Innovation, increments, and residuals: Definitions and examples

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Outline

1. Why should we / do we care?

2. How does “(re-)analysis” really work?

3. Conclusions

Balance the global (momentum, enthalpy, freshwater) budget !

Goal: use closed heat budgets to understand causes heat anomalies

Term-by-term budget analysis of origin of heat content anomalies through time:

$$\underbrace{\int_0^t \frac{H_t}{\rho_o C_p V}\, dt}_{\equiv(T-T_o)} = \underbrace{\int_0^t \frac{C_{adv}}{\rho_o C_p V}\, dt}_{\equiv T_{adv}} + \underbrace{\int_0^t \frac{C_{diff}}{\rho_o C_p V}\, dt}_{\equiv T_{diff}} + \underbrace{\int_0^t \frac{Q_{net}}{\rho_o C_p V}\, dt}_{\equiv T_Q}$$

Example: decomposition of advective term:

$$C_{adv} = -\rho_o C_p \int_{-D}^{\eta} \boldsymbol{\nabla}\cdot(\overline{\boldsymbol{u}T} + \overline{\boldsymbol{u}^* T})\, dz = \underbrace{-\rho_o C_p \int_{-D}^{\eta} \boldsymbol{\nabla}\cdot(\overline{\boldsymbol{u}}\overline{T})\, dz}_{\equiv C_{lin}} \underbrace{-\rho_o C_p \int_{-D}^{\eta} \boldsymbol{\nabla}\cdot(\overline{\boldsymbol{u}'T'} + \overline{\boldsymbol{u}^* T})\, dz}_{\equiv C_{bol}},$$

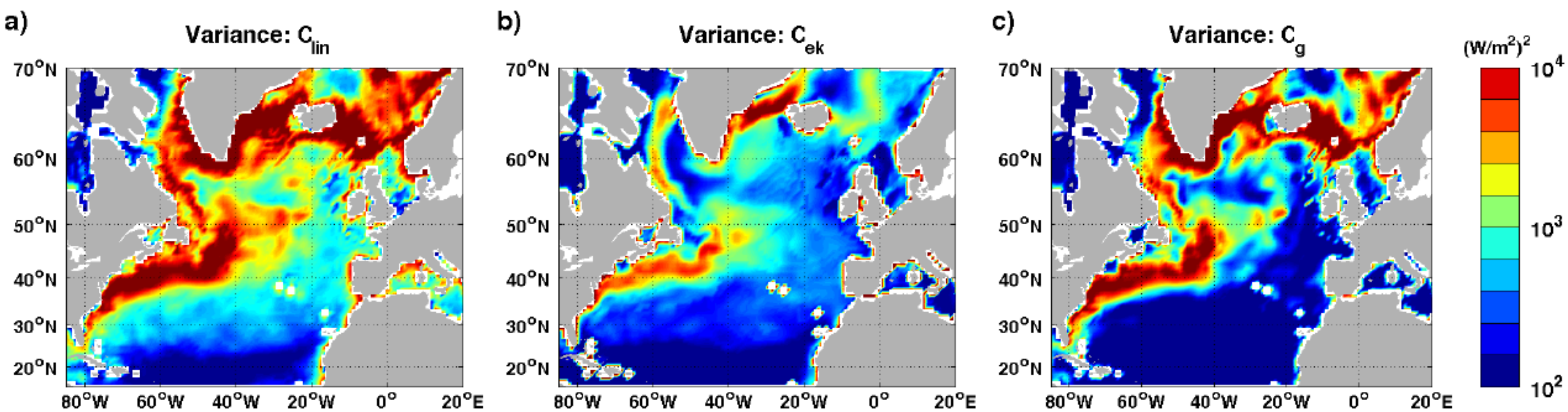
Buckley et al. (2013)

Goal: use closed heat budgets to understand causes heat anomalies

Another example:
decomposition of Ekman and geostrophic components:

$$C_{ek}(\mathbf{u}_{\mathbf{ek}}, w_{ek}, \theta) = C_{ek}(\bar{\mathbf{u}}_{\mathbf{ek}}, \overline{w}_{ek}, \bar{\theta}) + \underbrace{C_{ek}(\mathbf{u}_{\mathbf{ek}}{}', w'_{ek}, \bar{\theta})}_{C^{v}_{ek}} + \underbrace{C_{ek}(\bar{\mathbf{u}}_{\mathbf{ek}}, \overline{w}_{ek}, \theta')}_{C^{T}_{ek}} + \underbrace{C_{ek}(\mathbf{u}'_{\mathbf{ek}}, w'_{ek}, \theta')}_{C^{vT}_{ek}}$$

