An Oceanographer's View of Data Assimilation and Reanalysis

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The World Ocean Circulation Experiment (WOCE, roughly 1992-1997+) for the first time gave oceanographers near-global, but extremely diverse, measurements which are also inhomogeneous in space and time. The overall goal was to achieve a quantitative estimate of the ocean circulation in three dimensions, globally, with time resolution of days, for a duration approaching a decade.

From the beginning, it was recognized that these data would have to be combined with numerical GCMs were any kind of global, overall, picture to emerge.

Among the Data Types

WOCE & After



Numerical weather forecasters had been doing something similar since the middle 1950s, which they called "data assimilation." Their reaction to the oceanographic problem was troubling:

- (1) "We know all about that. Go away."
- (2) "What you want to do isn't possible." (This comment referred to modifying systematic errors in the background state. It emerged, finally, that "isn't possible" meant "we (I) don't know how to do it.")

In addition, much of the oceanographic community was, and remains, hostile to the whole notion---combining large numerical models with global data sets is an alien practice for what used to be a mainly sea-going community. In contrast, atmospheric scientists "grow up" with NWP and take it for granted. Oceanographers had (have) no counterpart of either the requirement of daily weather nor forecasts, nor the infrastructure that supports the effort.

An advantage was that we could look at it *ab initio*: what did one really want to do?

The disadvantages were that there was no infrastructure and little experience with global scale data sets, global GCMs, and estimation methods, and indeed a great deal of hostility in oceanographic institutions to the whole notion.

Whatever was to be done would come from a small academic group.

As climate became the main concern after the Global Weather Experiment (FGGE) it was recognized in the Met. Community that climate required homogeneous estimates of the atmosphere over decades, and this in turn led to the notion of "reanalysis", which I want to look at briefly, partly because some oceanographers have simply assumed it is appropriate for the ocean problem, and because for many people, it represents meteorological "truth". My personal sweeping generalizations/description.

- (1) One uses a fixed model and estimation methodology over 50-100 years.
- (2) The methodology is adapted from operational weather forecasting.

Consequences (problems for an oceanographer and others):

The whole system is dominated by huge changes in the observing system.

Global conservation principles (mass, heat, freshwater, energy,...) are not imposed.

Prediction methodologies are both suboptimal for an estimation problem, and "analysis" time model-data combinations lead to physical jumps and preclude even local budgets of heat, moisture, vorticity, etc. I am indebted to David Bromwich, Ohio State, for the comparisons that follow.

Mean annual Antarctic net precipitation (P-E) from ERA-40 reanalysis for various elevation areas.

> [Bromwich et al. 2007, adapted from Van de Berg et al. 2005]



Spurious trends in the high latitudes resulting from changes in the observing system, especially the assimilation of satellite observations in the late 1970s.

□ Jump in Antarctic P-E in 1978-79, particularly marked at high elevations.

- □ A related scenario in the 1990s-2000s?
- Dramatic increase in the amount and quality of satellite observations assimilated into the reanalyses (or available for assimilation).



Number of observations assimilated in ERA-Interim

Mean annual precipitation (P) 1989-2008



Mean annual evaporation (E) 1989-2008



1989-2008 linear trends in annual P-E

(D. Bromwich, Byrd Polar Research Center, Ohio)



Annual P, E and P-E over the grounded Antarctic Ice Sheet



mm y⁻¹ 240 ¬

220

200

180

160

140

120

PRECIPITATION (P)

Precipitation and PW changes over the Southern Ocean



Zonal means of precipitation and total precipitable water (PW) are examined for different <u>latitude bands</u>.



- Additional datasets are included for latitudes **40°S-60°S**:
 - Precipitation estimates from:
 - Global Precipitation
 Climatology Project (GPCP)
 - Climate Prediction Center Merged Analysis of Precipitation (CMAP)
- PW estimates from SSM/I (over ice-free ocean only)

Spurious trends in MERRA precipitation



The figure shows the 2-month running average difference between forecast <u>daily</u> precipitation from MERRA and from ERA-Int, spatially averaged over the 50°S-60°S latitude band.

