obtained by validation against new data for assimilation and independent satellite sea surface temperature data as shown in Figure 2E for the forecast of Figure 2B. An important kinematical and dynamical interconnection between the eastern and western Mediterranean is the deep flow of salty Levantine Intermediate Water (LIW), which was not directly measured but was inferred from data assimilative simulations (Figure 2F). The scientific focus of the Massachusetts Bay experiment was planktonpatchiness, in particular the spatial variability of zooplankton and its relationship to physical and phytoplankton variabilities (Figure 3B, G). The smallest scale measurements in the bay were turbulence measurements from an AUV (Figure 3F), which were also used to research the assimilation in real time of subgridscale data in the primitive equation model.

Concepts and Methods

By definition (see Introduction), data assimilation in ocean sciences is an estimation problem for the ocean state, model parameters, or both. The schemes for solving this problem often relate to estimation or control theories (see below), but some approaches like direct minimization, stochastic, and hybrid methods (see below) can be used in both frameworks. Several schemes are theoretically optimal, while others are approximate or suboptimal. Although optimal schemes are preferred, suboptimal



Figure 2 Strait of Sicily. (A) Schematic of circulation features and dominant variabilities. (B) Forecast of the surface temperature for 25 August 1996, overlaid with surface velocity vectors (scale arrow is 0.25 m s^{-1}). (C) Objectively analyzed surface standard error deviation associated with the aircraft sampling on 18 September 1996 (normalized from 0 to 1). (D) Surface values of the first nondimensional temperature variability mode. (E) Satellite SST distributions for 25 August 1996. (F) Main LIW pathways, features, and mixing on deep potential density anomaly iso-surface ($\sigma_{\theta} = 29.05$), over bottom topography (for more details, see Lermusiaux, 1999, and Lermusiaux and Robinson, 2001).



Figure 3 Massachusetts Bay. (A) Schematic of circulation features and dominant variabilities. (B) Chlorophyll-a (μ g m⁻³) at 10 m, with overlying velocity vectors. (C) Sampling pattern for the bay scales and external large-scales in the Gulf of Maine. (D) Forecast of the standard error deviation for the surface temperature (from 0°C in dark blue to a maximum of 0.7°C in red), with tracks for adaptive sampling. (E) 20 m values of the temperature component of the first nondimensional physical variability mode. (F) AUV turbulence data (Naval Underwater Warfare Center (NUWC)). (G) Vertical section of zooplankton (μ M m⁻³) along the entrance of Massachusetts Bay (for more details, see Robinson and the LOOPS group, 1999, and Lermusiaux, 2001).

methods are generally the ones in operational use today. Most schemes are related in some fashion to least-squares criteria which have had great success. Other criteria, such as the maximum likelihood, minimax criterion or associated variations might be more appropriate when data are very noisy and sparse, and when probability density functions are multimodal (see Stochastic and hybrid models below). Parameters are assumed from here on to be included in the vector of state variables. For more detailed discussions, the reader is referred to the article published by Robinson *et al.* in 1998 (see Further Reading section).

Estimation Theory

Estimation theory computes the state of a system by combining all available reliable knowledge of the system including measurements and theoretical models. The *a priori* hypotheses and melding or estimation criterion are crucial since they determine the influence of dynamics and data onto the state estimate.

At the heart of estimation theory is the Kalman filter, derived in 1960. It is the sequential, unbiased, minimum error variance estimate based upon a linear combination of all past measurements and dynamics. Its two steps are: (1) the forecast of the state vector and of its error covariance, and (2) the dataforecast melding and error update, which include the linear combination of the dynamical forecast with the difference between the data and model predicted values for those data (i.e., data residuals).

The Kalman smoother uses the data available before and after the time of interest. The smoothing is often carried out by propagating the future data information backward in time, correcting an initial Kalman filter estimate using the error covariances and adjoint dynamical transition matrices, which is usually demanding on computational resources.

In a large part because of the linear hypothesis and costs of these two optimal approaches, a series of approximate or suboptimal schemes have been employed for ocean applications. They are now described, from simple to complex.