$$C_{g}(\mathbf{u}_{\mathbf{g}}, w_{g}, \theta) = C_{g}(\bar{\mathbf{u}}_{\mathbf{g}}, \overline{w}_{g}, \bar{\theta}) + v\, \underbrace{C_{g}(\mathbf{u}'_{\mathbf{g}}, w'_{g}, \bar{\theta})}_{C^{v}_{g}} + \underbrace{C_{g}(\bar{\mathbf{u}}_{\mathbf{g}}, \overline{w}_{g}, \theta')}_{C^{T}_{g}} + \underbrace{C_{g}(\mathbf{u}'_{\mathbf{g}}, w'_{g}, \theta')}_{C^{vT}_{g}}$$



Buckley et al. (subm.)

Need adequate model output

Basic principles for sampling model simulation

Maintain high degree of integrity of output

E.g.:

Products of time-dependent fields should be time averaged as a product, using all model time steps to build the average

Griffies et al. (2009)

INTERNATIONAL COUNCIL FOR SCIENCE

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WORLD CLIMATE RESEARCH PROGRAMME

Sampling Physical Ocean Field in WCRP CMIP5 Simulations: CLIVAR Working Group on Ocean Model Development (WGOMD) Committee on CMIP5 Ocean Model Output

February 2009

ICPO Publication Series No.137

WCRP Informal Report No. 3/2009

Combining the knowledge reservoirs: "data assimilation", "reanalysis"

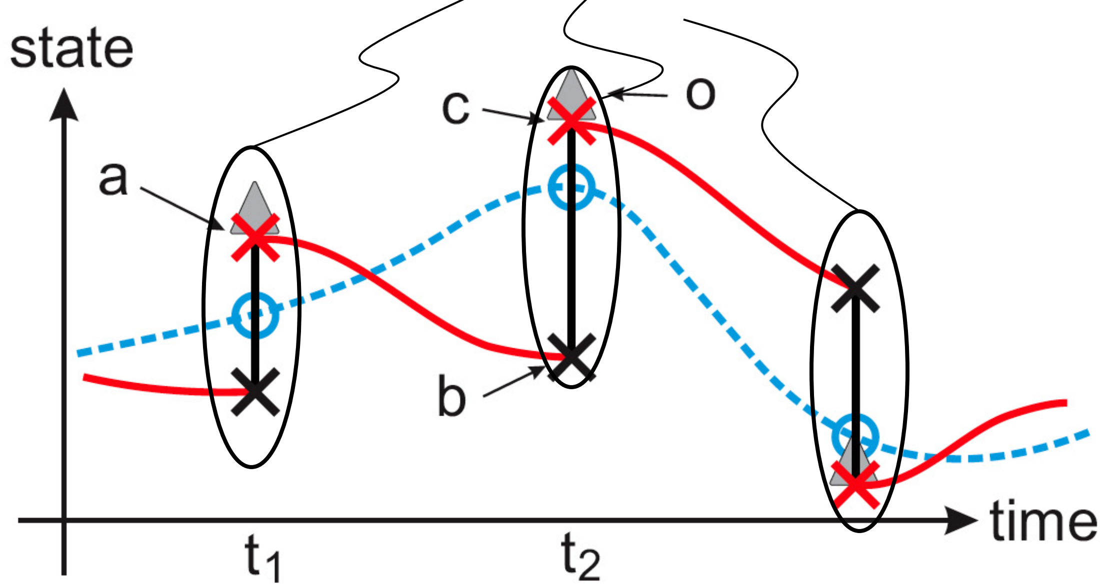
The *estimation (interpolation)* vs. *forecasting (extrapolation)* problem

- **Atmosphere**
  - Relatively abundant data sampling of the 3-dim. atmosphere
  - Most DA applications target optimal forecasting
  - ➔ find initial conditions which produce best possible forecast;
  - ➔ *dynamical consistency or property conservation *NOT* required*
- **Ocean**
  - Very sparse data sampling of the 3-dim. ocean
  - Understanding past & present state of the ocean is a major issue all by itself, the forecasting dependent upon it