1989-2008 linear trends in annual P (Southern Hemisphere)





Mean annual 10m zonal wind averaged over 180-75W, 40S-85S (Pacific sector of the Southern Ocean)



D. Bromwich, private comm. 2010

NOTE: We included ERA-Interim for completeness but there are known issues with the zonal and meridional wind fields in this reanalysis dataset (as well as in ERA-40). Caution is required here.

Trends in U10 (1989-2009) in m s-1 y-1



Zonal Wind Apparent Trends. Oceanographically, and climatologically, troubling.

reanalysis product	net fresh water imbalance [mm/year]		net heat flux imbalance [W/m²]		
	ocean-only	global	ocean-only	global	
NCEP/NCAR-I 1992-2010	159	62	-0.7	-2.2	
NCEP/DOE-II (1992-2004)	740	-	-10	-	
ERA-Interim (1992-2010)	199	53	-8.5	-6.4	
JRA-25 (1992-2009)	202	70	15.3	10.1	
CORE-II (1992-2007)	143	58			

The reanalyses are derived from *weather forecast* models in which global water/heat balances are of no special concern.

These are boundary conditions on the ocean and have a major influence. What is the runoff rate? How much does it vary? How much is climatological ice melt? Difficult to model the ocean state on climate time scales with these errors present.

(Consider the literature on sea level change---claiming accuracies of tenths of millimeters/year.)

Oceanographers (and glaciologists, hydrologists, etc.) are using these as "truth" and driving models, finding trends, etc. It would not be a serious zero order concern if the estimates were accompanied by error bars.

That the reanalysis differences are largest where there is least data is a commentary on (1) the dominance of data in the solutions, and (2) the secondary role of model skill (as far as we know). Probably should call it "model assimilation" rather than "data assimilation".



In conventional meteorological data assimilation, the state jumps at analysis times when the model forecast is shifted towards the observations. For forecasting, this behavior is of no concern, but it is fatal if one wishes to analyze heat, freshwater, momentum, vorticity, etc. budgets over the entire time span of estimation. Achieving time-evolving estimates of the oceanic state on decadal time-scales, consistent with known equations of motion, was a major WOCE priority.

Importance of a physically consistent solution

Atmospheric reanalyses contain large air-sea flux imbalances. For example, the NCEP/NCAR reanalysis has an ocean freshwater flux imbalance of **6.2 cm/yr**, about 20 times larger than the observed **3 mm/yr** sea level rise.

They also contain discontinuities during "assimilation" updates. For example, standard deviation of NCEP surface pressure analysis shows that 24% of the atmosphere's mass change is physically unaccounted for (I. Fukumori, JPL).

Change over 6-hours



Data Increment



0 10 20 mbar 0 2 4 Contrary to atmospheric data assimilation, whose primary objective is NWP, need climate solutions satisfy model equations exactly, for example, conserving tracer properties.

Example tracer application: CO2 Sea Air Flux

Estimate of CO2 flux during 97-98 El Niño (mol/m2/yr) based on Kalman filter-like solution---a prediction method



Observed estimate of CO₂ flux during 92-93 El Niño (mol/m²/yr)

Estimate based on smoothed solution---accounting for "future" data



McKinley, 2002



Feely et al., 1999

Interpolation ("smoothing" in control theory) is a very different problem than prediction ("extrapolation").

One sees numerous papers (and talks) saying: "a Kalman filter was used to make an estimate."

You're meant to be impressed.

But a Kalman filter is an optimal linear *predictor*, not a general purpose estimator. (How many people have actually read Kalman's (1960) paper?)



He was solving the ballistic missile impact problem.

Interpolation and extrapolation are fundamentally different. Recall the elementary problem of interpolating noisy data with a polynomial:



This is too simple to be more than a metaphor---but worth remembering.

Can climate trends be calculated from reanalysis data?

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Their answer is "no", but the inference has often been ignored.



TLT is temperature of the lower troposphere

Figure 2. TLT calculated from ERA40 for the period 1958–2001. The dashed line shows the corresponding warming trend. The full line indicates a corrected warming trend obtained by adding a factor to the data for the period 1958–1972 obtained from the difference between ERA40 and the NOSAT experiment, and by excluding data for the years 1972–1978. See color version of this figure in the HTML.

