A Kalman Filter for Ocean Monitoring

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Abstract: The feasibility of global ocean state estimation by sequential data assimilation is demonstrated. The model component of the assimilator is the GROB version of the MPIMET ocean circulation model HOPE. Assimilation uses the Fokker-Planck representation of the Kalman Filter. This approach determines the temporal evolution of error statistics by integration of the Fokker-Planck Equation. Phase space advection and diffusion are obtained from histogram techniques considering the model as a black box. For efficiency, the estimation procedure utilizes a combination of nudging and Kalman Filtering. The ocean state is estimated for the El Nino year 1997 by dynamical extrapolation of observed sea-surface temperatures and TAO/TRITON subsurface temperatures. The model-data combination yields improved estimates of the ocean’s mean state and a realistic record of El Nino related variability. The assimilator proves as an efficient, viable and thus practical approach to operational global ocean state estimation.

1.) Introduction

Ocean state estimation draws its wider societal as well as scientific significance from the central role of the oceans in Earth’s climate system. At a time when the impact of climate variability on societal infrastructures is increasingly felt, the need for comprehensive climate monitoring is generally accepted. While mankind is primarily affected by meteorological manifestations of climate variability, large-amplitude weather fluctuations oftentimes screen the atmospheric climate signal. In practice, atmospheric climate observation proves prohibitively intricate. Alternatively, estimates of the state of the ocean interior with its enormous capacity to store and distribute water, heat and radiatively active trace substances (such as carbon dioxide) provide direct evidence of the climate signal. As the dominating climate component, the ocean acts as a Markov Integrator of atmospheric noise, provides the memory of the climate system and sets time-scales of climate processes by (at least partly) predictable transport mechanisms. Thus, practical climate monitoring anchors on operational ocean state estimation.

Only a decade ago, an observational basis for the assessment of a temporally changing global ocean circulation was practically nonexistent. In fact, oceanography was plagued by a notorious undersampling problem and the ocean circulation was widely considered as a stationary flow. The most comprehensive data set of this era is the World Ocean Atlas (WOA) by Levitus and coworkers [1], a meticulous collection of hydrographic data from oceanographic archives all over the world. This atlas represents a global ocean density field that is best associated with the mean ocean circulation during the second half of the twentieth century. Temporal changes such as those at the roots of past, present and future climate variability are far beyond the scope of these data. Since then, ocean observation underwent an explosive development. Today, space-borne ocean observatories provide global data sets of the mesoscale state of the sea surface in near real-time. Oceanographic data paucity has been replaced by an almost overwhelming data stream [2]. Nevertheless, observational monitoring of the ocean interior remains technically difficult and costly for the foreseeable future. For mere book keeping
as well as for analysis and interpretation, ocean state estimation thus relies heavily on the dynamical extrapolation of observations by means of numerical models of the global ocean circulation.

Such models play a central role in the study of the climate system and its ocean component for more than three decades. As engineering devices with the capacity for otherwise impossible experimentation they provide a laboratory for the simulation, extrapolation and ultimately understanding of the observational record. So far, the most convincing demonstration of the potential of circulation modeling has been the discovery of the El Nino mechanism and its repercussions on remote regions of the globe. After Matsuno’s theoretical ground work [3] and the provision of observational evidence by Wyrtki [4], the essential dynamical processes were numerically simulated with simple shallow water models [5, 6]. Today, operational El Nino monitoring and forecasting are implemented at a number of institutions world wide and the variability of tropical circulations has become one of the best understood aspects of the climate system.

On the other hand, dedication of more complex models to the same problem has yet been unable to advance El Nino simulation and forecasting significantly. Nor has it been possible to gain comparable insights for the extratropics. While scientists are well aware of extratropical circulation variability such as the North Atlantic or Arctic Oscillation or the Antarctic Circumpolar Wave, numerical analyses have clearly been less yielding in these instances. Uncertainties of this kind also raise the question of the adequacy of contemporary numerical circulation models for longer term climate projections.

The major difficulty of global circulation modeling is the lack of a physically consistent and numerically soluble formulation of the circulation problem. Physically, the global ocean circulation poses the thermohydrodynamical problem for a viscous fluid on the rotating geoid. The gravest problem of circulation theory is certainly the absence of an energetically consistent formulation of the equations of motion for a viscous rotating fluid. While such formulations are well known for viscous nonrotating fluids and ideal rotating fluids, the derivation of the energy budget from the equations of motion of a dissipative rotating fluid remains a matter of scientific debate. As one consequence, wave-dissipation in rotating fluids is not very well understood. Moreover, viscosity plays a significant role for the numerical stability of circulation models. It is clearly desirable that parameterizations of subscale transports steer momentum, energy and vorticity along realistic, i.e. energetically and vortically consistent pathways in space-time and wave vector space. For contemporary circulation models, this matter remains essentially unsolved.