"jumps" are unphysical

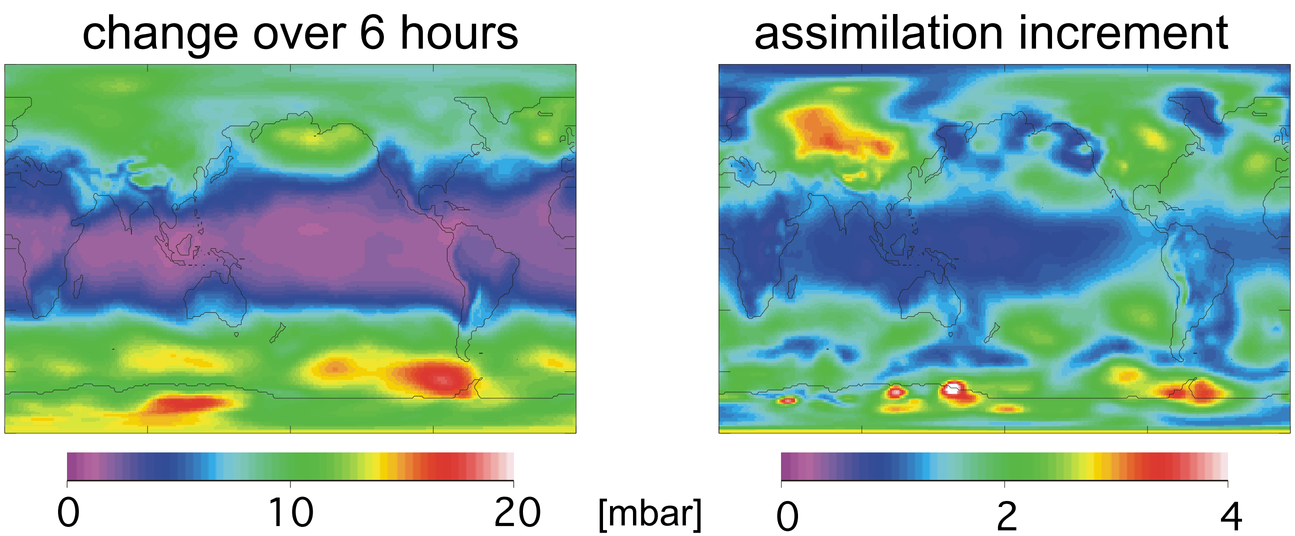
➔ use observations in an optimal way to extract max. information

➔ *dynamic consistency & property conservation *ESSENTIAL** for climate



Dynamical consistency: why does it matter:

(Large) imbalances in air-sea fluxes from atmospheric re-analysis products



Standard deviation of NCEP surface pressure shows that, on average, 24% of its mass change is physically unaccounted for.

reanalysis product	net fresh water imbalance [mm/year] "+" for ocean volume increase		net heat flux imbalance [W/m²] "+" for ocean cooling	
	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		

Problem statement & definitions

The **state & parameter estimation problem** statement

$$
\begin{aligned}
J =& \sum_{m=0}^{M} \Big[y(t) - \mathbf{E}\tilde{x}(t) \Big]^T \mathbf{R}^{-1}(t) \Big[y(t) - \mathbf{E}\tilde{x}(t) \Big] \\
&+ \sum_{m=0}^{M-1} \tilde{u}(t)^T \mathbf{Q}^{-1} \tilde{u}(t), \qquad t = m\,\Delta t
\end{aligned}
$$

differs from the **data assimilation problem**, as stated in NWP (a.k.a. **analysis** or **re-analysis**):

$$
\begin{aligned}
J_1 =& \Big[\tilde{x}(t_{now}) - \tilde{x}(t_{now}, -) \Big]^T \mathbf{P}^{-1}(t_{now}, -) \Big[\tilde{x}(t_{now}) - \tilde{x}(t_{now}, -) \Big] \\
&+ \Big[y(t_{now}) - \mathbf{E}(t_{now}) x(t_{now}) \Big]^T \mathbf{R}^{-1}(t_{now}) \Big[y(t_{now}) - \mathbf{E}(t_{now}) x(t_{now}) \Big]
\end{aligned}
$$

Problem statement & definitions

- Prior or background state estimate $\tilde{x}(t_{now}, -)$ obtained by running (in forecast mode) model over time τ
- New information/observations $y(t_{now})$ arrive at timt t_{now}

$$\mathbf{E}(t_{now})\, x(t_{now}) \,+\, n(t_{now}) \,=\, y(t_{now}),$$

$E(t_{now})$ observation matrix,
$n(t_{now})$ observation/representation error ("noise")

Obtain best linear unbiased estimator (BLUE), called **the analysis** (e.g., Kalman Filter, Optimal Interpolation):

$$\tilde{x}(t_{now}) \,=\, \tilde{x}(t_{now}, -) + \mathbf{P}^b \mathbf{H}^T \left[\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R}\right]^{-1} \Big(y(t_{now}) - \mathbf{E}x(t_{now}, -)\Big)$$

