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Data Assimilation: An Outlook

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Joint work (recently) with
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Outline

- Data in meteorology, oceanography and space physics
  - *in situ* & remotely sensed
- Basic ideas, data types, & issues
  - how to combine data with models
  - transfer of information
    – between variables & regions
  - filters & smoothers
  - stability of the forecast-assimilation cycle
- Parameter estimation
  - model parameters
  - noise parameters – at & below grid scale
- Novel areas of application
  - space physics
  - shock waves in solids
  - macroeconomics
  - paleoclimate
  - DADA
- Concluding remarks and bibliography
  - where we came from
  - where we're going

Main issues

- The solid earth stays put to be observed, the atmosphere, the oceans, & many other things, do not.
- Two types of information:
  - direct → observations, and
  - indirect → dynamics (from past observations);

  both have errors.
- Combine the two in (an) optimal way(s)
- Advanced data assimilation methods provide such ways:
  - sequential estimation → the Kalman filter(s), particle filters, and
  - control theory → the variational & adjoint method(s)
- The two types of methods are essentially equivalent for simple linear systems (the duality principle)

Main issues (continued)

- The two types of methods are essentially equivalent for simple linear systems (the duality principle)
- Their performance differs for large nonlinear systems in:
  - accuracy, and
  - computational efficiency
- Study optimal combination(s), as well as improvements over currently operational methods (OI, 4-D Var, PSAS, EnKF).

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Atmospheric data

Drifting buoys: P_s – 267

Cloud-drift: V – 2x2259

Aircraft: V – 2x1100

Ship & land surface: P_s, T_s, V_s – 4x3446

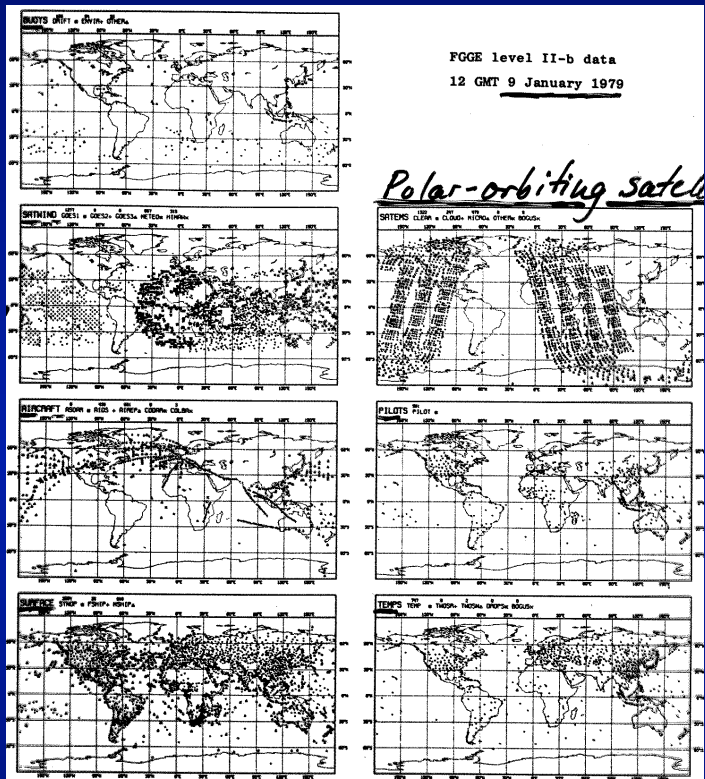


Fig. 1 An example of the different observing systems in use during the Global Weather Experiment.

Abbreviations used:

Aireps	Standard wind observations from aircraft
Asdars, Aids	High quality wind observations from aircraft
Buoys	Surface pressure observations from drifting buoys
Colba	Constant level balloons
Drops	Radiosondes dropped from aircraft
Pilots	Wind measurements from ascending balloons
Satems	Temperature measurements from polar orbiting satellites
Satwind	Cloud drift wind measurements from geostationary satellites
Ships	Surface observations from ships
Synops	Surface observations from land
Temps	Temperature, humidity and wind measurements from radiosondes

Bengtsson, Ghil & Källén (eds.): *Dynamic Meteorology, Data Assimilation Methods* (1981)

Polar orbiting satellites: T – 5x2048

Balloons : V – 2x581x10

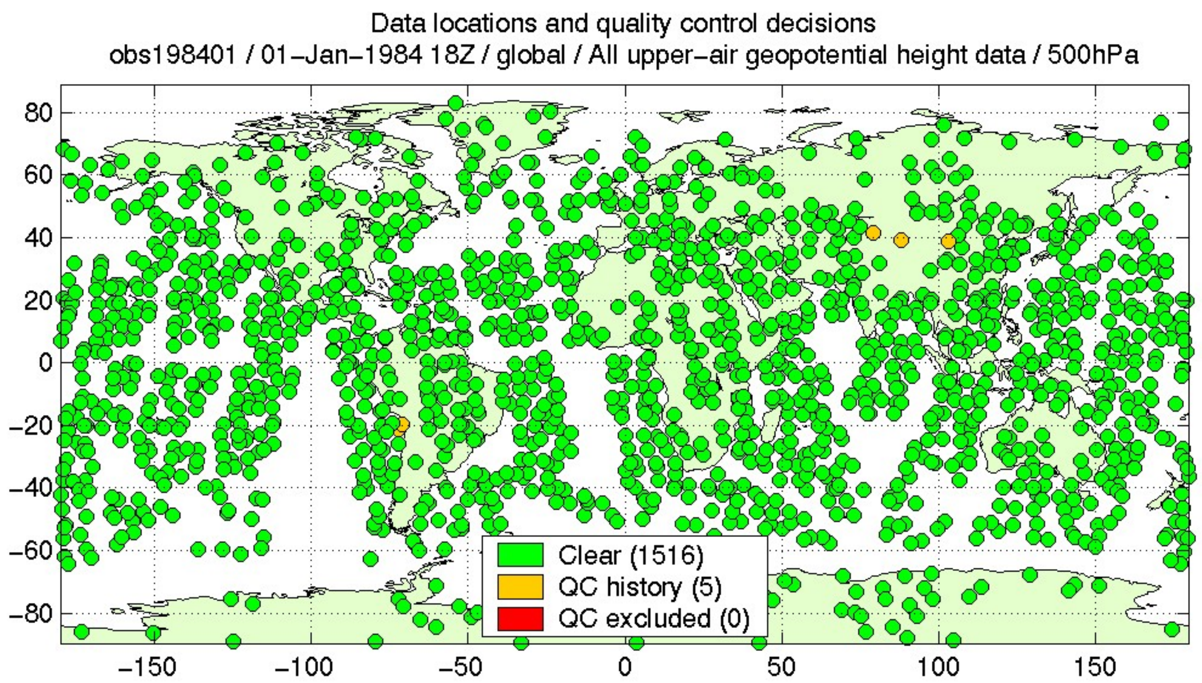
Radiosondes : T, V - 3x749x10

Total no. of observations = 0(10^5) scalars per 12h–24h

⁂ 0(10^2) observations/[(significant *d-o-f*) x (significant Δt)]

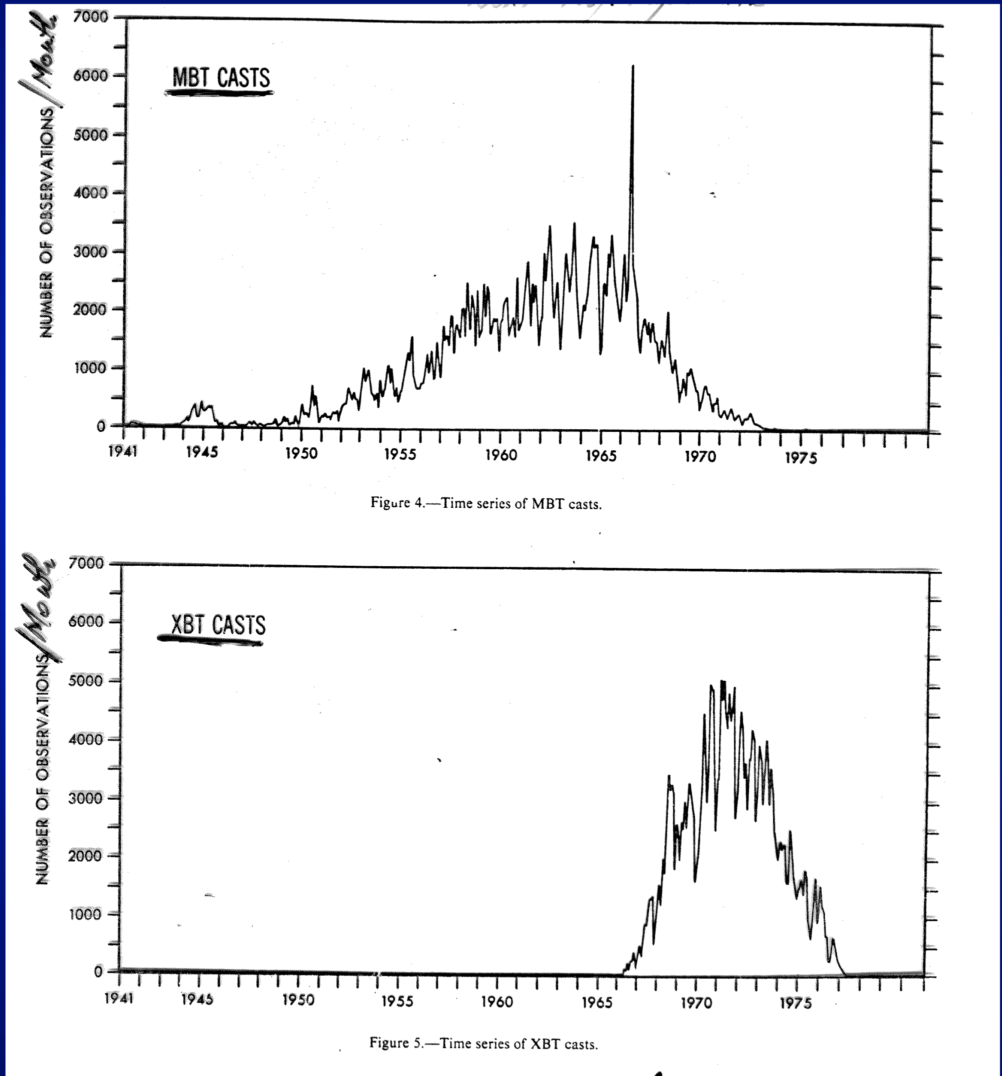
Nowadays 0(10^7) obs. & more d-o-f of interest, too!