Satellite orbits reveal a complex fine structure of the planet’s shape and considerable uncertainties particularly about the marine geoid still exist. For most purposes of circulation modeling, however, an approximation in terms of a spheroid or even a sphere is probably sufficient. A source of dissatisfaction with 3-dimensional spheroidal or spherical circulation equations are difficulties in analytically obtaining simple stationary solutions which reflect characteristic circulation features such as geostrophy and thermal wind balance. Moreover, linearizations in these coordinates do generally not admit separation of variables. Hence, it has yet been impossible to study analytically the propagation of acoustic, gravity and Rossby wave disturbances together with the stability of simple flows in a common, 3-dimensional framework. For numerical integration, such problems are insignificant. Nevertheless, most contemporary numerical circulation models compromise geometric-dynamic integrity in favor of a multi-β-plane approximation to the geometry of the geoid. This approach codes Laplace operators as sum of second order derivatives and ignores first order contributions from nontrivial Christoffel symbols.

A third set of issues of circulation modeling is associated with the nonlinearity of fluid dynamics. Nonlinear field theories inevitably couple variability on the smallest space- and time-scales with the largest scales available. For numerical as well as theoretical purposes, processes on small spatial and fast temporal scales should be eliminated from circulation equations. In the first place, this applies to acoustics. The widely favored sound filter invokes the Boussinesq approximation to inertia and weight of the fluid. While this approach has been quite successful in the study of internal gravity waves and Rayleigh-Benard instability, its vorticity-inconsistency becomes a problem in long-term
integrations of circulation modeling. Furthermore, Rayleigh-Benard (or static) instability involves fast convective motions on small spatial scales. Such convective events are generally not resolved in global circulation models and their crucial role for the thermohaline circulation is represented by appropriate parameterizations. Hence, models assume the ocean to be in hydrostatic equilibrium and simply neglect internal vertical accelerations relative to Earth’s gravitational acceleration. However, this straightforward introduction of hydrostatics generates a problem. Now, momentum density is a 2-dimensional vector while the mass flux vector of the continuity equation remains 3-dimensional. Such a violation of the first law of motion will generally be uncritical for stationary flows or order-of-magnitude estimates. However, for the long-term integrations of circulation modeling, such a formulation is not entirely satisfactory.

The Boussinesq approximation, hydrostatics and the so-called “traditional approximation” of inertial forces define Richardson’s Primitive Equations [7]. Currently, these equations provide the physical basis for most global circulation models. While the Primitive Equations account consistently for velocities and thermodynamics of equilibrium circulations, they do not pose a Newtonian dynamical problem.

The present study utilizes GROB HOPE, a coarse version of the numerical Hamburg Ocean Primitive Equations model of MPI-MET [8]. This model is based on a C-grid discretization of the Primitive Equations for UNESCO seawater [9] and allows various convection parameterizations which account for different characteristics of this process in the open ocean and in the bottom boundary layer down submarine slopes. GROB HOPE includes sea ice dynamics with viscous-plastic rheology parameterizing cracking, ridging, rafting and deformation of sea ice. The model is forced by buoyancy fluxes and wind stresses at the sea surface as well as the freshwater discharges of Earth’s 50 largest rivers.

In long term experiments (integration time: 1000 years) with climatological forcing resolving the annual cycle, the model assumes an essentially drift-free cyclostationary state after a few centuries which reproduces the major water masses and gyre structures of the global ocean circulation as well as the sea ice cover and its seasonal variation at high latitudes. While this model circulation exhibits the characteristic degree of realism of state-of-the-art simulations it also displays a number of typical deficits. The model fails to maintain the observed Pacific Intermediate Waters. Furthermore, while the poleward Atlantic heat transport is certainly of the observed order of magnitude, its maximum of 0.8 PW is still somewhat lower than the 1.1 PW suggested by observations. On the other hand, the mass transport by the Antarctic Circumpolar Current with 180 Sverdrup in the Drake Passage is higher than the observed 140 Sverdrup. The path of the Gulf Stream which is crucial for the European climate and weather turns out to be quite sensitive to the details of the atmospheric forcing and the chosen parameterization of subscale transports. For an extensive discussion of the strengths and weaknesses of the GROB HOPE circulation, see [8]. At this time, the versatility of numerical circulation models is sufficiently developed to simulate a wide variety of preconceived scenarios. However, beyond this illustrative role, state-of-the-art models generally lack the capacity of scientific discrimination between competing predictions and projections. To a large part, these uncertainties can be resolved by the systematic combination of models with observations.

Such combination and confrontation of models with extensive and novel observational data sets has been the outstanding factor in forecast-improvement by numerical weather prediction over the last thirty years. With maturing numerical ocean circulation models and a growing understanding of the variability of the ocean circulation this approach has now also become attractive to the oceanographic and climate communities. Given the characteristics of model data and observations in Earth System Modeling, the integration of information from different sources poses a considerable data engineering problem. Frequently, observations do not refer to prognostic model variables while other parameters such as vertical velocities are practically unobservable. Moreover, observations are typically distributed highly irregular in space-time. And data sets from both sources, model and observation, are large. The mathematics of the optimizing synthesis of large data sets are the objective of estimation theory [11]. To avoid the mutual enhancement of model- and data-error, estimation theory has been (and still is)
developing a number of what are called data assimilation algorithms. Generally, these algorithms fall into two classes: variational and sequential techniques. The equivalence of both methods is readily demonstrated in simple cases.