Problem statement & definitions

$$\tilde{x}(t_{now}) = \tilde{x}(t_{now}, -) + \mathbf{P}^b \mathbf{H}^T \left[\mathbf{H} \mathbf{P}^b \mathbf{H}^T + \mathbf{R} \right]^{-1} \Big(y(t_{now}) - \mathbf{E}\, x(t_{now}, -) \Big)$$
$$= \tilde{x}(t_{now}, -) + \mathbf{K} \cdot \Big(y(t_{now}) - \mathbf{E}\, x(t_{now}, -) \Big)$$

- K: **gain matrix**
- $\tilde{y}(t_{now}) = y(t_{now}) - \mathbf{E}\, x(t_{now}, -)$: **innovation vector** or **residuals**: new information contained in the observations

Interpretation:
Gain matrix **K** *weighs* the innovation vector $\tilde{y}(t_{now})$
according to observational & prior uncertainties
to produce the analysis $\tilde{x}(t_{now})$

Problem statement & definitions

For example (limiting cases):

- large obs. error $\longrightarrow$ small weights $\longrightarrow \tilde{x}(t_{now}) \approx x(t_{now}, -)$
- small obs. error $\longrightarrow$ large weights $\longrightarrow \tilde{x}(t_{now}) \neq x(t_{now}, -)$

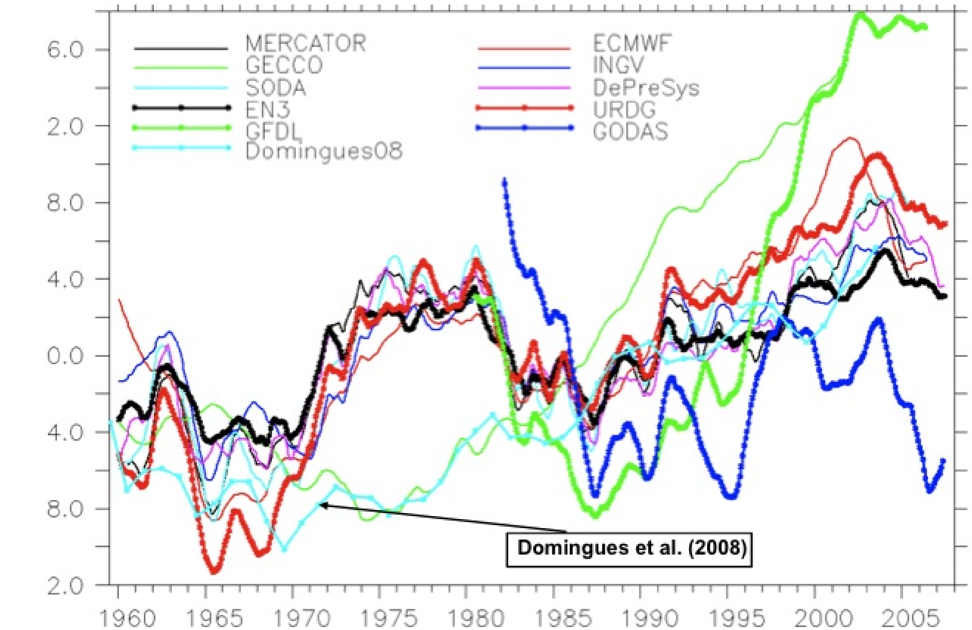
Key point to understand: The analysis step

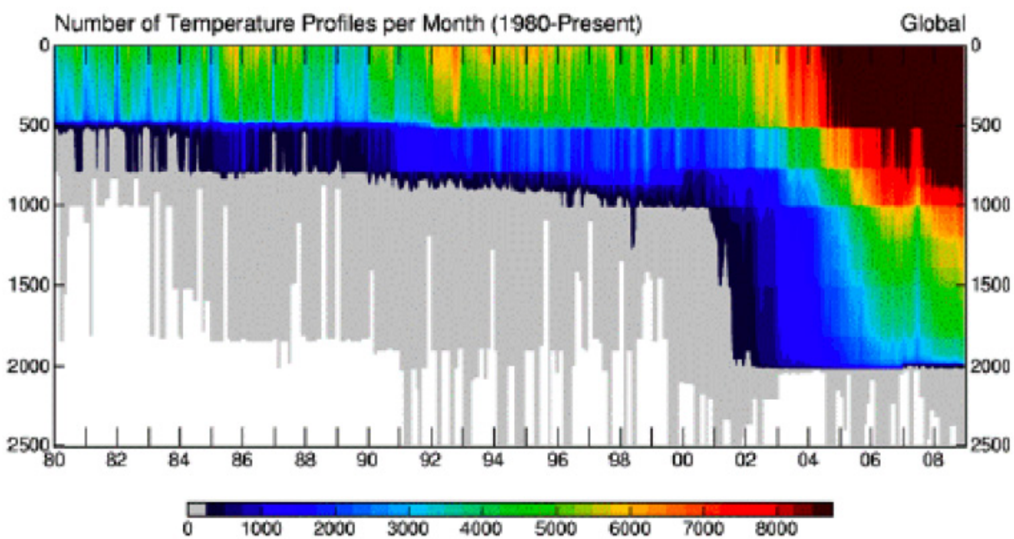
$$x(t_{now}, -) \quad \longrightarrow \quad x(t_{now}) = x(t_{now}, -) + \mathbf{K} \cdot \Big(y - \mathbf{E}\, x \Big)$$