Observational network



Quality control – preliminary & as part of the assimilation cycle

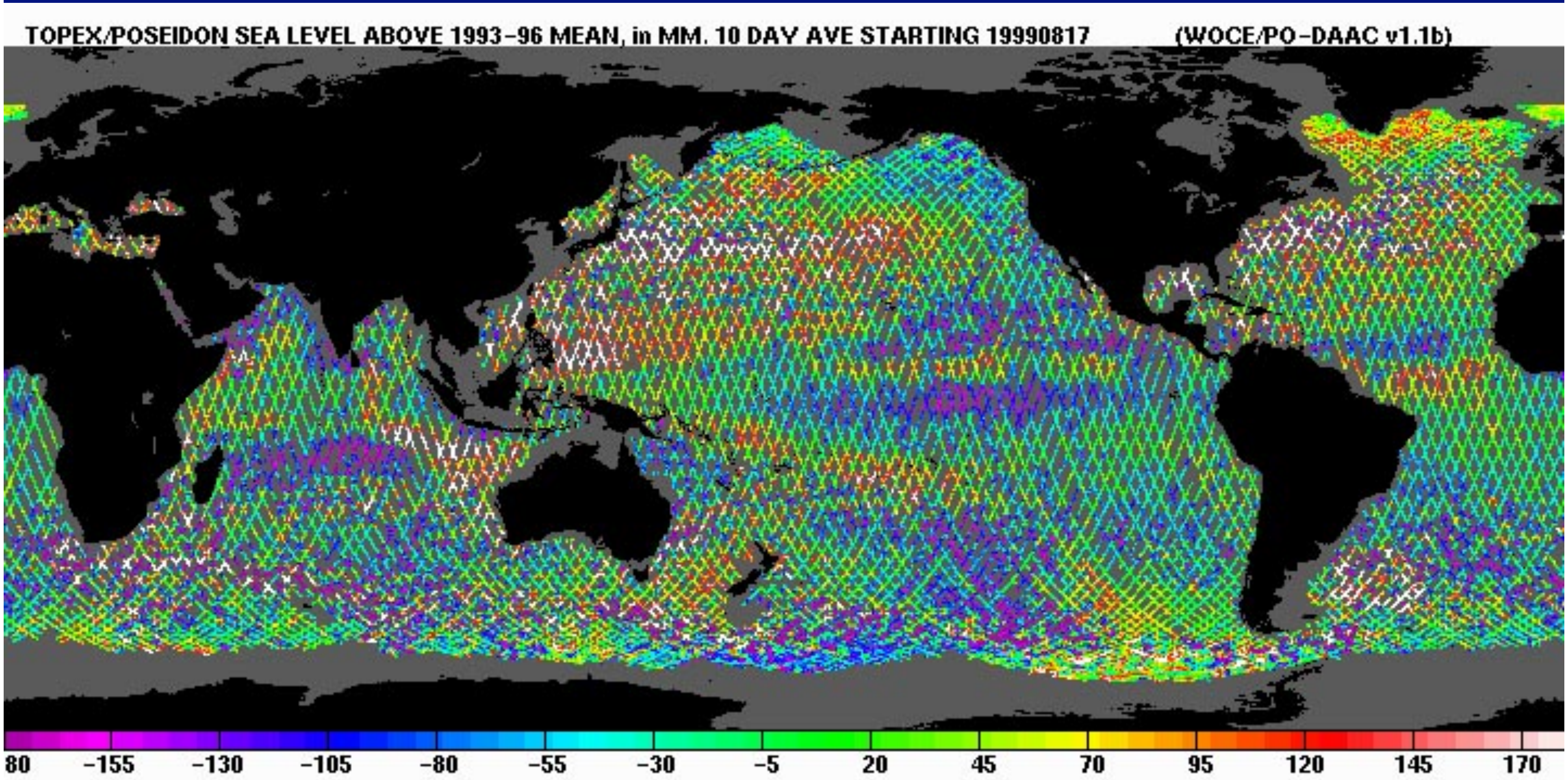
Ocean data – past



Total no. of
(oceanographic observations)/
(meteorological observations)
= $O(10^{-4})$ for the past; &
= $O(10^{-1})$ for the future :
Syd Levitus (1982).

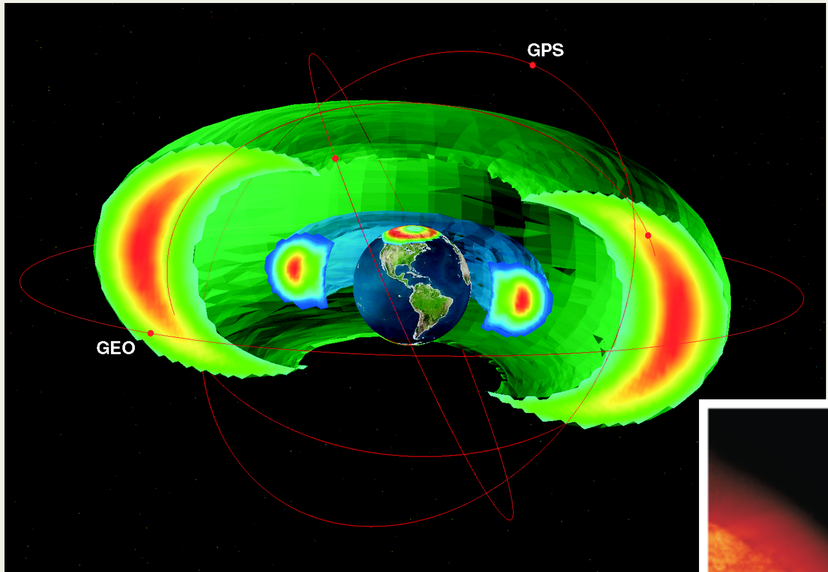
Ocean data – present & future

Altimetry ⇒ sea level; scatterometry ⇒ surface winds & sea state;
acoustic tomography ⇒ temperature & density; etc.



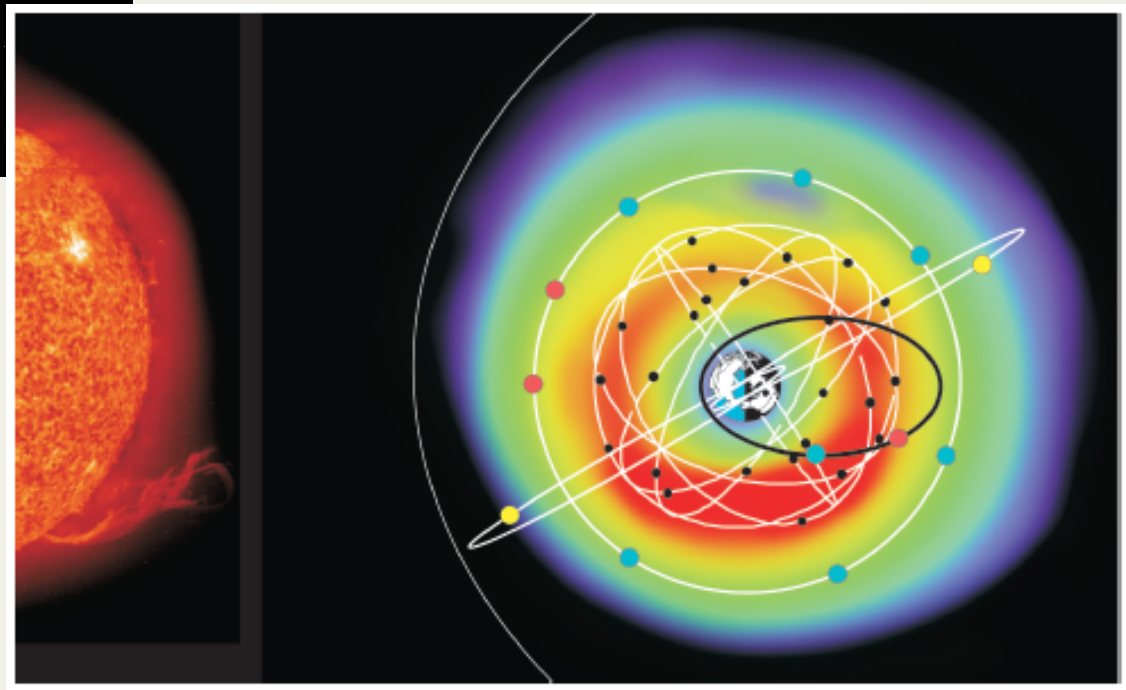
Courtesy of Tong ("Tony") Lee, JPL

Space physics data



Two decades ago …

… and now



Space platforms in Earth’s magnetosphere

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Basic ideas of data assimilation and sequential estimation - I

Simple illustration

We want to estimate
T – the temperature of this room, based on the readings
T_1 and T_2 of two thermometers,

by a linear estimate $\hat{T} = \alpha_1 T_1 + \alpha_2 T_2$

The interpretation will be:
$T_1 = T^f$ - **first guess** (of numerical forecast model)
$T_2 = T^o$ - **observation** (R/S, satellite, etc.)
$\hat{T} = T^a$ - **objective analysis**

Basic ideas of data assimilation and sequential estimation - II

If the observations T_1 and T_2 are unbiased, and we want $\hat{T}$ to be unbiased, then $\alpha_1 + \alpha_2 = 1$,

so one can write

$\hat{T} = T_1 + \alpha_2(T_2 - T_1)$: updating (sequential).