Variational assimilation, namely the Adjoint Method, is based on an application of inverse modeling techniques to the estimation problem. Variation of control parameters minimizes a cost function formed by the model-data misfit. This approach lends itself particularly to the estimation of equilibrium states and processes of finite duration. Computation of the cost gradient with respect to the controls calls for what is often referred to as the temporally backward integration of the adjoint model. For complex models, coding of the model adjoint is a substantial task, well comparable to coding the model itself. The practical relevance of adjoint assimilation in Earth System Modeling therefore arose only after the advent of the theory of automatic differentiation and the subsequent development of automatic adjoint code compilers. With global circulation models, the Adjoint Method finds presently wide application in sensitivity studies.

Sequential methods such as the Kalman Filter are more specifically tailored to the needs of monitoring and prediction. These updating schemes emerge from the application of the theory of stochastic processes to estimation and yield an estimate of minimum variance. On update, the relative weight of model and data is determined by the Kalman Gain which is computed from data and model error dynamics. To this end, the model error is considered as a stochastic process. The dynamics of such processes can be equivalently formulated in the Langevin (or Heisenberg) representation and in the Fokker-Planck (or Schrödinger) representation. The Langevin picture addresses the space-time behavior of the process in terms of its moments. In practice, this refers generally to the covariance only. Formally, the temporal development of the covariance is uniquely determined by the model dynamics. However, the practical derivation of the covariance dynamics for a complex model such as a global ocean circulation model readily becomes everything but straightforward. This applies particularly to nonlinear models, the issue of boundary and initial conditions for the covariance, stability questions and the problem of temporally backward assimilation. Nevertheless, at this time the literature on Kalman Filter assimilation in Earth System Modeling and other branches of engineering is almost exclusively dominated by the Langevin approach.

Alternatively, a stochastic process may be considered in phase-space in terms of its probability density. Provided the process is Markovian and jumps remain small in an appropriate sense, the dynamics of this probability density are governed by the Fokker-Planck Equation. The advection- and diffusion-coefficients of this linear parabolic differential equation are determined by model dynamics and observational error statistics. In general, these coefficients are also difficult to obtain from a complex model. However, for sufficiently short update intervals, phase-space advection and diffusion can be determined phenomenologically from the model output by histogram techniques. In this framework, the assimilation method provides practical answers to the issues of phase-space reduction, model nonlinearity, initial and boundary conditions for higher moment dynamics as well as stability. Moreover, the existence of the Backward Fokker-Planck Equation will permit the generalization of sequential assimilation to include the temporally backward extrapolation of data information. The mathematical aspects of the Fokker-Planck representation of sequential Kalman Filter assimilation have been developed in detail.

With the typical volume of model output and observational record in Earth System Modeling, computational demands for assimilation with least-square optimality are always quite high. For a reduction of the computational burden, the present estimation utilizes a combination of Kalman Filter assimilation and simple “nudging”. While subsurface temperatures from the TAO/TRITON array will be assimilated sequentially, observations of global sea-surface temperatures are essentially inserted into the model at daily intervals. The feasibility of this simplistic technique is by no means trivial. Older model generations were generally unable to “digest” essentially unprocessed data and model-data inconsistencies would readily emerge in various regions of space-time and phase space. It will here be shown that the quality of contemporary models and data sets is sufficiently high for
nudging to be beneficial for the ocean state estimate.

2.) Fokker-Planck Picture of the Kalman Filter.

Societal and scientific needs in Earth System Monitoring are presently best met by an operational, steady combination and confrontation of substantial, yet incomplete observations with complex, but nevertheless approximate numerical models. This combination aims to fill data gaps by dynamical extrapolation of observations on the basis of physical laws incorporated in the model and simultaneously constrain model uncertainties by operating the model in close vicinity of observations. One source of information is used to compensate the deficits of the other and thus arrive at a comprehensive state estimate including an assessment of model- and observation-quality. The assimilation algorithms of estimation theory are information integration techniques which prevent the mutual enhancement of errors from different sources and maximize the benefit from imperfect models and data. As an engineering tool, data assimilation accepts or rejects a hypothesis (the model) while a constructive evaluation of structural model deficits remains beyond its scope.

![Figure 1: Flow Chart for Sequential Data Assimilation](image)

The key idea of sequential assimilation is to integrate the model until an observation becomes available. At this time, model integration is halted and the state of the system is updated by an appropriate combination of model prediction and observation. Subsequently, this update provides the initial value for the continued model integration (fig.1). Hence, the main task in sequential data assimilation is the determination of the temporal development of the relative weight of model prediction and observation.

The state of the system under consideration (here: the global ocean) is given by a finite- (generally: very high) dimensional vector $Y(t, x)$ where $t$ denotes time and $x = (x(1), x(2), x(3))$ the 3-dimensional spatial coordinate. In numerical ocean models, time and space coordinates will generally be members of a discrete, 4-dimensional grid. The time-development of the state of the system is governed by the model dynamics

$$\frac{d}{dt}Y_m(t) = \Lambda(Y_m, t)$$

where the index $m$ refers to the model and $\Lambda$ is a generally nonlinear operator of $Y_m$ with

$$\Lambda(Y_m = 0, t) = 0$$

and some explicit time-dependence representing external forcing. For simplicity, spatial coordinates have been suppressed in (1). It is now assumed that the model is sufficiently “good” so that the
time-development of the true, i.e. observed system is given by the equations of motion

\[ \frac{d}{dt} Y_o(t) = \Lambda(Y_o, t) + W_0 \]

(2)

where the index \(o\) refers to observation, while \(\Lambda\) is the same operator as in (1) and \(W_0\) an additive noise of known probability distribution. The possibly nonstationary noise is assumed to have zero average, finite spatial and no temporal correlation, i.e. it is assumed to be temporally white

\[ < W_0(t, x) >= 0, \quad < W_0(t, x) W_0(t + \tau, x + r) >= Q(t, r) \delta(\tau). \]

Physically, this noise accounts for model deficits. Equation (2) is the Langevin representation of a (nonlinear) stochastic differential equation.