Direct insertion consists of replacing forecast values at all data points by the observed data which are assumed to be exact. The blending estimate is a scalar linear combination, with user-assigned weights, of the forecast and data values at all data points. The nudging or Newtonian relaxation scheme 'relaxes' the dynamical model towards the observations. The coefficients in the relaxation can vary in time but, to avoid disruptions, cannot be too large. They should be related to dynamical scales and *a priori* estimates of model and data errors. In optimal interpolation (OI), the matrix weighting the data residuals, or gain matrix, is empirically assigned. If the assigned OI gain is diagonal, OI and nudging schemes can be equivalent. However, the OI gain is usually not diagonal, but a function of empirical correlation and error matrices.

The method of successive corrections performs multiple but simplified linear combination of the data and forecast. Conditions for convergence to the Kalman filter have been derived, but in practice only a few iterations are usually performed. Frequently, the scales or processes of interest are corrected one after the other, e.g., large-scale first, then mesoscale.

Control Theory

All control theory or variational approaches perform a global time-space adjustment of the model solution to all observations and thus solve a smoothing problem. The goal is to minimize a cost function penalizing misfits between the data and ocean fields, with the constraints of the model equations and their parameters. The misfits are interpreted as part of the unknown controls of the ocean system. Similar to estimation theory, control theory results depend on *a priori* assumptions for the control weights. The dynamical model can be either considered as a strong or weak constraint. Strong constraints correspond to the choice of infinite weights for the model equations; the only free variables are the initial conditions, boundary conditions and/or model parameters. A rational choice for the cost function is important. A logical selection corresponds to dynamical model (data) weights inversely proportional to *a priori* specified model (data) errors.

In an 'adjoint method', the dynamical model is a strong constraint. One penalty in the cost function weights the uncertainties in the initial conditions, boundary conditions, and parameters with their respective *a priori* error covariances. The other is the sum over time of data-model misfits, weighted by measurement error covariances. A classical approach to solve this constrained optimization is to use Lagrange multipliers. This yields Euler-Lagrange equations, one of which is the so-called adjoint equation. An iterative algorithm for solving these equations has often been termed the adjoint method. It consists of integrating the forward and adjoint equations successively. Minimization of the gradient of the cost function at the end of each iteration leads to new initial, boundary, and parameter values. Another iteration can then be started, and so on, until the gradient is small enough.

Expanding classic inverse problems to the weak constraint fit of both data and dynamics leads to generalized inverse problems. The cost function is usually as in adjoint methods, except that a third term now consists of dynamical model uncertainties weighted by *a priori* model error covariances. In the Euler-Lagrange equations, the dynamical model uncertainties thus couple the state evolution with the adjoint evolution. The representer method is an algorithm for solving such problems.

Direct Minimization Methods

Such methods directly minimize cost functions similar to those of generalized inverse problems, but often without using the Euler-Lagrange equations. **Descent methods** iteratively determine directions locally 'descending' along the cost function surface. At each iteration, a minimization is performed along the current direction and a new direction is found. Classic methods to do so are the steepest descent, conjugate-gradient, Newton, and quasi-Newton methods. A drawback for descent methods is that they are initialization sensitive. For sufficiently nonlinear cost functions, they are restarted to avoid local minima.

Simulated annealing schemes are based on an analogy to the way slowly cooling solids arrange themselves into a perfect crystal, with a minimum global energy. To simulate this relatively random process, a sequence of states is generated such that new states with lower energy (lower cost) are always accepted, while new states with higher energy (higher cost) are accepted with a certain probability.

Genetic algorithms are based upon searches generated in analogy to the genetic evolution of natural organisms. They evolve a population of solutions mimicking genetic transformations such that the likelihood of producing better data-fitted generations increases. Genetic algorithms allow nonlocal searches, but convergence to the global minimum is not assured due to the lack of theoretical base.

Stochastic and Hybrid Methods

Stochastic methods are based on nonlinear stochastic dynamical models and stochastic optimal control. Instead of using brute force like descent algorithms, they try to solve the conditional probability density equation associated with ocean models. Minimum error variance, maximum likelihood or minimax estimates can then be determined from this probability density. No assumptions are required, but for large systems, parallel machines are usually employed to carry out Monte Carlo ensemble calculations. Hybrid methods are combinations of previously discussed schemes, for both state and parameter estimation; for example, error subspace statistical estimation (ESSE) schemes. The main assumption of such schemes is that the error space in most ocean applications can be efficiently reduced to its essential components. Smoothing problems based on Kalman ideas, but with nonlinear stochastic models and using Monte Carlo calculations, can then be solved. Combinations of variational and direct minimization methods are other examples of hybrid schemes.