violates the conservation equations for tracers and momentum!

Challenges (e.g. summarized in several OceanObs' 09 whitepapers)

Comparison of different multi-decadal "re-analyses" (CLIVAR/GSOP)



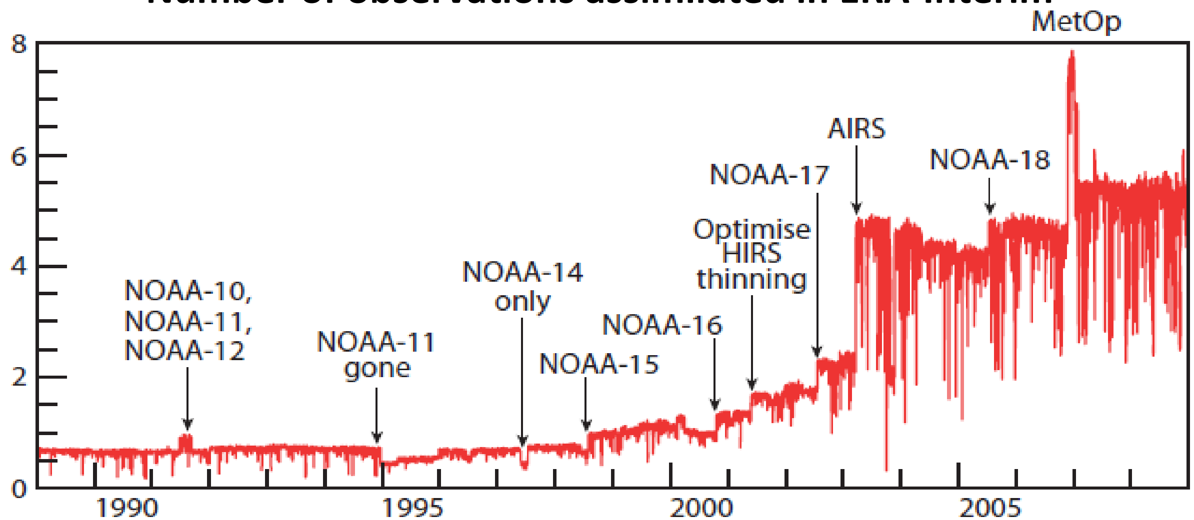


- Convergence of estimates with increasing number of observations?
- If not, why not?
- Consequences for attempt to understand circulation changes…
- Narrowing of transport uncertainties to "*useful*" numbers remains hard

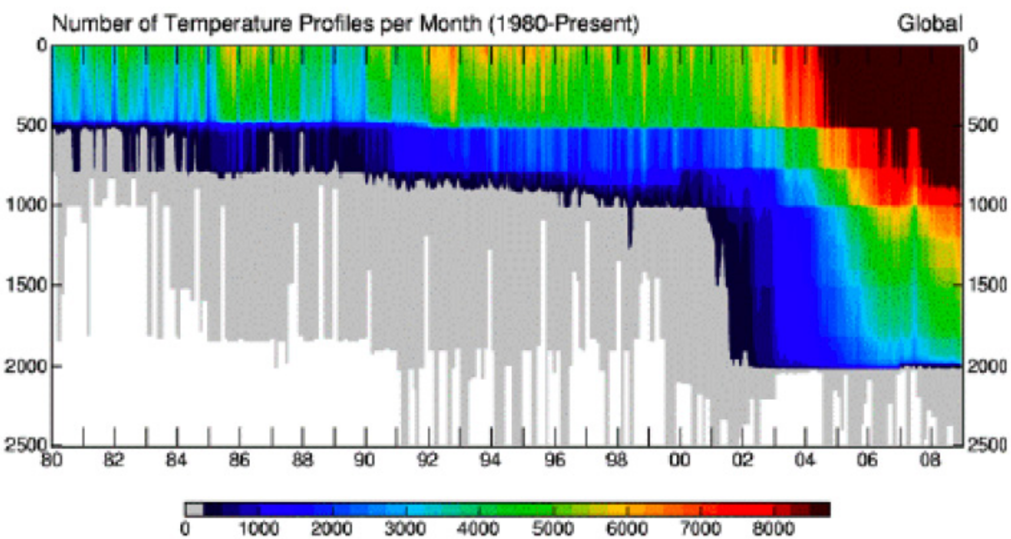
Recent(!) changes in the atmosphere and ocean observing systems

An important issue is that changes in the global observing system aren't just a thing of the past (pre-1980s), but remain relevant today.