The model error

\[ y(t, x) = Y_o(t, x) - Y_m(t, x) \]

appears under a variety of names in different applications of assimilation theory. Variational techniques generally term this quantity “misfit” while numerical weather prediction refers to the model error as “innovation”. By definition, the model error satisfies the Langevin equation

\[ \frac{d}{dt} y(t) = \Lambda(y + Y_m, t) - \Lambda(Y_m, t) + W_0. \]

With the help of the mean value theorem, the dynamical operator is rewritten as

\[ \Lambda(y + Y_m, t) - \Lambda(Y_m, t) = y \Lambda'(Y_m, t) + R \]

where the residual \(R\) comprises terms higher than second order. Writing now

\[ \Lambda(y + Y_m, t) - \Lambda(Y_m, t) = \Lambda(y, t) - \Lambda(y, t) + y \Lambda'(Y_m, t) + R \]

and using again the mean value theorem on \(\Lambda(y, t)\) together with \(\Lambda(0, t) = 0\), one arrives at

\[ \frac{d}{dt} y(t) = \Lambda(y, t) + W \]

(3)

where the new noise \(W\) comprises \(W_0\) and terms of second and higher order. It is readily seen that

\[ < W(t, x) >= 0. \]

The error dynamics (3) account for nonlinearities and provide the basis for the histogram technique to be invoked below.

For simplicity, data are here assumed to represent prognostic model variables directly. Furthermore, measurements are made at specific observation points \(X = (X(1), X(2), X(3))\) which are generally much less in number than model grid points \(x\) and do not coincide with these. Interpolation to model points will generally be straightforward and observation points are here assumed to coincide with model points. In the context of monitoring and prediction, observations typically become available at specific times which are termed “analysis times” in numerical weather prediction. At these times, sequential data assimilation halts the model integration and updates the system’s state vector with observational information. This update is given in terms of a convolution-type integral

\[ Y(t, x) = Y_m(t, x) + \int_0^t \int d\tau dX G(\tau, x, X) y(\tau, X) \]

(4)

where the kernel \(G(\tau, x, X)\) is called the gain. For the update (4), the gain accounts for all observations prior to analysis time and hence only represents the temporally forward propagation of data.
information. In this sense, the kernel in (4) represents the “retarded gain”. It is equally possible to ask: at which state did the system initially start, if it is at the observed state on analysis time. The account of the temporally backward propagation of data information requires the inclusion of the “advanced gain”. Sequential assimilation admits the dynamical extrapolation of data information into both, past and future. The corresponding algorithm, namely a meaningful representation of the advanced gain becomes particularly transparent in the phase space representation. Its formal details will be discussed elsewhere.

There is a number of expressions for the gain-kernel in (4) which all lead to a different variance for the state estimate. The estimate has minimum variance if the gain is given by the Wiener-Hopf equation

\[ K(t, x, X) = \int_0^t d\tau \int dX_0 G(\tau, x, X_0) K(t - \tau, X, X_0) \]  

where

\[ K(t, x_1, x_2) = \langle y(t, x_1) y(t, x_2) \rangle - \langle y(t, x_1) \rangle \langle y(t, x_2) \rangle. \]

is the error covariance with brackets indicating the ensemble mean and unbraced indices denoting different points, i.e. different 3-tuples (and not different vector components). The gain defined by equation (5) is called the Kalman Gain and the sequential data assimilation algorithm given by (4) and (5) is called the Kalman Filter [20]. It follows from (5) that the central problem of Kalman Filter assimilation is the determination of the temporal development of the error covariance \( K(t, x_1, x_2) \).

Formally, the covariance matrix and its temporal behavior are uniquely determined by the model error dynamics (3). In practice, however, exploitation of this equation encounters a number of serious problems. Covariance dynamics on the basis of (3) are determined at every model grid point. If model integration requires \( N \) operations per time-step, integration of the covariance dynamics requires additional \( N^2 \) operations. An order of magnitude estimate of the number of operations for a contemporary ocean circulation model such as GROB HOPE is \( N \approx 10^5 \). Even taking into account the rate of increase in available computing capacities, integration of the complete covariance dynamics in the Langevin picture becomes prohibitive for global circulation models. Furthermore, these models typically involve strong nonlinearities. For mean quantities such as the the error covariance, this non-linearity leads to a hierarchy problem since the mean of a product does not equal the product of the means. The difficulties and ambiguities of practical closures of such hierarchies are well known from turbulence theory [21]. Additional complications arise from the lack of initial and boundary conditions for the dynamics of higher moments and for the determination of stability and uniqueness conditions of the assimilation procedure. These problems represent some of the reasons for the prevalence of the Adjoint Method in Earth System estimation.