Can one predict from these solutions?



IPCC AR4 scenarios for Arctic September ice cover 100 years into the future. (I. Eisenman, J. Wettlaufer, 2007) Models were all tuned to recent conditions.

Climate models now contain nearly 1 million lines of computer code and have been assembled over 50 years by hundreds of individuals.

What does ECCO (Estimating the Circulation and Climate of the Ocean) do? A whole family of ocean estimates from a consortium that at various times has included MIT, JPL, SIO, U. Hamburg. Finally funded beginning about 1997.

Goal: A practical system in which the estimates would include all data of any type, be consistent with known equations of motion, and central conservation principles. Doing it has proved: Difficult, expensive, and slow. But it has been accomplished.



A generic time-stepping system can always be written as:

$$\mathbf{x}(t+1) = \mathcal{L}[\mathbf{x}(t), \mathbf{Bq}(t), \mathbf{\Gamma} \mathbf{u}(\mathbf{t})]$$

The underlying equations can be any of the famous partial differential equation sets of mathematical physics: Maxwell, Schrodinger, Navier-Stokes, elastic, general relativity, orbital, ballistic,.... Or such non-physical systems as financial (econometric), ecological and biological systems.

All have non-linear regimes, but Navier-Stokes is perhaps the most complicated set----they represent a non-linear field theory.

Navier-Stokes equations of a stratified, rotating, spherical shell of complex lateral boundary and bottom topography typically a starting point for oceanographers. But *any set* capable of representation on a digital computer can be handled.

$$\frac{du}{dt} - \frac{uv\tan\phi}{a} + \frac{uw}{a} - 2\Omega\sin\phi v = \frac{1}{a\cos\phi}\frac{\partial p}{\rho\partial\lambda} + F_u$$
$$\frac{dv}{dt} + \frac{u^2\tan\phi}{a} + \frac{vw}{a} + 2\Omega\sin\phi u = \frac{1}{a}\frac{\partial p}{\rho\partial\phi} + F_v$$
$$\frac{dw}{dt} - \frac{u^2 + v^2}{a} = -\frac{\partial p}{\rho\partial z} - g$$
$$\frac{1}{a\cos\phi}\left(\frac{\partial u}{\partial\lambda} + \frac{\partial(v\cos\phi)}{\partial\phi}\right) + \frac{\partial w}{\partial z} = 0$$
$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \frac{u}{a\cos\phi}\frac{\partial \rho}{\partial\lambda} + \frac{v}{a}\frac{\partial \rho}{\partial\phi} + \frac{w\partial \rho}{\partial z} = 0$$

where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{u}{a\cos\phi}\frac{\partial}{\partial\lambda} + \frac{v}{a}\frac{\partial}{\partial\phi} + w\frac{\partial}{\partial z}.$$

$$\mathbf{x}(t+1) = \mathcal{L}[\mathbf{x}(t), \mathbf{B}\mathbf{q}(t), \mathbf{\Gamma}\mathbf{u}(\mathbf{t})]$$

Typically, the "state vector" $\mathbf{x}(t)$ would consist of u,v,w,p, and p (or equivalent). The notation $\mathbf{Bq}(t)$ denotes for technical reasons, the boundary and initial conditions and the $\mathbf{u}(t)$ are the adjustable parameters of the problem (the "controls"). The model: has about 100,000 lines of code:

$$\mathbf{x}(t+1) = \mathcal{L}[\mathbf{x}(t), \mathbf{Bq}(t), \mathbf{\Gamma} \mathbf{u}(\mathbf{t})]$$

in ECCO, the MIT GCM

Cost, or objective, function: $J = \sum_{m=1}^{M-1} (\mathbf{y}(t) - \mathbf{E}(t)\mathbf{x}(t))^T \mathbf{R}(t)^{-1} (\mathbf{y}(t) - \mathbf{E}(t)\mathbf{x}(t)) + \mathbf{x}(0)^T \mathbf{P}(0)^{-1}\mathbf{x}(0) + \sum_{m=0}^{M-2} \mathbf{u}(t)^T \mathbf{Q}(t)^{-1}\mathbf{u}(t), \quad t = m\Delta t, m = 0, \dots, M-1$

Constrained least-squares. Minimize J with respect to the state vector, while making sure the model remains identically satisfied and the adjustments, **u**(t), are as small as possible. The mathematics of Navier-Stokes is gone at this stage. Major assumption at this point is that minimizing J makes sense and is connected to an assumption of unimodal probability density functions. *No* evidence of zero-order failure of near-Gaussian assumption in either data or model error.