If T_1 and T_2 are uncorrelated, and have known standard deviations,

$A_1 = \sigma_1^{-2}$, $A_2 = \sigma_2^{-2}$,

then the minimum variance estimator[(*)] is

$$\hat{T} = T_1 + \frac{A_2}{A_1 + A_2}(T_2 - T_1),$$

and its accuracy is

$\hat{A} = (A_1 + A_2) \geq \max\{A_1, A_2\}$.

(*) BLUE = Best Linear Unbiased Estimator

(Extended) Kalman Filter (EKF)

True Evolution (deterministic + stochastic)

$$\mathbf{x}^t(t_{i+1}) = M_i[\mathbf{x}^t(t_i)] + \eta(t_i)$$
$$\mathbf{Q}_i\delta_{ij} \equiv \mathbb{E}(\eta_i\eta_j^T)$$

Observations

$$\mathbf{y}_i^0 = H_i[\mathbf{x}^t(t_i)] + \varepsilon_i$$
$$\mathbf{R}_i\delta_{ij} \equiv \mathbb{E}(\varepsilon_i\varepsilon_j^T)$$
$\mathbf{d} = \mathbf{y}_i^0 - H_i[\mathbf{x}^f(t_i)]$ - innovation vector

$$\Delta\mathbf{x}^{f,a} \equiv \mathbf{x}^{f,a} - \mathbf{x}^t$$
$$\mathbf{P}^{f,a} \equiv \mathbb{E}[(\Delta\mathbf{x}^{f,a})(\Delta\mathbf{x}^{f,a})^T]$$
$\mathrm{tr}\mathbf{P}^{f,a} =$ global error

Stage 1: Prediction (deterministic)

$$\mathbf{x}^f(t_i) = M_{i-1}[\mathbf{x}^a(t_{i-1})]$$
$$\mathbf{P}^f(t_i) = \mathbf{M}_{i-1}\mathbf{P}^a(t_{i-1})\mathbf{M}_{i-1}^T + \mathbf{Q}(t_{i-1})$$

Stage 2: Update (Probabilistic)

$$\mathbf{x}^a(t_i) = \mathbf{x}^f(t_i) + \mathbf{K}_i(\mathbf{y}_i^0 - H_i[\mathbf{x}^f(t_i)])$$
$$\mathbf{P}^a(t_i) = (\mathbf{I} - \mathbf{K}_i\mathbf{H}_i)\mathbf{P}^f(t_i)$$
$$\mathbf{K}_i = \mathbf{P}^f(t_i)\mathbf{H}_i^T[\mathbf{H}_i\mathbf{P}^f(t_i)\mathbf{H}_i^T + \mathbf{R}_i]^{-1}$$
subject to $\partial_{\mathbf{K}}\mathrm{tr}\mathbf{P}^a = 0$

$\mathbf{M}$ and $\mathbf{H}$ are the linearizations of M and H

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Basic concepts: barotropic model

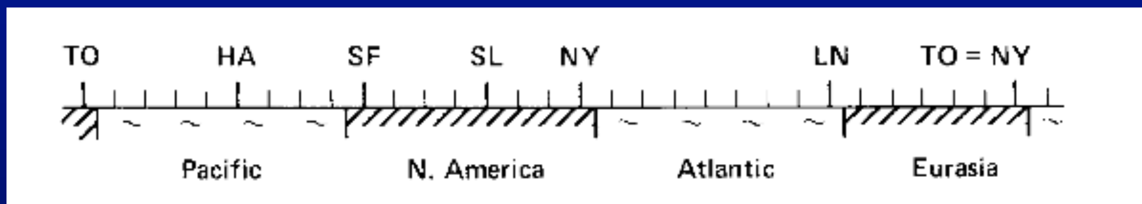
Shallow-water equations in 1-D, linearized about (U, 0, Φ), $fU = -\Phi_y$
U = 20 ms^{-1}, f = 10^{-4}s^{-1}, $\Phi = gH$, $H \approx$ 3 km.

$$u_t + Uu_x + \phi_x - fv = 0$$

$$v_t + Uv_x + fu = 0$$

$$\phi_t + U\phi_x + \Phi u_x - fUv = 0$$

PDE system discretized by finite differences, periodic B. C.
H$_k$: observations at synoptic times, over land only.



Ghil *et al*. (1981), Cohn & Dee (Ph.D. theses, 1982 & 1983), etc.

Conventional network

Relative weight of observational *vs.* model errors

$P_\infty = QR/[Q + (1 - \Psi^2)R]$

(a) $Q = 0 \Rightarrow P_\infty = 0$

(b) $Q \neq 0 \Rightarrow$ (i), (ii) and (iii):

(i) "good" observations

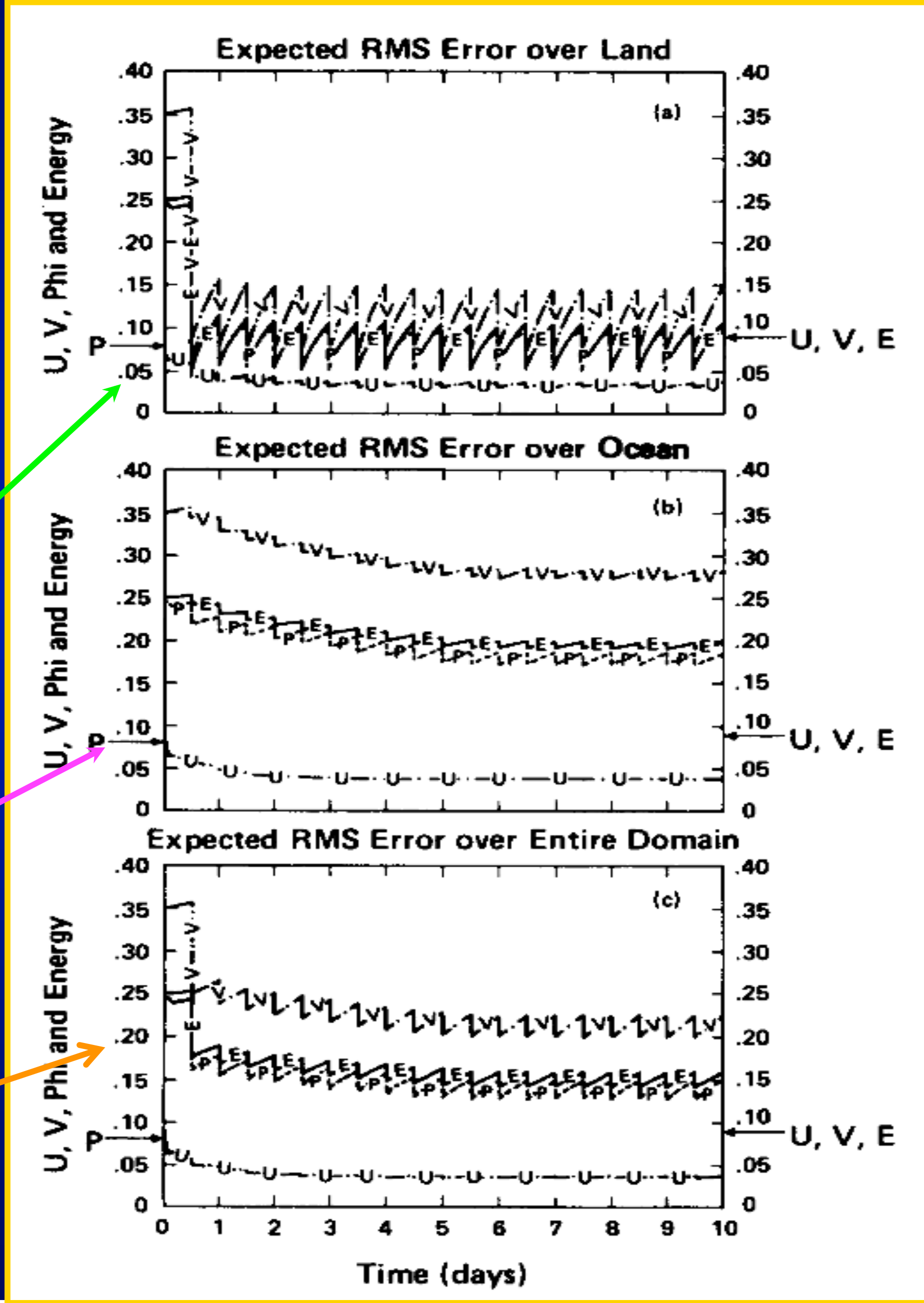
$R << Q \Rightarrow P_\infty \approx R$;

(ii) "poor" observations

$R >> Q \Rightarrow P_\infty \approx Q/(1 - \Psi^2)$;

(iii) always (provided $\Psi^2 < 1$)

$P_\infty \leq \min\{R, Q/(1 - \Psi^2)\}$.