An alternative approach to the Kalman Filter utilizes the phase space or Fokker-Planck representation of stochastic processes. In this framework, a detailed assimilation algorithm for application in Earth System estimation has been developed by Belyaev and coworkers [19, 22]. The starting point of this formulation is the joint probability distribution

\[ p(t, \eta_1, \eta_2; X_1, X_2) \]

for the two-component projection \( \eta \) of the model error \( y \)

\[ \eta = (\eta_1, \eta_2) = (y(t, X_1), y(t, X_2)) \]

to have the value \( \eta_1 \) at observation point \( X_1 \) and the value \( \eta_2 \) at observation point \( X_2 \) at time \( t \). In terms of this probability the error covariance (5) takes the form

\[ K(t, X_1, X_2) = \int d^2 \eta_1 \eta_2 p - \int d^2 \eta_1 \eta_1 p \int d^2 \eta_2 p. \]  

Determination of the error covariance thus requires the calculation of joint probability distributions \( p \) and this operation sets the magnitude of necessary computing capacities. Notice that (6) defines
the error covariance only for pairs of observation points. In Earth System estimation, the number $M$ of these points is typically orders of magnitude smaller than the number $N$ of model grid points. Using the symmetry of the joint probability distribution, the covariance matrix for $M$ observations has $M(M+1)/2$ independent members. Given 1000 data points (which still is a fairly small data set in Earth System observation), the error covariance calls for the computation of half a million probability functions. While this number is clearly much smaller than $N^2 \approx 10^{10}$, it still poses a considerable computational task.

In the phase space picture, the error $\eta$ is viewed as a Markov process. The temporal development of the conditional probability distribution of such a process is governed by the Master Equation $[18]$. For Markov processes with small jumps this equation is well approximated by the Fokker-Planck Equation $[18, 23, 24]$. In the present case this equation takes the form

$$\partial_t p = -\partial^m \Lambda_n p + \frac{1}{2} \partial^m (q_{mn} \partial^m p)$$

(7)

where the usual summation convention for indices $m, n, \ldots = 1, 2$ is implied. The vector

$$J_n = \Lambda_n p - \frac{1}{2} q_{mn} \partial^m p$$

denotes the advective-diffusive probability flux in phase space with advection velocity $\Lambda_n$ and diffusion $J_n = -\frac{1}{2} q_{mn} \partial^m p$. In this sense, the Fokker-Planck Equation (7) expresses the conservation of probability in phase space. Temporally, this linear parabolic equation governs the development of the conditional probability $p(t_2, \eta_2 | t_1, \eta_1)$ of the error $\eta$ to have the value $y_2$ at time $t_2$ and location $X_2$ given its value $y_1$ at time $t_1 < t_2$ at location $X_1$. The required joint probability follows from the solution of the Fokker-Planck Equation by Bayes’ Rule

$$p(t, \eta_2, \eta_1) = p(t, \eta_2 | t, \eta_1) p(t, \eta_1).$$

It is noted that there is also a Backward Master Equation $[18, 24]$. The small jump approximation to this equation leads to the Adjoint Fokker-Planck Equation which governs the temporally reversed development of the error distribution. Hence, the Adjoint Fokker-Planck Equation provides the basis for the determination of the Advanced Kalman Gain.

For the solution of the Fokker-Planck Equation (7) the phase space advection $\Lambda_n(t, \eta)$ and the diffusion tensor $q_{mn}(t, \eta)$ have to be known. These parameters are determined by error dynamics and data stochastics according to

$$\Lambda_n(t, \eta) = \langle \Lambda_n(t, \eta) | \eta = y > = \tau^{-1} \int d^2 \eta' (\eta_m - \eta_n') p(t, \eta | t', \eta')$$

with $\tau = t - t'$ for $t' < t$ for the advection while one has for the diffusion tensor

$$q_{mn}(t, \eta) - Q_{mn}(t, \eta) = \langle \Lambda_m(t, \eta) \Lambda_n(t, \eta) | \eta = y > = \tau^{-1} \int d^2 \eta' (\eta_m - \eta'_m)(\eta_m - \eta'_n) p(t, \eta | t', \eta')$$

where $Q_{mn}$ denotes the data covariance. With these definitions, the Fokker-Planck Equation (7) is readily seen to be equivalent to the Langevin Equation (3). Multiplying (7) from the left by $\eta$ and integrating over phase space one obtains

$$\frac{d}{dt} < \eta_n > = \langle \Lambda_n(t, \eta) >$$

in agreement with the two-component projection of the ensemble average of (3).

In principle, the advection- and diffusion-terms are determined by the Langevin representation (3) of the error dynamics. However, particularly for strongly nonlinear dynamics such a derivation encounters serious formal difficulties and a unique and practical solution to this problem is currently
not known. In view of the typical problem in Earth System Monitoring, Belyaev and coworkers \cite{22} propose an alternative, phenomenological determination of these parameters. In Earth System Monitoring the time-interval between consecutive samples is typically short compared to the time scales of the processes under observation. Under these conditions it becomes possible to consider the model as a black box and determine the transition (i.e. conditional) probabilities by histogram techniques from model input and output. To this end, the number $N'$ of all grid points is counted for which $\eta$ has the value $y'$ at time $t'$. At the later time $t = t' + \tau$ all former $y'$-points $N$ are counted for which $\eta$ now has the value $y$. The conditional probability is then given by the ratio

$$p(t, \eta | t', \eta') = \frac{N}{N'}.$$  

Since $0 \leq N \leq N'$, this expression always satisfies the condition

$$0 \leq p(t, \eta | t', \eta') \leq 1$$

necessary for being interpreted as a probability density. With the help of this probability, the advection and diffusion parameters are readily obtained by phase space integration according to the above formulas.