There are many sensible ways to measure the deviation of a model from data:

$$\mathsf{J} = \sum_{i} \left(\sum_{j} E_{ij} x_j - y_i \right)^2 W_{ii}, \quad \sum_{i} \left| \sum_{j} E_{ij} x_j - y_i \right|, \\ \min \max_{i} \left| \sum_{j} E_{ij} x_j - y_i \right|$$

The most common is least-squares---for a number of reasons: it is analytically tractable, minimization is connected to maximum likelihood estimation in Gaussian systems, sometimes the central limit theorem operates to one's advantage, and there is a 200year history of development and use including parallel computation codes. (Not necessary--it's convenient, but sometimes not appropriate.) One solution, with some advantages: Adjoin the model (using Lagrange multipliers—the adjoint solution). Idea known for about 200 years:

$$J' = \sum_{m=1}^{M-1} (\mathbf{y}(t) - \mathbf{E}(t)\mathbf{x}(t))^T \mathbf{R}(t)^{-1} (\mathbf{y}(t) - \mathbf{E}(t)\mathbf{x}(t)) + \mathbf{x}(0)^T \mathbf{P}(0)^{-1} \mathbf{x}(0) + \sum_{m=0}^{M-2} \mathbf{u}(t)^T \mathbf{Q}(t)^{-1} \mathbf{u}(t) - 2\sum_{m=1}^{M-1} \mu(t)^T ([\mathbf{x}(t) - \mathbf{L}\mathbf{x}(t - \Delta t), \mathbf{B}\mathbf{q}(t - \Delta t), \mathbf{\Gamma}\mathbf{u}(t - \Delta t)]),$$

$$t = m\Delta t, m = 0, \dots, M-1$$

constrained (but nonlinear) least-squares. What one is trying to do. The rest is computational detail! *The physics lies with the writing of the model, and in the choice of J and of the weight matrices. The latter determines the nature of the solution, but its critical nature is often overlooked, as it is not mathematically exciting and tabloids like Nature won't publish error analyses.*



If proceed naively, can form the "normal" equations whose solution defines the stationary point. Highly recommended if can afford it. In practice, do not solve them explicitly this way, but if a solution can be found, it will satisfy these equations.

$$\frac{1}{2} \frac{\partial J}{\partial u(t)} = \mathbf{Q}(t)^{-1} \mathbf{u}(t) + \left(\frac{\partial \mathbf{L}}{\partial u(t)}\right)^{T} \Gamma^{T} \mu(t+1) = \mathbf{0}$$
Trouble is that L is a
Fortran code. How do you
differentiate such a
thing?

$$\mathbf{x}(t) - \mathbf{L}[\mathbf{x}(t-1), \mathbf{Bq}(t-1), \Gamma \mathbf{u}(t-1)] = \mathbf{0},$$

$$1 \le t \le tf$$

$$\frac{1}{2} \frac{\partial J}{\partial \mathbf{x}(0)} =$$

$$\mathbf{P}(0)^{-1}[\mathbf{x}(0) - \mathbf{\hat{x}}(0)] + \left(\frac{\partial \mathbf{L}}{\partial \mathbf{x}(0)}\right)^{T} \mu(1) = \mathbf{0},$$

$$\frac{1}{2} \frac{\partial J}{\partial \mathbf{x}(t)} = \mathbf{E}(t)^{T} \mathbf{R}(t)^{-1}[\mathbf{E}(t)\mathbf{x}(t) - \mathbf{y}(t)] - \mu(t)$$

$$+ \left(\frac{\partial \mathbf{L}}{\partial \mathbf{x}(t)}\right)^{T} \mu(t+1) = \mathbf{0}, \quad 1 \le t \le tf - 1$$

$$\frac{1}{2} \frac{\partial J}{\partial \mathbf{x}(t_{f})} =$$

$$\mathbf{E}(t_{f})^{T} \mathbf{R}(t_{f})^{-1}[\mathbf{E}(t_{f})\mathbf{x}(t_{f}) - \mathbf{y}(t_{f})] - \mu(t_{f}) = \mathbf{0}.$$