Examples

This section presents a series of recent results that serve as a small but representative sample of the wide range of research carried out as data assimilation was established in physical oceanography.

General Circulation from Inverse Methods

The central idea is to combine the equations governing the oceanic motion and relevant oceanic tracers with all available noisy observations, so as to estimate the large-scale steady-state total velocities and related internal properties and their respective errors. The work of Martel and Wunsch in 1993 exemplifies the problem. The three-dimensional circulation of the North Atlantic (Figure 4A) was studied for the period 1980-85. The observations available consisted of objective analyses of temperature, salinity, oxygen, and nutrients data; climatological ocean-atmosphere fluxes of heat, water vapor, and momentum; climatological river runoffs; and current meter and float records. These data were obtained with various sensors and platforms, on various resolutions, as illustrated by Figure 4B. A set of steady-state equations were assumed to hold *a priori*, up to small unknown noise terms. The tracers were advected and diffused. The advection velocities were assumed in geostrophic thermalwind balance, except in the top layer where Ekman transport was added. Hydrostatic balance and mass continuity were assumed. The problem is inverse because the tracers and thermal wind velocities are known; the unknowns are the fields of reference level velocities, vertical velocity, and tracer mixing coefficients.

Discrete finite-difference equations were integrated over a set of nested grids of increasing resolutions (Figure 4A). The flows and fluxes at the boundaries of these ocean subdivisions were computed from the data (at 1° resolution). The resulting discrete system contained c. 29000 unknowns



Figure 4 (A) Domain of the model used in the inverse computations. Weak dynamical constraints were imposed on the flow and tracers, and integrated over a set of nested grids, from the full domain (heavy solid lines) to an ensemble of successive divisions (e.g., dashed lines) reaching at the smallest scales the size of the boxes labeled by numbers. (B) Locations of the stations where the hydrographic and chemical component of the data set were collected (model grid superposed). (C) Inverse estimate of the absolute sea surface topography in centimeters (contour interval is 10 cm). (D) Inverse estimate of the standard error deviation (in cm) of the sea surface topography shown in (C). (Reproduced with permission from Martel and Wunsch, 1993.).

and 9000 equations. It was solved using a tapered (normalized) least-squares method with a sparse conjugate-gradient algorithm. The estimates of the total flow field and of its standard error are plotted on Figure 1C and D. The Gulf Stream, several recirculation cells and the Labrador current are present. In 1993, such a rigorous large-scale, dense, and eclectic inversion was an important achievement.

Global versus Local Data Assimilation via Nudging

Malanotte-Rizzoli and Young in 1994 investigated the effectiveness of various data sets to correct and control errors. They used two data sets of different types and resolutions in time and space in the Gulf Stream region, at mesoscale resolution and for periods of the order of 3 months, over a large-scale domain referred to as global scale.

One objective was to assimilate data of high quality, but collected at localized mooring arrays, and to investigate the effectiveness of such data in improving the realistic attributes of the simulated ocean fields. If successful, such estimates allow for dynamical and process studies. The global data consisted of biweekly fields of sea surface dynamic height, and of temperature and salinity in three dimensions, over the entire region, as provided by the Optimal Thermal Interpolation Scheme (OTIS) of the US Navy Fleet Numerical Oceanography Center. The local data were daily current velocities from two mooring arrays. The dynamical model consisted of primitive equations (Rutgers), with a suboptimal nudging scheme for the assimilation.

The global and local data were first assimilated alone, and then together. The 'gentle' assimilation of the spatially dense global OTIS data was necessary for the model to remain on track during the 3-month period. The 'strong' assimilation of the daily but local data from the Synoptic Ocean Prediction SYNOP was required to achieve local dynamical accuracies, especially for the velocities.

Small-scale Convection and Data Assimilation

In 1994, Miller et al. addressed the use of variational or control theory approaches (see earlier) to assimilate data into dynamical models with highly nonlinear convection. Because of limited data and computer requirements, most practical ocean models cannot resolve motions that result from static instabilities of the water column; these motions and effects are therefore parameterized. A common parameterization is the so-called convective adjustment. This consists of assigning infinite mixing coefficients (e.g., heat and salt conductivities) to the water at a given level that has higher density than the water just below. This is carried out by setting the densities of the two parcels to a unique value in such a way that heat and mass are conserved. In a numerical model, at every time step, water points are checked and all statically unstable profiles replaced by stable ones.