Advection of information

Upper panel (NoSat):

Errors advected off the ocean

ϕ_{300}

Lower panel (Sat):

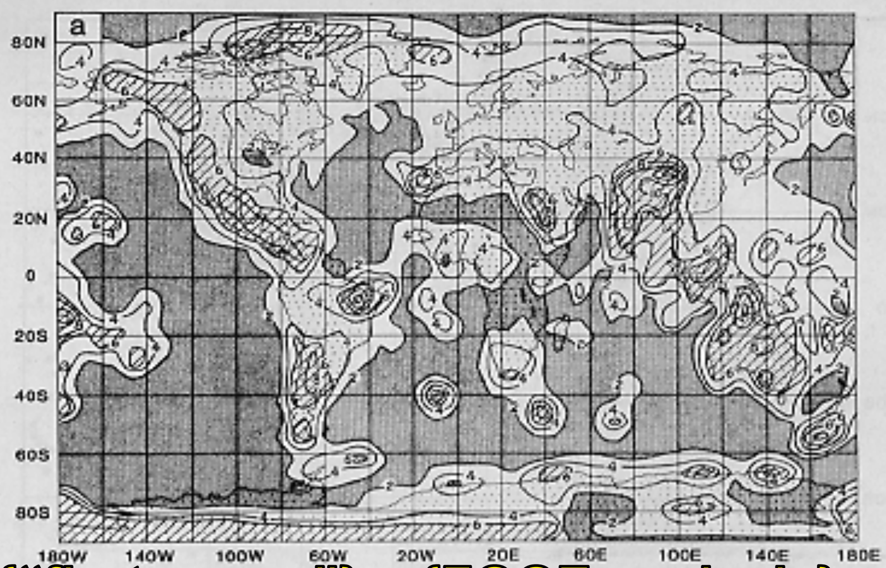
Errors drastically reduced, as info. now comes in, off the ocean

ϕ_{300}

Halem, Kalnay, Baker & Atlas

(*Bull. Amer. Meteorol. Soc.*, 1982)

{6h fcst} – {conventional (NoSat)}



{"first guess"} – {FGGE analysis}

FIG. 5. The rms difference between the 6 h forecast of the 300 mb geopotential height field and the analysis for the period 5–21 January 1979. Contour interval is 20 m. a) Rms difference between the NOSAT analysis and forecast. b) Rms difference between the FGGE analysis and forecast.

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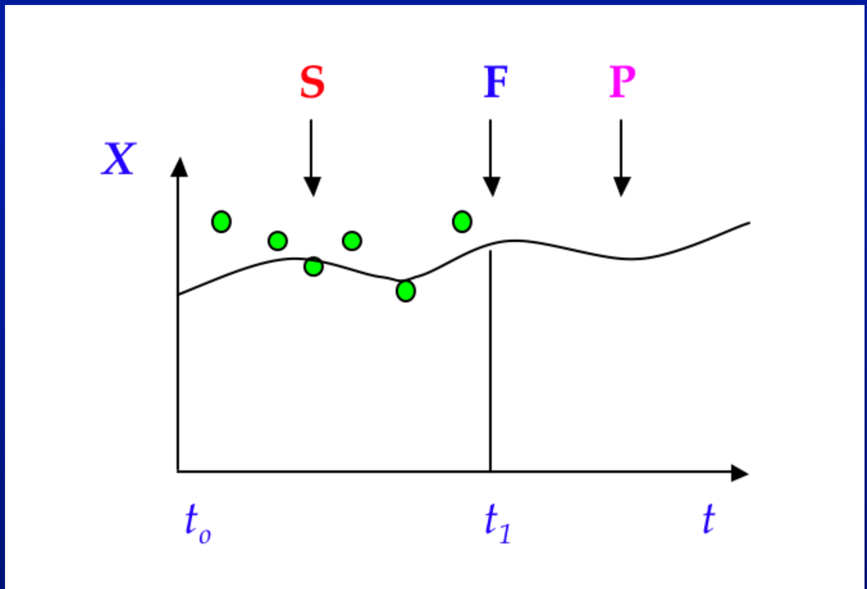
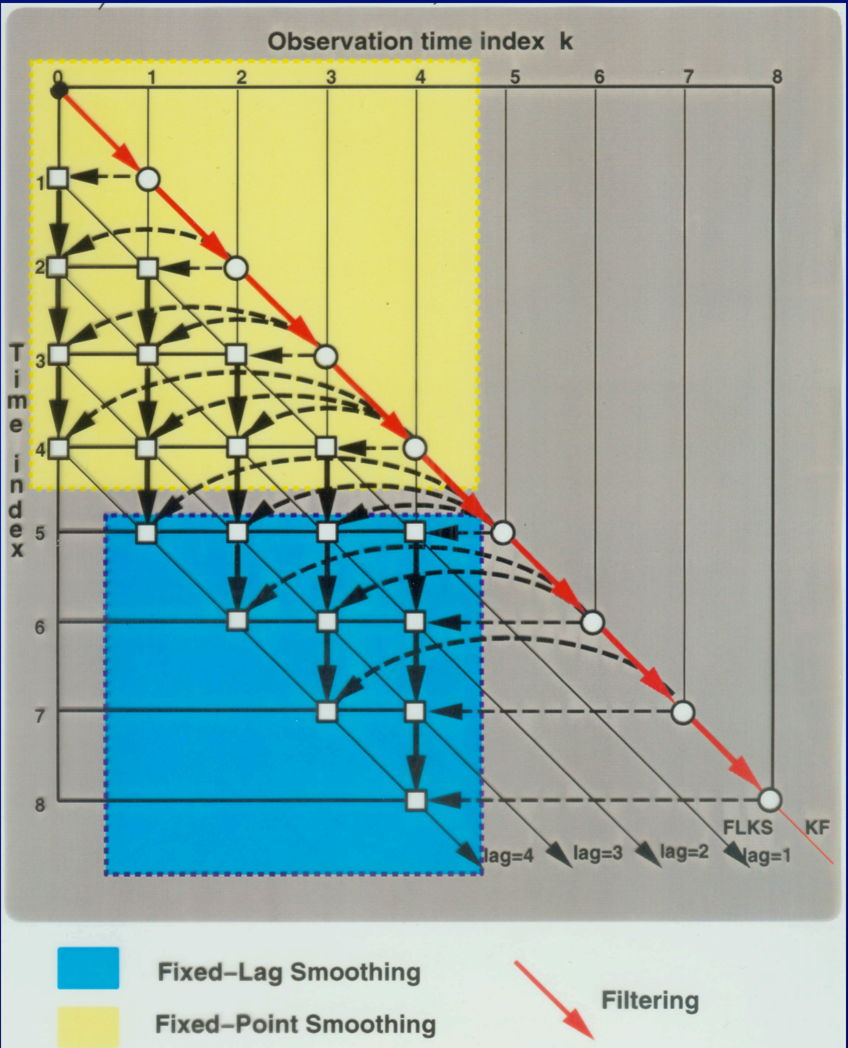
The main products of estimation(*)

- Filtering (F) – "video loops"
- Smoothing (S) – full-length feature "movies"
- Prediction (P) – NWP, ENSO



(*) N. Wiener (1949, MIT Press)

Kalman smoother



For a fixed interval, weak constrained 4-D Var is equivalent to the sequential ("Kalman") smoother.

Cohn, Sivakumaran & Todling (*MWR*, 1994)

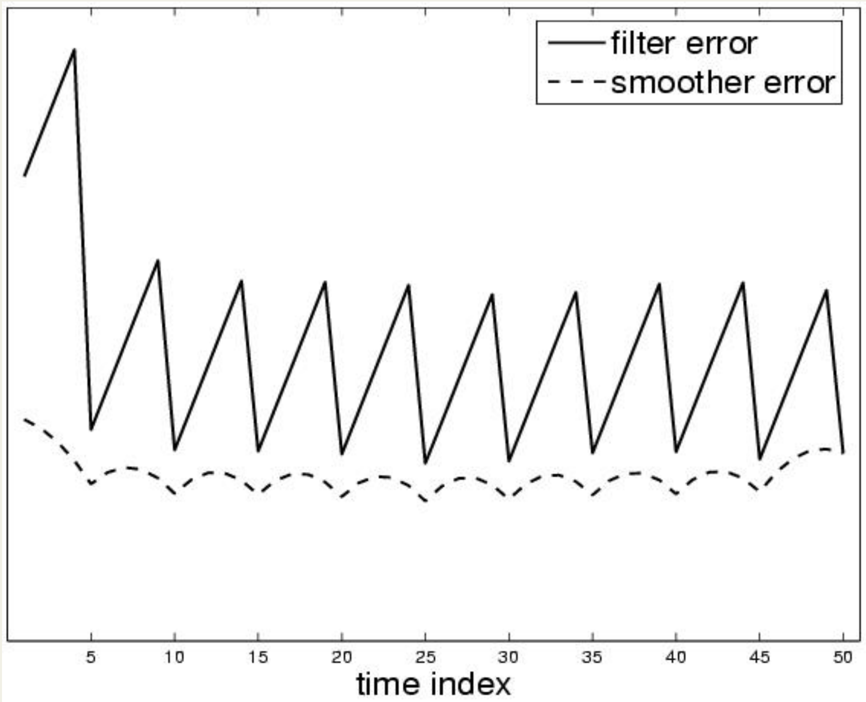
Smoothing *vs.* Filtering: The Backward Sequential Smoother (BSS)

- A "smoother" **is** smoother than a filter.
- But which smoother is - smoothest
  - cheapest
  - easiest to implement?