What made the method practical for ECCO was the development before, and within, ECCO of automatic differentiation (AD) tools, capable of taking the forward model code, and producing the code for the adjoint model. (R. Giering, A .Griewank,, J. Restrepo, P. Heimbach and others). A story in its own right.

Sciavicco and Siciliano, 2000



ECCO is solving a problem in control theory. A robotic arm is prototypical.



Perhaps hundreds of degrees of freedom. We have hundreds of millions+.

Some of us set out to solve this problem. Eventually became known as ECCO (Estimating the Circulation and Climate of the Ocean)



observation	instrument	product/source	area	period	dT
Mean dynamic topography (MDT)	GRACE SM004-GRACE3EGM2008/DNSC07	CLS/GFZ (A.M. Rio) N. Pavlis/Andersen & Knudsen	global global	time-mean	mean
Sea level anomaly (SLA)	 TOPEX/POSEIDON Jason ERS, ENVISAT GFO 	NOAA/RADS & PO.DAAC NOAA/RADS & PO.DAAC NOAA/RADS & PO.DAAC NOAA/RADS & PO.DAAC	65°N/S 82°N/S 65°N/S 65°N/S	1993 - 2005 2001 - 2011 1992 - 2011 2001 - 2008	daily daily daily daily
SST	• blended, AVHRR (O/I) • TRMM/TMI • AMSR-E (MODIS/Aqua)	Reynolds & Smith GHRSST GHRSST	Global 40°N/S Global	1992 - 2011 1998 - 2004 2001 - 2011	monthly daily daily
SSS	Various in-situ	WOA09 surface	Global	climatology	monthly
In-situ T, S	 Argo, P-Alace XBT CTD SEaOS TOGA/TAO, Pirata 	Ifremer D. Behringer (NCEP) various SMRU & BAS (UK) PMEL/NOAA	"global" "gobal" sections SO Tropics	1992 - 2011 1992 - 2011 1992 - 2011 2004 - 2010 1992 - 2011	daily daily daily daily daily
Mooring velocities	• TOGA/TAO, Pirata • Florida Straits	PMEL/NOAA NOAA/AOML	Trop. Pac. N. Atl.	1992 - 2006 1992 - 2011	daily daily
Climatological T,S	• WOA09 • OCCA	WOA09 Forget, 2010	"global" "global"	1950 - 2000 1950 - 2002	mean mean
sea ice cover	 satellite passive microwave radiometry 	NSIDC (bootstrap)	Arcitc, SO	1992 - 2011	daily
Wind stress	QuickScat	NASA (Bourassa)SCOW (Risien & Chelton)	global	1999 – 2009 climatolggy	daily monthly
Tide gauge SSH	Tide gauges	NBDC/NOAA	sparse	1992 - 2006	monthly
Flux constraints	from ERA-Interim, JRA-25, NCEP, CORE-2 variances	Various	global	1992 - 2011	2-day to 14-day
Balance constraints			global	1992 - 2011	mean
bathymetry		Smith & Sandwell, ETOPO5	global	-	-



In the ECCO configuration, the state vector is of dimension approximately 6.7 million at each time step (restart information at one time step is 20 million values).

Taking 1 hour time steps over 15 years, one has approximately 10^{12} physical state vector elements. Control vector has order 200 million elements over 15 years. Number of observational constraints is about 300 million (10⁸). If include the meteorological variables, there are several billion observations.

In the ECCO2 configuration (1/6 degree spatially), the state vector dimensionality is much greater and hence the optimization is far more approximate.

We stressed the largest computers at NCAR, GFDL, NASA, US Navy,...