Number of observations assimilated in ERA-Interim



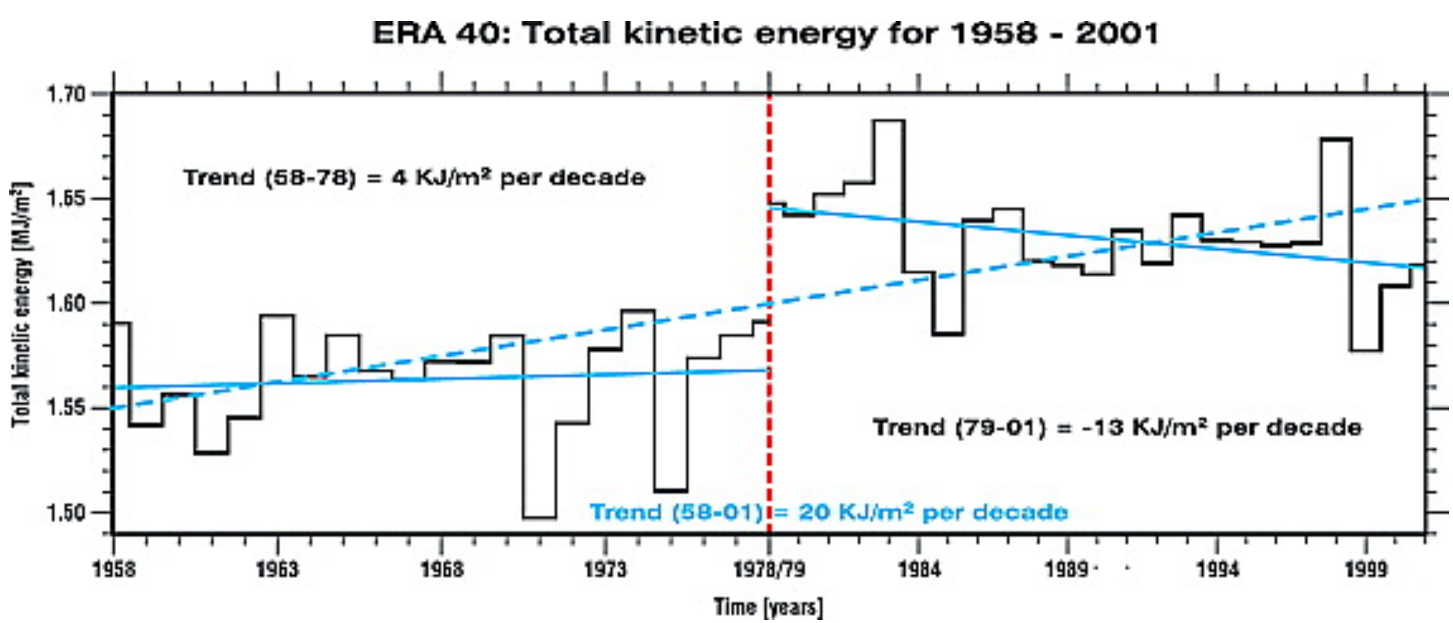
[Dee et al., 2009, *ECMWF Newsletter* (119)]



Lessons from atmospheric reanalysis:
"Can climate trends be calculated from reanalysis data?"