It is now possible to solve the Fokker-Planck Equation numerically. As a linear parabolic differential equation in the 2-dimensional unbounded plane, the equation is efficiently integrated by the Peaceman-Rachford scheme \cite{25}. For details of this integration concerning initial conditions, positive definiteness and normalizability of the solution see \cite{14}. The resulting probability density determines the error covariance at all observational points $X$ according to (6) and the covariance at all model grid points is constructed from this expression by interpolation \cite{14}. Using this error covariance, the Wiener-Hopf Equation (5) is solved for the Kalman Gain and the model is finally updated according to (4).

3.) Ocean State Estimation

The feasibility of operational global ocean state estimation will here be demonstrated by combining simulations of the numerical circulation model GROB-HOPE with observations of global sea-surface temperatures (SST) and observed subsurface temperatures from the TAO/TRITON array for the El Nino year 1997. Besides a globally realistic mean state, the objective of the estimate is the improvement of the model’s El Nino simulation.

GROB HOPE has 20 layers in the vertical with high resolution of 10 layers in the upper 500m. In the horizontal, the model uses a spatially inhomogeneous grid obtained from a conformal transformation of the geographical coordinates. At the present stage of model development and availability of computer capacities, the disadvantages of an inhomogeneous horizontal grid are easily outweighed by its advantages. For one, polar singularities are avoided by transformation of the model poles to a continental site. Secondly, the spatial inhomogeneity of the horizontal grid allows high resolution in regions of interest (up to 25 km for the Arctic Ocean in the present case) while low resolution is accepted for remote regions (300 km near the equator in the present case). This design avoids well-known open boundary problems of fine-resolution regional or nested models. While the low-resolution regions provide a model-consistent climatology, the high-resolution regions admit even the study of mesoscale processes. In spite of this versatility, the machine requirements for GROB HOPE are those of a global model with a spatially homogeneous $3^\circ \times 3^\circ$ grid. This design permits a time step of 2.4 hours. With its coarse spatial resolution in the tropics, the GROB version of HOPE does not especially qualify for El Nino simulation. It is here to be shown that assimilation of observations is able to offset these design limitations. Success in this framework provides a demonstration of the capacities of sequential assimilation. For operational purposes, on the other hand, data will always be assimilated into the best model available.
After an initial spin-up period of 2 years with restoring to the 3-dimensional buoyancy climatology of WOA the model is integrated from 1948 to the present with surface forcing derived from the NCEP reanalysis [26]. Atmospheric data are interpolated onto the GROB HOPE grid and surface buoyancy-and momentum-fluxes are calculated by bulk formulae [8] depending on both, the atmosphere and the ocean. Hence, the eventual ocean forcing is determined by the particular realization of the ocean state by the model while the present ocean-only set-up is unable to account for a feedback of the ocean on the atmosphere. For a reduction of trends in the deep ocean, integration over the NCEP period is repeated. Furthermore, model surface salinities are nudged to a mean annual cycle taken from WOA with a time constant of a little over a year (385d). Use of a mean annual cycle rather than an annual mean accounts for the seasonal variation in the hemispheric distribution of convective
activity. With this forcing the model is integrated to 31 December 1997. The period from 1 January 1997 to 31 December 1997 is taken as the control run in the present experiment and the model state at 31 December 1996 provides the initial condition for the assimilation. It is noted that model runs considered here do not address the prediction problem. Surface data transfer external El Nino information to the ocean model.

Fig. 2 shows the monthly mean of the net surface heat flux of the control configuration for December 1997. This heat flux is determined by atmospheric data from the NCEP reanalysis and oceanic data from GROB HOPE. The main feature is the characteristic seasonal separation of the (southern) summer- and (northern) winter-hemisphere: the ocean gains heat in summer and loses heat during winter. A particular detail in the North Atlantic is associated with model problems in simulating a realistic Gulf Stream path: off the American east coast, the ocean is unrealistically warm leading to a pronounced heat loss while the ocean is unrealistically cold in the region of the so-called North West Corner leading in turn to a pronounced heat gain by the ocean. Similar aberrations are seen in the Kuroshio region, the confluence of the Malvinas and Brazil Currents off the South American east coast and for the Agulhas Current near the Cape of Good Hope. The paths of these currents are essentially determined by vorticity dynamics and mismatches of NCEP derived forcing and model simulation are due to ambiguities in the vorticity dynamics of the Primitive Equations. Given the NECP fluxes, GROB HOPE fails to simulate mesoscale details of the state of the underlying ocean surface realistically.