Ensemble Kalman Filter – EnKF (*)
Markov chain Monte Carlo – MCMC
Resampled Particle Filter – RPF

(*) to distinguish it from the
Extended Kalman Filter – EKF

T. M. Chin, M. J. Turmon, J. B. Jewell (JPL)
& M. Ghil (*MWR*, 2007)

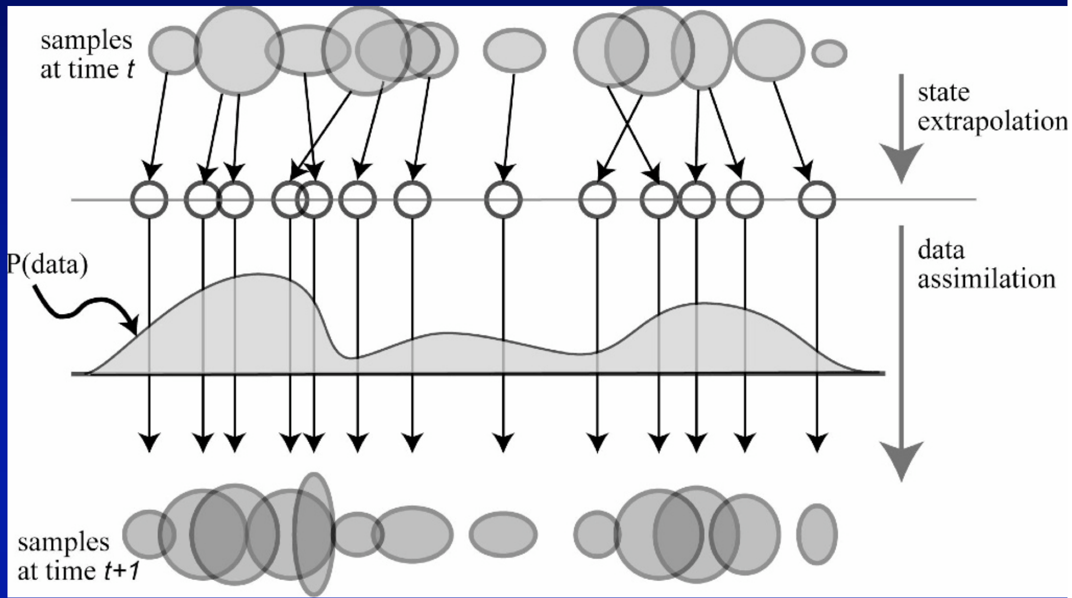


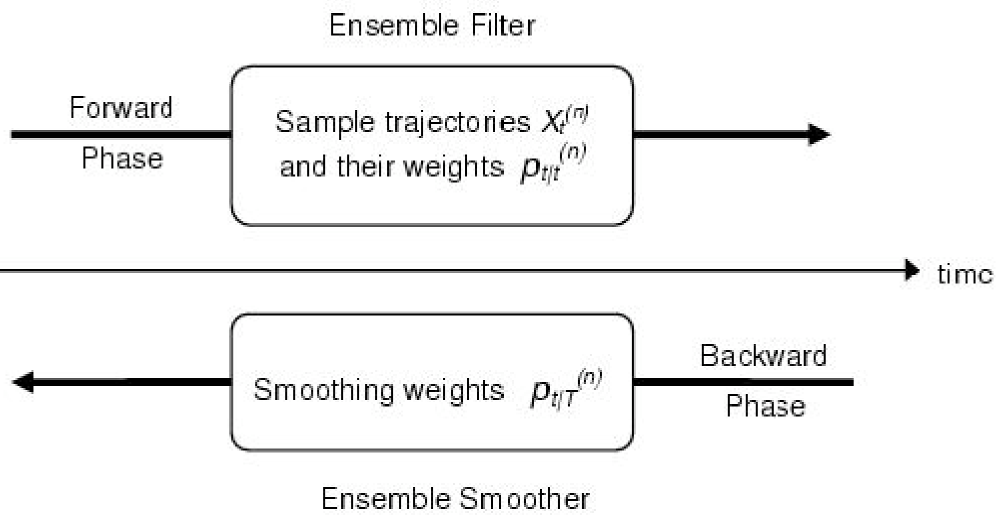
EnKF, RPF, MCMC and the BSS

The BSS retrospectively updates a set of weights for ensemble members.

It can

- work with either EnKF- or RPF-generated ensembles;
- is relatively inexpensive; and
- works well for highly nonlinear, illustrative examples:
  - the double-well potential, &
  - the Lorenz (1963) model.



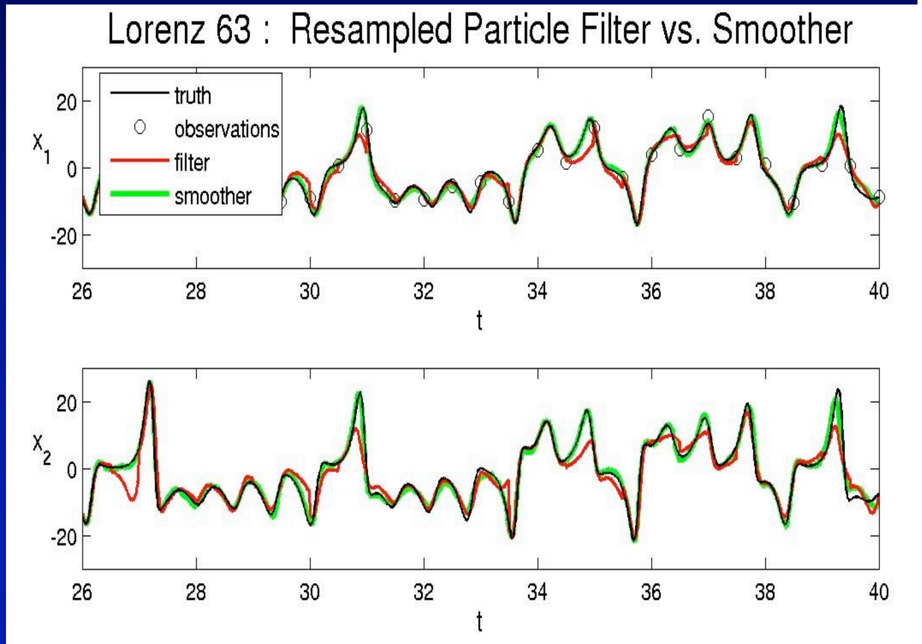


BSS Performance for the Lorenz (1963) System

Data: x_1 and x_3, every $\Delta t = 0.5$

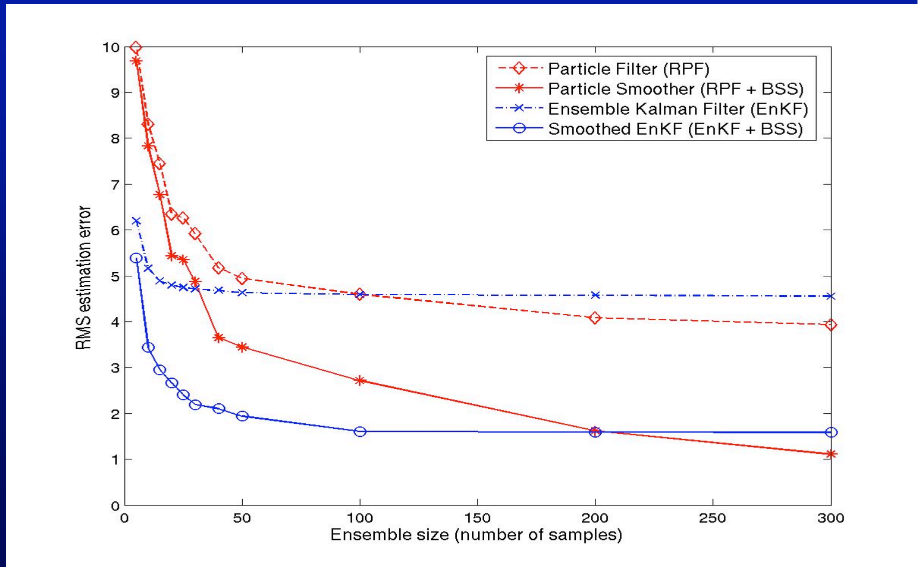
Upper panel: RPF vs. smoother

Smoother follows ob'ns (○) better in x_1 and is more realistic in x_2.



Lower panel: RPF *vs.* EnKF,
& filter (- - -) *vs.* smoother (----)

Smoother better than filter, & EnKF better than RPF for very small ensemble size N, but RPF takes over as N increases.



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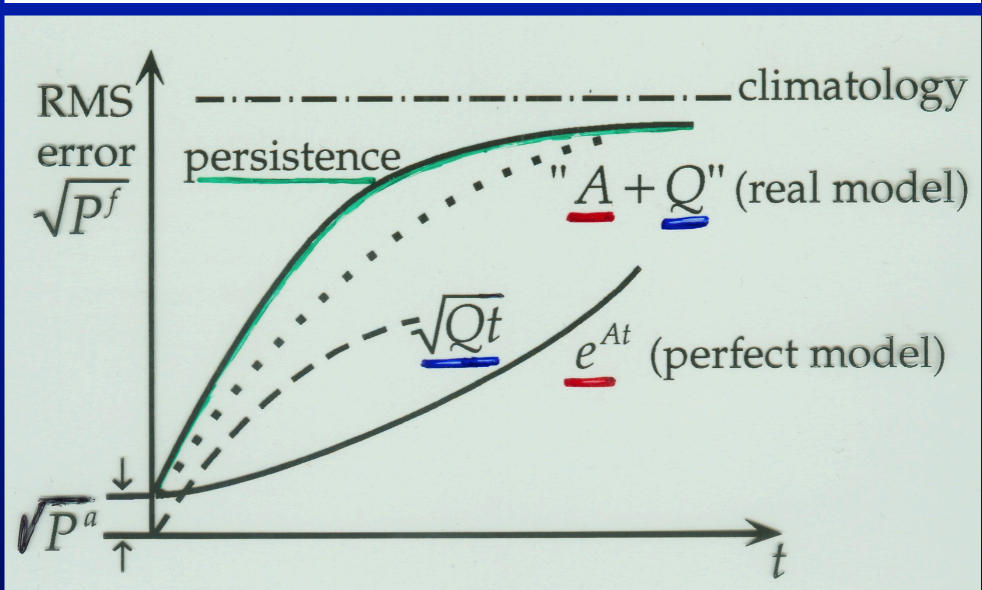
Error components in forecast–analysis cycle

$$\underbrace{P^f}_{\substack{\text{first-guess}\\ \text{error}}} \cong \underbrace{P^a}_{\substack{\text{analysis}\\ \text{error}}} + \Delta t(\underbrace{2AP^a}_{\substack{\text{id. twins}\\ \text{error}\\ \text{growth}}} + \underbrace{Q}_{\substack{\text{modeling}\\ \text{error}}})$$

$$(\Psi = e^{A\Delta t} \cong \underline{1 + A\Delta t})$$



The relative contributions to error growth of

- **analysis error**
- **intrinsic error growth**
- **modeling error (stochastic?)**