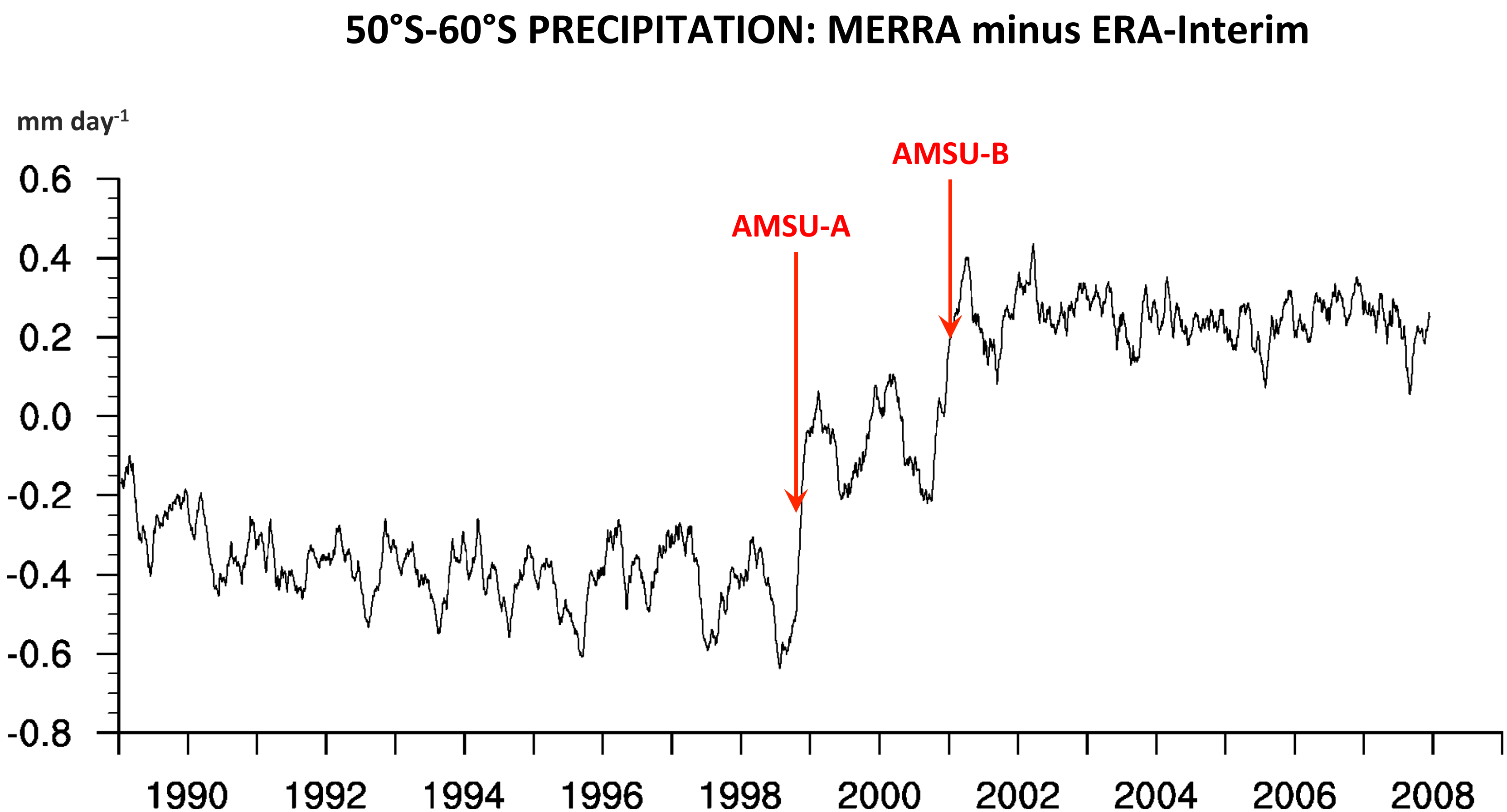
- Large warming trend in ERA40 an artifact of large changes in observational coverage at the end of the 1970s
- Large uncertainty in the calculation of trends from present reanalyses
- Present observing system was set up to support weather forecasting, not directly suitable for climate monitoring
- Systematic errors in the assimilating models add complications
- Limited resources currently devoted to address these problems!!

Why should the ocean estimation problem be any different?



Bengtsson et al. (2004)

Spurious trends in MERRA precipitation

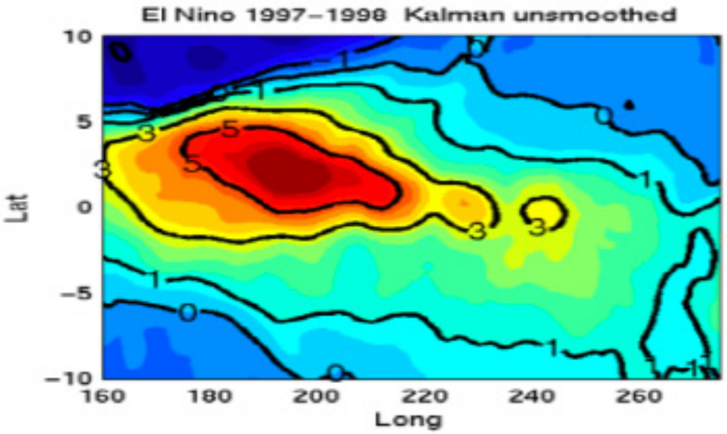


2-month running average difference between forecast daily precipitation from MERRA and from ERA-Interim, spatially averaged over the 50°S-60°S latitude band.