It will now be shown that nudging of observed SST into the model improves the state estimate considerably. To this end, GROB HOPE is restarted from 31 December 1996 and daily mean Reynolds SST of the NCEP data set are inserted into the model’s top layer at a time constant of one day. During this one year integration, model-data incompatibilities do not develop. This is also true for GROB HOPE runs with SST nudging over the full NCEP period (not shown). Fig. 3 depicts the monthly mean net surface heat flux for December 1997 with SST nudging. In comparison to fig. 2, it is seen that aberrations of the major current systems are significantly reduced and the estimate of mesoscale features of the state of the sea surface improves without penalty.

Nudging effects are not confined to the upper ocean alone. In convectively active regions surface temperature information is rapidly communicated to the abyss. For the present integration period of one year the deep ocean remains of course unable to adjust to the “injected” information. Nevertheless, with these data and for this model, nudging becomes a practical option of ocean state estimation by an efficient and yet robust model-data combination. Other presently available observations are of similar quality: sea-level data from space-borne altimeters and space-based observations of sea-ice cover. By nudging observations of this type into a global ocean circulation model, it is currently possible to arrive efficiently at a comprehensive and realistic estimate of the global state of the sea surface at mesoscale resolution.

For the assessment of the state of the interior ocean consider the equatorial temperature field during the El Nino episode of 1997/98. Fig. 4 shows the temperature difference Nudge-WOA along the equator for December 1997 where “Nudge” refers here to the GROB HOPE simulation of the global ocean circulation with NCEP forcing and nudging of daily SST observations, i.e. the run also portrayed in fig. 3.

In the abyssal Pacific, simulation and observation are seen to differ by typically less than half a degree. While the simulation is systematically colder than WOA, structural mismatches do not emerge. The agreement is less satisfactory in the abyssal Indic and Atlantic. In the near-surface Pacific, the model clearly exhibits the characteristic El Nino pattern. Relative to the WOA climatology, the eastern and central Pacific are colder while the West is anomalously warm. Comparison with observed subsurface temperatures [27] shows that the model simulates the phase of the process quite realistically. Since phase information is directly provided by forcing data, this model response is primarily indicative of the consistency of the simulation of near-surface wave propagation with with surface boundary conditions.
Other features of fig.4 exhibit a lesser degree of realism. The warm anomaly in the surface waters of the central Pacific cannot be found in the observational record [27]. Here, the mixed-layer model of GROB HOPE fails to mix the heat supplied at the surface, sufficiently deep into the upper ocean. In the model, heat mainly penetrates to greater depth by slow diffusion processes. In the ocean, however, these transfers are dominated by turbulent mixing. As another consequence of the mixing parameterization, GROB HOPE underestimates mixed-layer depths throughout the year and thus fails to account for Kelvin wave downwelling during El Nino. Thermocline temperatures beneath the mixed layer are about 2°C Celsius too warm. Here, the model diffuses too much heat to depths of approximately 500m in the eastern equatorial Pacific which penetrates westward at approximately 250m. This mismatch is the result of unrealistically strong downward diffusion of heat and unrealistically weak upwelling of cold waters.

For Primitive Equation models, vertical transfers pose a greater problem. Nonhydrostatic mixing processes have to be parameterized and such parameterizations are by no means trivial. The mixed-layer model of GROB HOPE is tuned to yield realistic mixing depths at moderate latitudes and compromises for the equatorial mixed layer are accepted. The alternative would be a far more complex and machine-intensive mixed-layer model. Moreover, vertical velocities are determined from mass conservation, independent of the momentum budget. Possible problems and ambiguities are smeared out by diffusion. Hence, models have a tendency to use diffusion where space-time- and phase-space-characteristics of the real ocean are determined by advection and propagation.

Sequential assimilation of subsurface temperatures improves this state estimate significantly. Subsurface temperature data are taken from the TAO/TRITON array which consists of approximately 70 moorings in the tropical Pacific between 8°S and 8°N. The buoys record a number of atmospheric parameters, sea surface temperatures and subsurface temperatures at 10 irregularly spaced depths in the upper 500m. Records are transmitted to shore in real-time via the ARGOS satellite system. TAO/TRITON has become one of the most successful ground-based ocean observatories for two major reasons. In the first place, the relatively quiescent tropical waters allow the long-term deployment of buoys. For the more energetic high latitude oceans, the physical lifetime of a similar array would be significantly shorter than time scales of ocean processes of interest. Secondly, the observed variability is readily interpreted in terms of Matsuno’s theory. Since 1985, the TAO/TRITON array has become an integral part of operational services as well as ocean and climate research.

In contrast to the surface boundary condition, nudging of regional TAO/TRITON data is not an option. This array is physically embedded in the global ocean circulation and its data interact physically with their neighborhood in space-time as well as in phase space. In the Fokker-Planck picture of the Kalman Filter this is accounted for by phase space advection and diffusion which are updated at every assimilation step. To this end, model integration is halted at the end of each month and the model temperature field is updated by observed TAO temperatures. After the update, model integration resumes and continues for one month when model temperatures are updated again. Thus, model operation is constrained to the vicinity of the observed state of the ocean.