The main issues of using such convective schemes with variational data assimilation are that: (1) the dynamics is no longer governed by smooth equations, which often prevents the simple definition of adjoint equations; (2) the optimal ocean fields may evolve through 'nonphysical' states of static instability; and (3), the optimization is nonlinear, even if the dynamics are linear. Ideally, the optimal fields should be statically stable. This introduces a set of inequality constraints to satisfy. An idealized problem was studied so as to provide guidance for realistic situations. A simple variational formulation had several minima and at times produced evolutions with unphysical behavior. Modifications that led to more meaningful solutions and suggestions for algorithms for realistic models were discussed. One option is the 'weak' static stability constraint: a penalty that ensures approximate static stability is added to the cost function with a very small error or large weight. In that case, static stability can be violated, but in a limited fashion. Another option is the 'strong constraint' form of static stability which can be enforced via Lagrange multipliers. Convex programming methods which explicitly account for inequality constraints could also be utilized.

Global Ocean Tides Estimated from Generalized Inverse Methods

In 1994, Egbert *et al.* estimated global ocean tides using a generalized inverse scheme with the intent of removing these tides from the data collected by the TOPEX/POSEIDON satellite and thus allowing the study of subtidal ocean dynamics.

A scheme for the inversion of the satellite crossover data for multiple tidal constituents was applied to 38 cycles of the data, leading to global estimates of the four principal tidal constituents (M_2 , S_2 , K_1 and O_1) at about 1° resolution. The dynamical model was the linearized, barotropic shallow water equations, corrected for the effects of ocean selfattraction and tidal loading, the state variables being the horizontal velocity and sea surface height fields. The data sets were linked to measurement models and comprehensive error models were derived.

The generalized inverse tidal problem was solved by the representer method. Representer functions are related to Green's functions: they link a given datum to all values of the state variables over the period considered. These representers were computed by solving the Euler-Lagrange equations in parallel. The size of the problem was reduced by winnowing out the full set of 6350 crossovers to an evenly spaced subset of 986 points (see Figure 5A). The resulting representer matrix was then reduced by singular value decomposition.

The amplitude and phase estimates for the M_2 constituent are shown in Figure 5B. The M_2 fields are qualitatively similar to previous results and amphidromes are consistent. However, when compared with previous tidal model estimates, the inversion result is noticeably smoother



Figure 5 (A) TOPEX/POSEIDON crossover points and subsampling. Representers were calculated only for the windowed subset of 986 satellite crossover points (large filled dots), but differences from all 6355 crossover points (small dots and large filled dots) were included in the data-misfit penalty. (B) Generalized inverse estimate of the amplitude and phase of the M_2 tidal constituent. The phase isolines are plotted in white over color-filled contours of the amplitude. Contour interval is 10 cm for amplitude and 30° for phase. (Reproduced with permission from Egbert *et al.* 1994.).

and in better agreement with altimetric and ground truth data.

Conclusions

The melding of data and dynamics is a powerful, novel, and versatile methodology for parameter and field estimation. Data assimilation must be anticipated both to accelerate research progress in complex, modern multiscale interdisciplinary ocean science, and to enable marine technology and maritime operations that would otherwise not be possible.

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See also

Biogeochemical Data Assimilation. Coastal Circulation Models. Current Systems in the Mediterranean sea. CTD. Elemental Distribution: Overview. Expendable Sensors. Florida Current, Gulf Stream and Labrador Current. Forward Problem in Numerical Models. Inverse Models. Mesoscale Eddies. Ocean Circulation. Open Ocean Convection. Patch Dynamics. Regional and Shelf Sea Models. Tides. Upper Ocean Time and Space Variability.

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DEEP CONVECTION

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Introduction

Density of ocean water generally increases with depth except at the surface where stirring by waves and convection creates a well-mixed homogeneous layer. Breaking waves alone can mix the upper 5–10m, but convection, forced by an increase in

density at the surface via heat loss or evaporation, can greatly increase the mixed layer depth. During winter, heat loss from the surface of the ocean is high and convectively mixed surface layers are the norm in the extratropical oceans. The deepest (> 1500 m) are found in the Labrador Sea, the Greenland Sea, and the Golfe du Lion in the Mediterranean Sea, because of two special features. First, they are near land where cold continental air flows over the water to create the necessary high heat loss. Second, the circulation in each is weakly cyclonic which helps to maintain the convecting water where the high heat loss occurs. The combination of these