Assimilation of observations: Stability considerations

Free-System Dynamics (sequential-discrete formulation)**:** ***Standard breeding***

Forecast state:

model integration from a

previous analysis

$$\mathbf{x}^f_{n+1} = M(\mathbf{x}^a_n)$$

Corresponding perturbative (tangent linear) equation

$$\delta\mathbf{x}^f_{n+1} = \mathbf{M}\delta\mathbf{x}^a_n$$

Observationally Forced System Dynamics (sequential-discrete formulation)**:** ***BDAS***

If observations are available and we assimilate them:

Evolutive equation of the system, subject to forcing by the assimilated data

$$\mathbf{x}^a_{n+1} = \left[\mathbf{I} - \mathbf{K}H \circ\right] M(\mathbf{x}^a_n) + \mathbf{K}\mathbf{y}^o_{n+1}$$

Corresponding perturbative (tangent linear) equation, if the same observations are assimilated in the perturbed trajectories as in the control solution

$$\delta\mathbf{x}^a_{n+1} = \left[\mathbf{I} - \mathbf{K}\mathbf{H}\right]\mathbf{M}\delta\mathbf{x}^a_n$$

- The matrix (**I – KH**) is expected, in general, to have a stabilizing effect (Ghil *et* al., 1981);
- The free-system instabilities, which dominate the error growth during the forecast step , can be reduced during the analysis step.

Carrassi, Ghil, Trevisan & Uboldi (CHAOS, 2008)

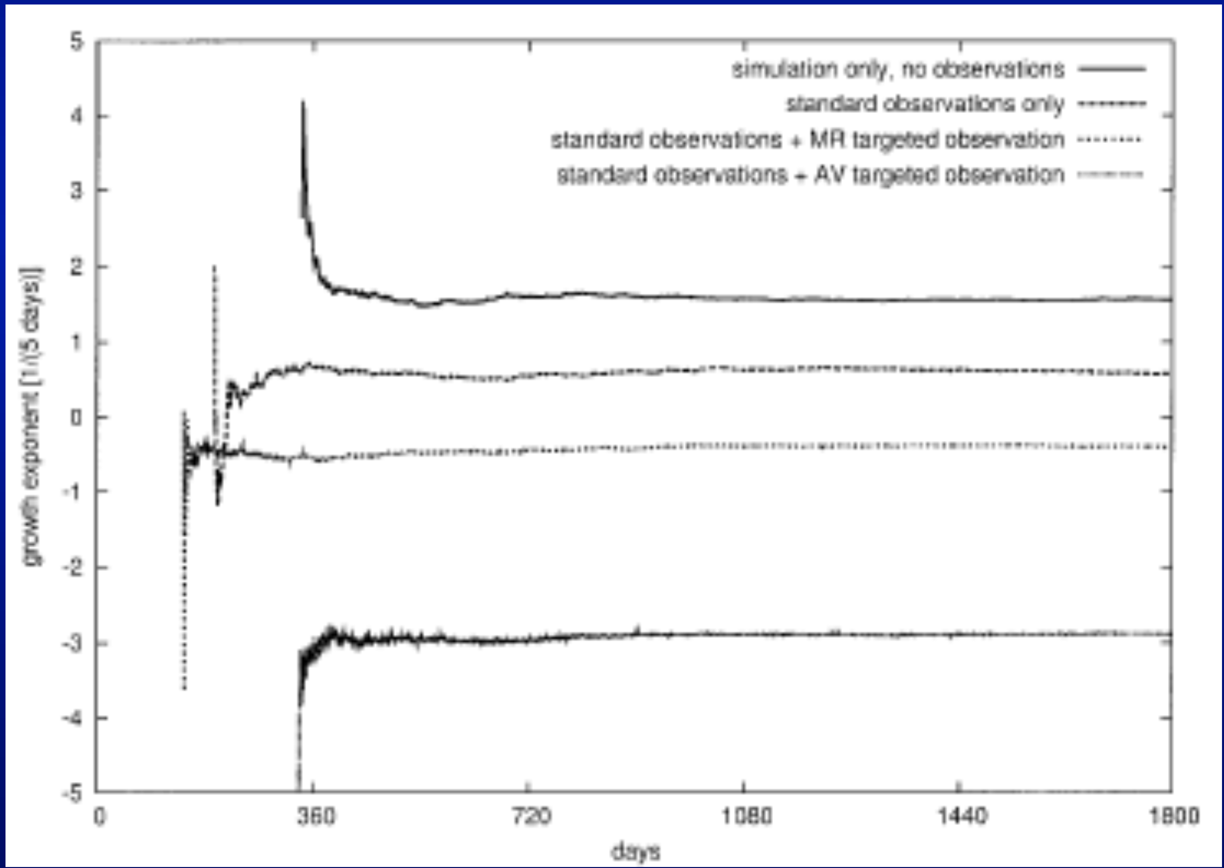
Stabilization of the forecast–assimilation system – I

Assimilation experiment with a low-order chaotic model

- Periodic 40-variable Lorenz (1996) model;
- Assimilation algorithms: replacement (Trevisan & Uboldi, 2004), replacement + one adaptive obs'n located by multiple replication (Lorenz, 1996), replacement + one adaptive obs'n located by BDAS and assimilated by AUS (Trevisan & Uboldi, 2004).

BDAS: Breeding on the Data Assimilation System

AUS: Assimilation in the Unstable Subspace



Trevisan & Uboldi (*J. Atmos. Sci.*, 2004)

Stabilization of the forecast–assimilation system – II

Assimilation experiment with the 40-variable Lorenz (1996) model

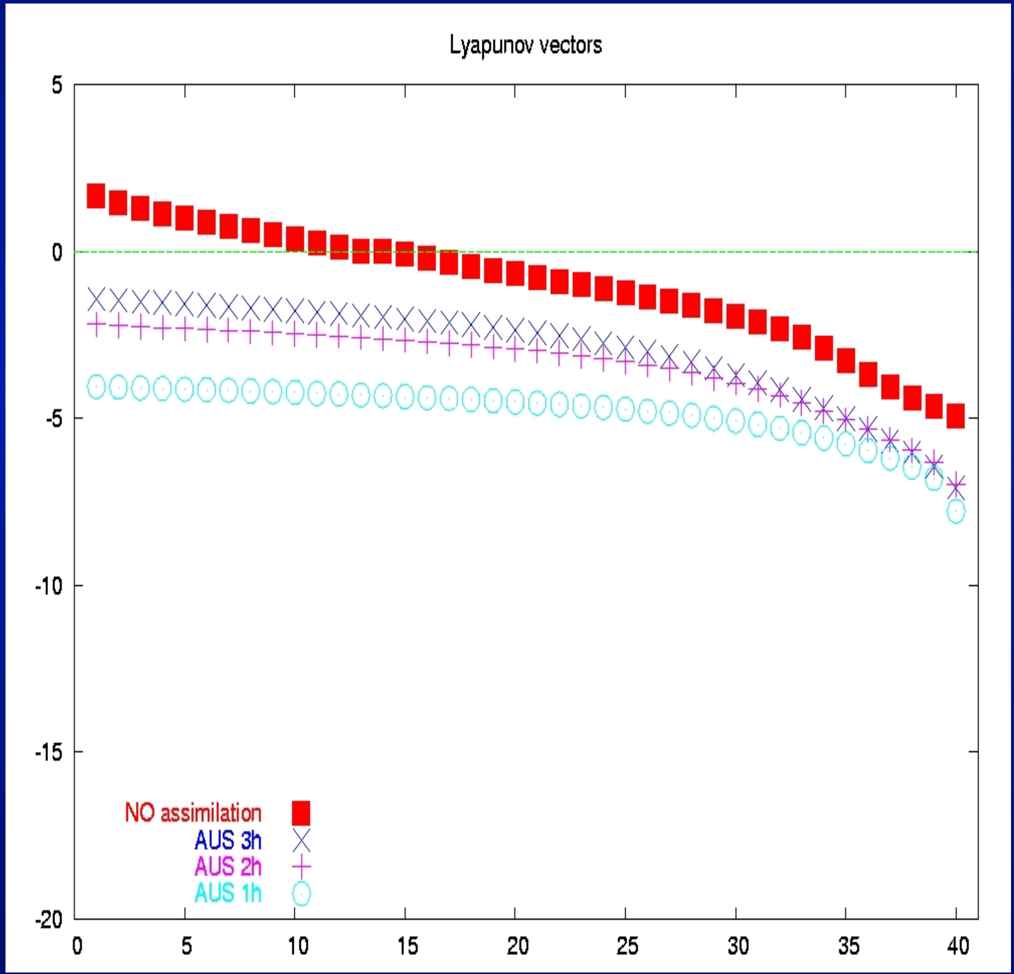
Spectrum of Lyapunov exponents:

Red: free system

Dark blue: AUS with 3-hr updates

Purple: AUS with 2-hr updates

Light blue: AUS with 1-hr updates



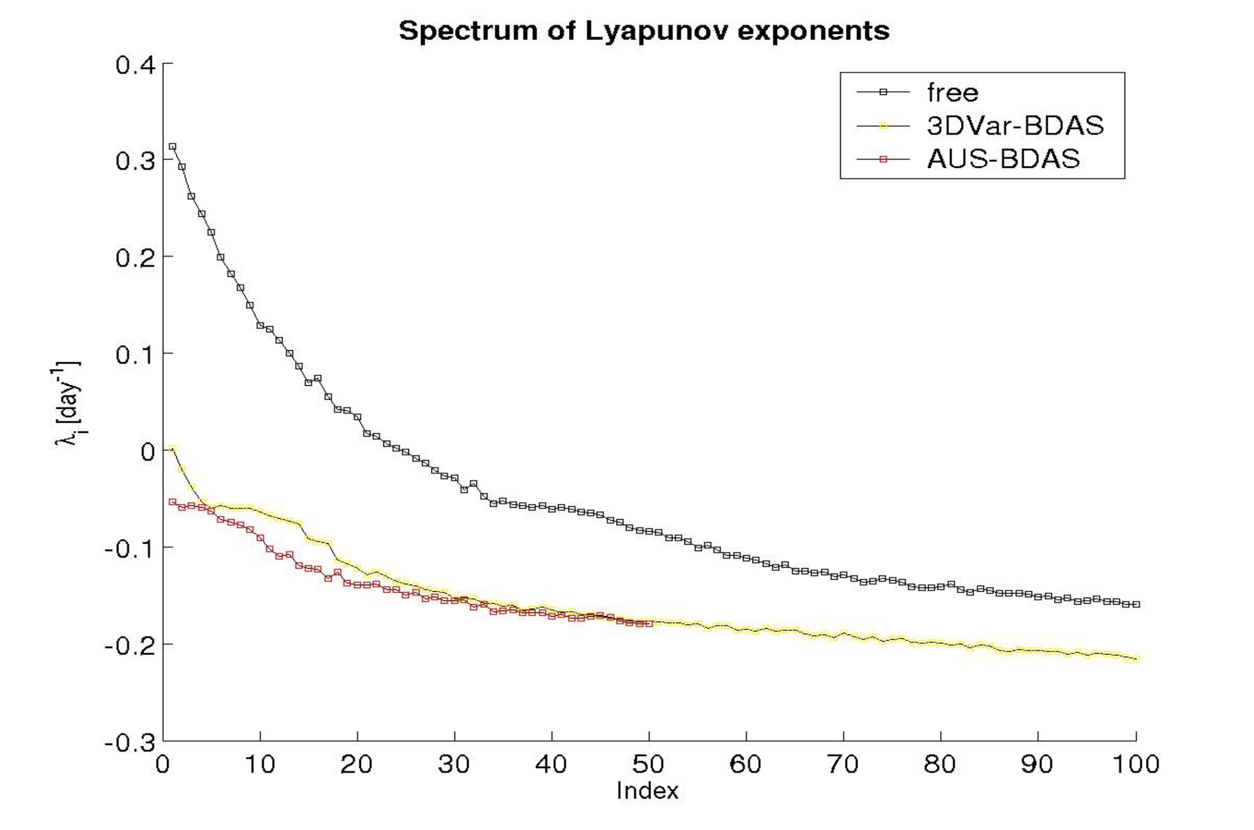
Carrassi, Ghil, Trevisan & Uboldi, (*CHAOS*, 2008)

Stabilization of the forecast–assimilation system – III

Assimilation experiment with an intermediate atmospheric circulation model

- 64-longitudinal x 32-latitudinal x 5 levels periodic channel QG-model (Rotunno & Bao, 1996)
- Perfect-model assumption
- Assimilation algorithms: 3-DVar (Morss, 2001); AUS (Uboldi *et al.,* 2005; Carrassi *et al.*, 2006)

Observational forcing ⇒ Unstable subspace reduction



➤ ***Free System***

Leading exponent:

$\lambda_{max} \approx 0.31$ days^{-1};

Doubling time ≈ 2.2 days;

Number of positive exponents:

$N^+ = 24$;

Kaplan-Yorke dimension ≈ 65.02.

➤ ***3-DVar–BDAS***

Leading exponent:

$\lambda_{max} \approx 0.002$ days^{-1};

Kaplan-Yorke dimension ≈ 1.1

➤ ***AUS–BDAS***

Leading exponent:

$\lambda_{max} \approx -0.52\text{x}10^{-3}$ days^{-1}

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Parameter Estimation

a) Dynamical model

$dx/dt = M(x, \mu) + \eta(t)$

$y^o = H(x) + \varepsilon(t)$

Simple (EKF) idea – augmented state vector

$d\mu/dt = 0$, $X = (x^T, \mu^T)^T$

b) Statistical model

$L(\rho)\eta = w(t)$, L – AR(MA) model, $\rho = (\rho_1, \rho_2, \ldots. \rho_M)$

Examples: 1) Dee *et al*. (*IEEE*, 1985) – estimate a few parameters in the covariance matrix $Q = E(\eta, \eta^T)$; also the bias $<\eta> = E\eta$;

2) POPs - Hasselmann (1982, Tellus); Penland (1989, *MWR*; 1996, *Physica D*); Penland & Ghil (1993, *MWR*)

3) $dx/dt = M(x, \mu) + \eta$: Estimate both M & Q from data (Dee, 1995, *QJ*), Nonlinear approach: Empirical mode reduction (EMR: Kravtsov *et al*., *J. Clim*., 2005; Kondrashov *et al*., *J. Clim*., 2005, *J. Atmos. Sci*., 2006; Kravtsov *et al*., in Palmer & Williams (Eds.), Cambridge U. P., 2010; Strounine *et al*., *Physica D*, 2010)

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Sequential parameter estimation

- "**State augmentation**" method – uncertain parameters are treated as additional state variables.
- Example: one unknown parameter μ

$$\bar{x}_k = \begin{pmatrix} x_k \\ \mu_k \end{pmatrix} = \begin{pmatrix} F(x_{k-1}, \mu_{k-1}) \\ \mu_{k-1} \end{pmatrix} + \begin{pmatrix} \epsilon_k \\ \epsilon^{\mu}_{k-1} \end{pmatrix}$$

$$y^o_k = \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} x_k \\ \mu_k \end{pmatrix} + \epsilon^0 = \bar{H}\bar{x}_k + \epsilon^0$$

$$\bar{x}^a_k = \bar{x}^f_k + \bar{K}(y^o_k - \bar{H}\bar{x}^f_k); \quad \bar{K} = \bar{P}^f \bar{H}^T (\bar{H}\bar{P}^f \bar{H}^T + R)^{-1}$$

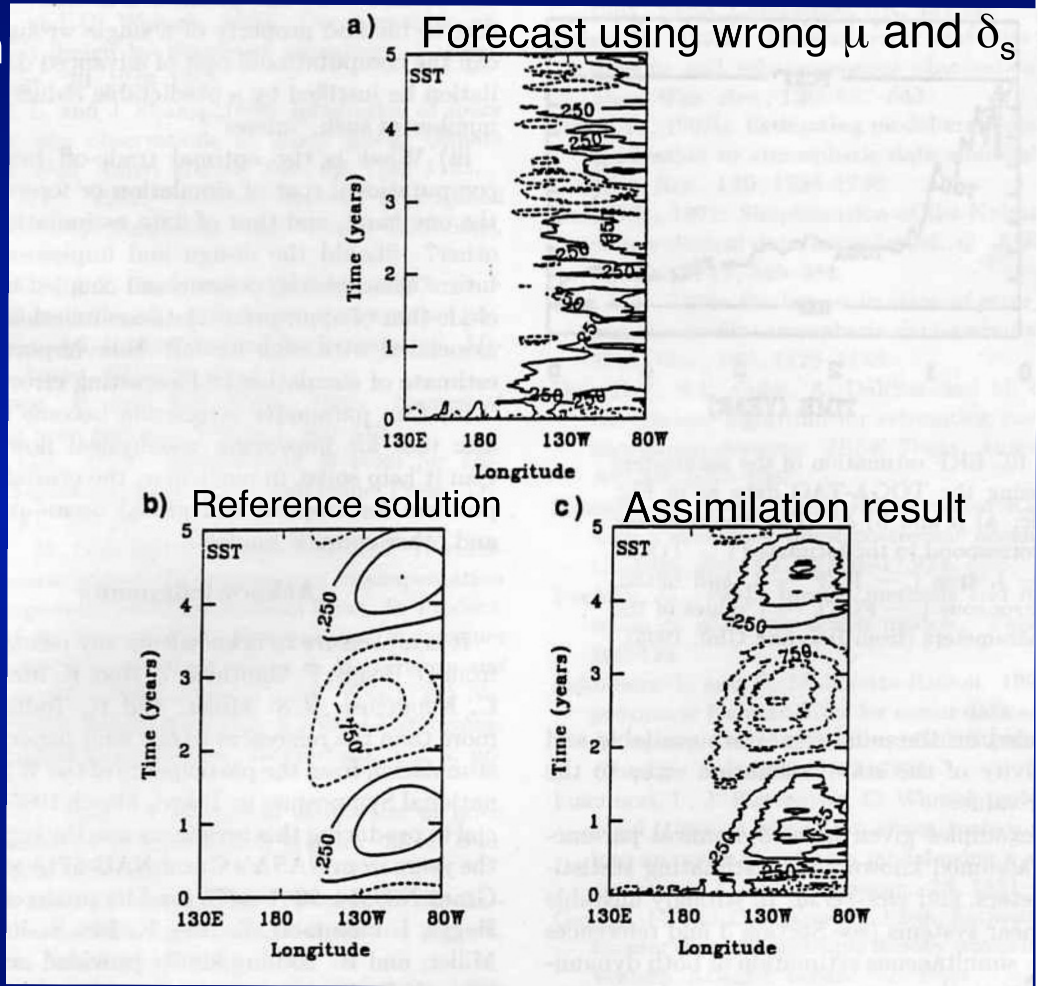
- **The parameters are not directly observable, but** the **cross-covariances** drive parameter changes from innovations of the state:

$$\bar{P}^f = \begin{pmatrix} P^f_{xx} & P^f_{x\mu} \\ P^f_{\mu x} & P^f_{\mu\mu} \end{pmatrix}; \quad \bar{K} = \begin{pmatrix} P^f_{xx} H^T \\ P^f_{\mu x} H^T \end{pmatrix} (H P^f_{xx} H^T + R)^{-1}$$