Fig.5 shows the monthly mean temperature difference Assimilation-Nudge along the equator for December 1997. The data are seen to have three major effects on the estimate: the surface becomes colder, the mixed layer warmer and the thermocline colder. These modifications lead to a significantly higher degree of realism for the estimate. Assimilation ensures that heat supplied at the surface, is uniformly mixed into the upper layer and cold water is upwelled into the thermocline. In response to the data information, the model replaces diffusion dominated dynamics with mixing and advection. However, it is also seen that the assimilation still exhibits some pockets of warm water below 500m although far less than fig.4. Primarily, these pockets are a consequence of the lower boundary condition chosen for vertical transition probabilities: the model is assumed to be true at 500m. Obviously, there is room for improvement.

A different view of these data effects is given in fig.6. The figure shows a time series of monthly mean temperature profiles at a location in the eastern equatorial Pacific for 1997. Simulated (black)
and assimilated (red) profiles are compared. The simulation is clearly diffusion dominated, unable to produce a mixed layer and leaking too much heat into the thermocline. The assimilation also fails to produce well-defined mixed layers during the first part of 1997. Before the arrival of the downwelling
Kelvin wave in the eastern Pacific, mixed layers here are shallow (typically 25m). Their absence in the assimilation during the first part of the year is a consequence of the poor vertical resolution of GROB HOPE. With the arrival of the Kelvin wave, assimilation produces the characteristic signature of turbulent mixing in the upper ocean with realistic mixed-layer depth. At the same time, the thermocline is cooled by upwelling of colder water and temperature gradients at the mixed-layer base increase.

It is mentioned (corresponding plots not shown) that the model extrapolates data information beyond the temperature field in the TAO/TRITON region. By December 1997, temperatures as far as 30° latitude on both hemispheres are modified by the assimilation. In phase space, model dynamics extrapolate temperature observations onto sealevel, salinity and the velocity field and improve the estimate for the complete state of the ocean. On the other hand, without continued assimilation the model loses memory of the data information from the upper equatorial Pacific after a time period of three to six months.

4.) Summary

Societal needs of climate monitoring call for the installation of global ocean state estimation in the framework of an operational service similar to national weather prediction agencies. Novel ocean observation techniques provide a global data base for such estimates. For a number of parameters, these observations are available almost in real-time and at mesoscale resolution. Assimilators utilize numerical circulation models to dynamically extrapolate measurements in space-time and phase space and, at the same time, constrain model uncertainties.

Given the data volume in ocean observation and modeling, requirements in computing resources are high. For efficiency, it is significant that model and data quality is sufficiently developed to allow nudging the model to essentially unprocessed data at short time constants. This applies particularly to the sea surface where data wealth is largest and determines primarily the surface forcing with a high degree of realism. The forcing problem that plagued ocean model development 20 years ago has been resolved.

Dynamical extrapolation of interior ocean data requires advanced assimilation techniques. Monitoring problems are best addressed by sequential methods such as the Kalman Filter. Typically, observations do not coincide with the corresponding model solution and may even be incompatible
with model dynamics. The Kalman Filter finds the initial value for model restart that is both, as close as possible to the data and compatible with model dynamics. To this end, the phase space representation of the filter solves (a large number of) simple, 2+1 dimensional, linear Fokker-Planck equations which represent model dynamics in terms of phase space advection and diffusion. Determination of these parameters by an elementary histogram method circumvents a number of highly complex, but essentially technical issues of the stochastics of nonlinear systems. For numerical analysis, the method proves efficient and reliable.

At this time, models alone are generally unable to simulate the global ocean circulation with satisfactory realism. However, they do capture large-scale features such as gyres, water masses and their seasonal and longer-term variation quite realistically if they are determined by large-scale features of topography and external forcing. Problems typically emerge with the dynamical control of the density field. In the present study, this is demonstrated for equatorial mixing and upwelling and the paths of major ocean currents. On the other hand, the assimilation has shown that models are not antagonistic to (temporary) operation in closer vicinity of the data. At this development stage, model operation in the assimilation mode is capable of delivering practically relevant global ocean state estimates provided a continuous inflow of data is guaranteed.

Some improvement in model performance is readily obtained by fairly simple measures. Higher vertical resolution is oftentimes possible within the framework of given computing resources. Significant increase of the overall horizontal resolution requires generally an upgrade of computer resources. For the performance of HOPE at higher spatio-temporal resolution, see [8]. Moreover, the modeling community continuously develops increasingly appropriate parameterizations of subscale processes and models are updated accordingly.

On the other hand, as long as models are unable to account for basic laws of nature such as the first law of motion, long-term projections with little or no data input after initialization will remain questionable. In this context, it is noted that the “Newtonization” of Richardson’s equations is actually more or less trivial: vertical integration of the Primitive Equations for an incompressible (multilayer) fluid leads again to a Newtonian set of equations of motion. In this framework, vertical variability appears as internal variability of the spatially strictly 2-dimensional fluid. Minor questions arise from the hierarchy problem that results from vertical integration of the nonlinear advection term. Since stratification is represented by the multilayer structure, low-order cut-offs of the advection hierarchy suffice for most purposes of circulation modeling. This shallow water approach to the circulation problem can be formulated with geometric-dynamic integrity and energetic consistency in both, the viscous nonrotating limit and the ideal rotating limit. The theory also admits comprehensive analytical studies of wave-circulation interaction. Currently, physically consistent global circulation models on the basis of shallow water theory are not available.

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