Meridional Heat Transport---Global Integrals



C. Wunsch / Dynamics of Atmospheres and Oceans xxx (2009) xxx-xxx



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Fig. 8. U_{20} (SV) in each month across subsection 2B (upper panel). Dashed line is the running annual mean and dotted horizonta line is the temporal mean. U_{2A} (dashed) and the total, U_2 are shown in the lower panel, U_2 is almost identical to U_1 in Fig. 9 Vertical line denotes the time of the Niño3 index maximum, and the INSTANT interval is shown by the arrows.

1 .

Fig. 4. Temperature (-C) at 118 m in the model in January 1992 showing the topography of the passages and the meridional sections used here. Section 1, at the western boundary, is not sub-divided; Section 2 is divided into 3 parts, with 28 being the sum of 28 and 20. Subsections 38 and 48 are not discussed here.

Stammer, Ueyoshi, Köhl, Large, Josey, Wunsch, 2004.



Change in control vector (wind stress) as a result of optimization.

Figure 9. Mean (a) surface zonal wind stress and (b) meridional wind stress fields as they result from the optimization over the period 1992 through 2001 (in N/m²). (c) Mean changes in ECCO meridional wind stress relative to the prior NCEP fields estimated over the six-year period 1992–2001 (in N/m²), and (d) for the meridional component (in N/m²). (e) Mean difference in ERS zonal wind stress from 1992 through 1997 minus net NCEP surface heat fluxes from the same period. (f) The same as Figure 9e, but for the meridional stress. Positive values are eastward and northward, for zonal and meridional components, respectively. The white lines in the lower two rows of the figure are the zero contour.



G. Gebbie, 2003 Resolved eddy field, open boundaries, constrained Subduction Experiment Area.





Snapshot 1 June 1993



SOSE misfits



SOSE vertically integrated mass flux.

Southern Ocean State Estimate (SOSE), Mazloff et al., JPO, 2010. 1/6 degree horizontal resolution. Open boundary to north.



Many other applications:

McGillicudy, et al. Time evolving nutrient fields are a consequence both of the physics and the complex biogeochemical interactions. Very short and very long time scales



Figure 4. Snapshots of (a) potential density, (b) nitrate, (c) nitrate anomaly, and (d) new production extracted from Figure 3 in a subdomain of the Sargasso Sea. Nitrate anomaly is defined as the difference between simulated nitrate and the nitrate field computed from the simulated density field and the climatological nitrate-density relationship (to which the nitrate field is relaxed below the euphotic zone).

From M. Follows, S. Dutkiewicz, 2006 Total phytoplankton biomass (micromoles nitrogen) monthly for a climatological year of ECCO-GODAE v2.177



(Dutkiewicz et al., 2008

Future Issues:

Major issues of affordability, including CPU time and storage. For some purposes, exact derivatives (adjoints)are not required Can the "semi-automatic" AD tools be made more nearly fully automatic? An "open source" AD exists (openAD, NSF funded), but requires users to make it practical.

Biggest issue---useful error estimates. Formally, we know precisely what to do: In a linearized system the filtersmoother operation produces explicit uncertainty covariance matrices. But:

If there are N elements in the state vector (typically $N\sim10^8$), must run the model 2N+2 times at every time step (!).

Monte Carlo ensembles (how big does the ensemble need to be? How does one generate it so as to span the uncertainty space? Rarely discussed beyond just doing something.)

Solve the Fokker-Planck equations for the probability density. Dimension?

Inverse Hessian (second derivatives from AD) map formally on to covariance calculations

See papers by A. Majda and others....

Need:

Coupled "smoothed"/interpolated systems: ocean, ice, atmosphere: quantities such as ocean surface salinities or heat content provide the best available constraints on atmospheric behavior. *Not* a forecasting problem.

Proper use of coupled systems is beyond the capability of a small academic group: the MIT ECCO effort, including model and method development, data flow and quality control, calculation, and scientific analysis, is fewer than about 8 full-time people, and includes students and postdocs. Supported in 3-year increments, mainly by NASA. Not sustainable in the long-term.

Who will step forward?

"When are oceanographers going to start using the sophisticated DA methods developed by meteorologists?"

Said to me and colleagues, repeatedly, at DA meetings. Has led to some furious responses.

"When are meteorologists going to use more appropriate methods for determining the climate state?" Thank you.