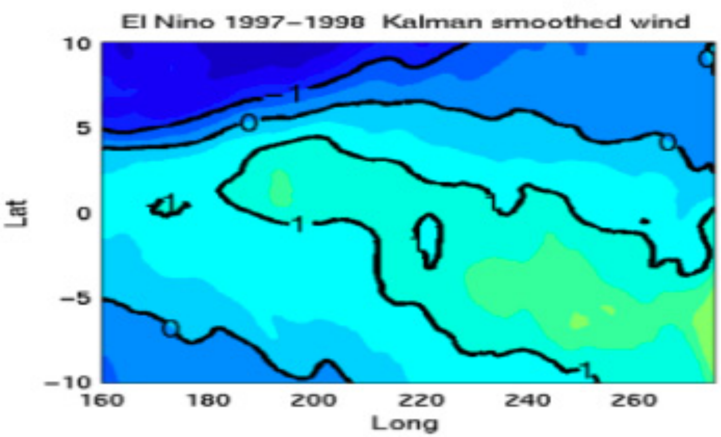
Dynamical consistency: why does it matter:

Driving offline tracer simulations (e.g. CO_2)

Filtered estimate of CO_2 flux during 97-98 El Niño (mol/m^2/yr)

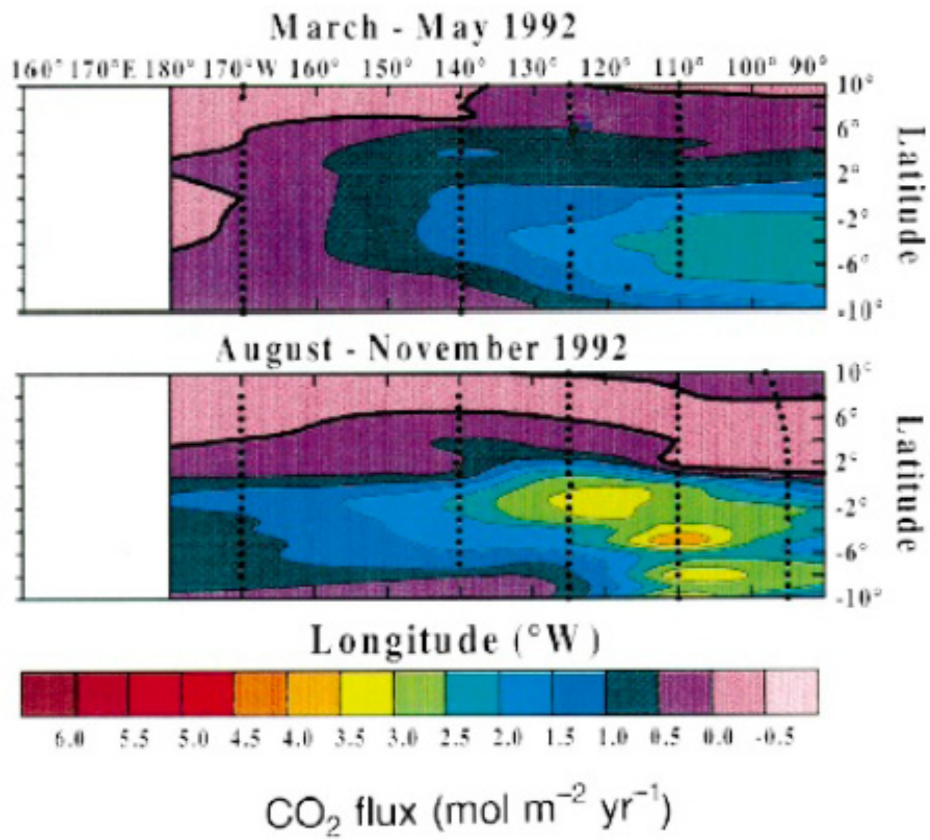


Smoothed estimate of CO_2 flux



McKinley, 2002

Observed estimate of CO_2 flux during 92-93 El Niño



Feely et al., 1999

Conclusions

- *sequential/filtering* methods solve not the same problem as *estimation/smoother* methods
  - break dynamical consistency
  - tracer conservation no longer fulfilled
  - NWP is not the same thing as "reconstruction"

- for climate science applications need to account for and understand the analysis increments

- if needed, at a minimum make analysis step / innovation vector part of the basic diagnostics and budget calculations
  - also has value to diagnose systematic model deficiencies