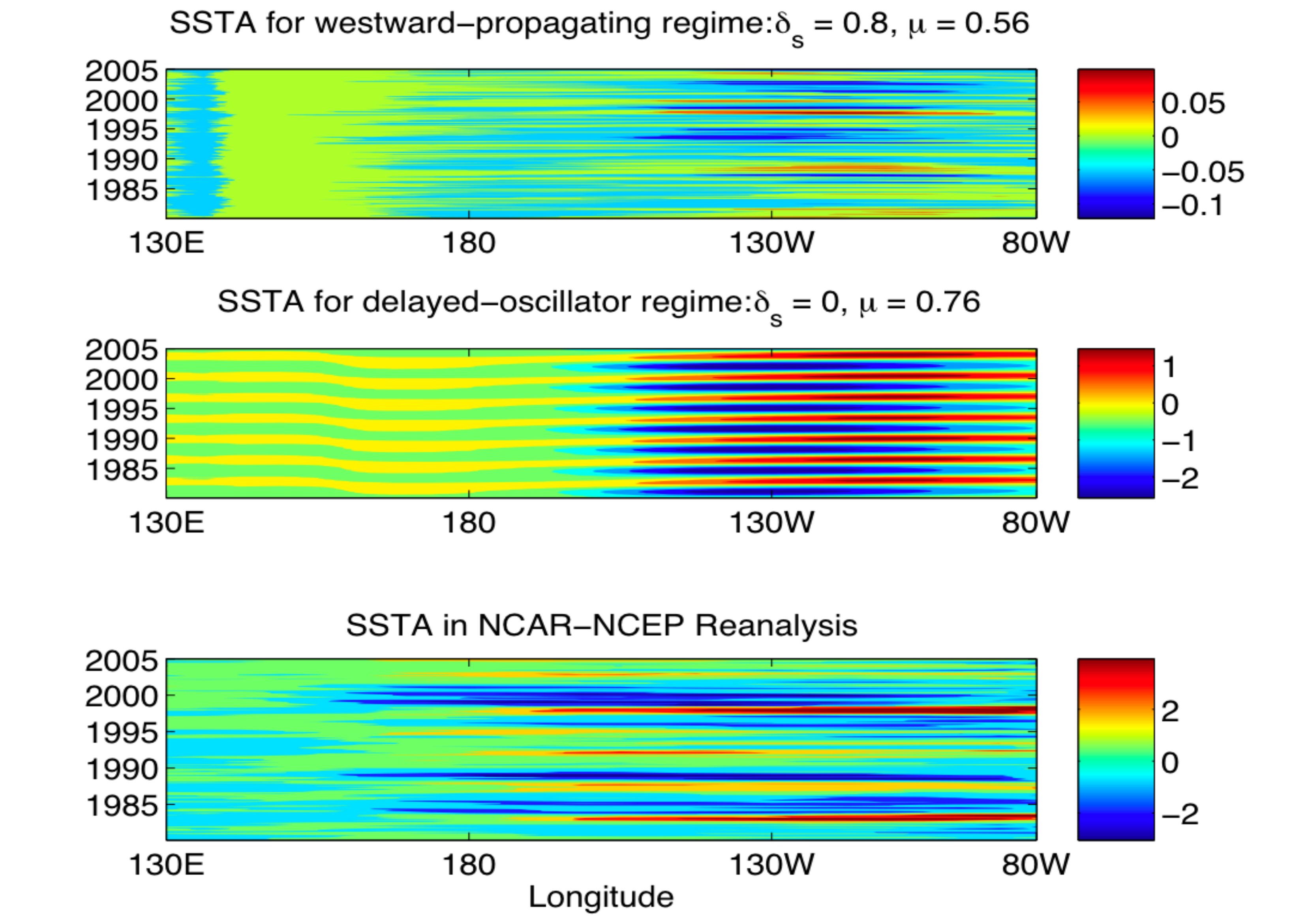
- Parameter estimation is always a **nonlinear problem,** even if the model is **linear** in terms of the model state: use **Extended Kalman Filter (EKF).**

Parameter estimation for coupled O-A system

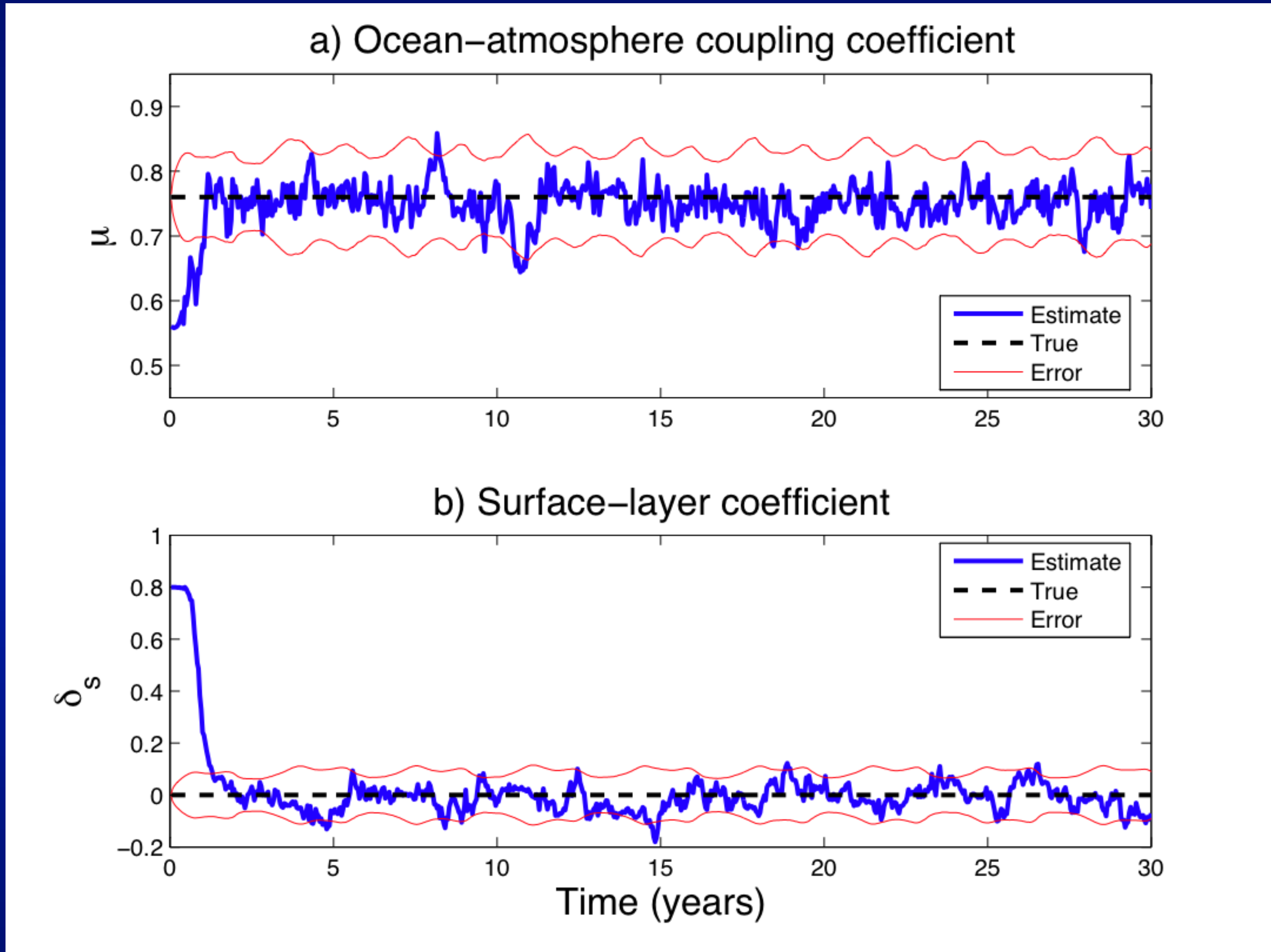
- Intermediate coupled model (ICM: Jin & Neelin, *JAS*, 1993)
- Estimate the state vector $W = (T', h, u, v)$, along with the coupling parameter μ and surface-layer coefficient δ_s by assimilating data from a single meridional section.
- The ICM model has errors in its initial state, in the wind stress forcing & in the parameters.
- Hao & Ghil (1995, *Proc. WMO Symp. DA Tokyo*); Ghil (1997, *JMSJ*); Sun *et al*. (2002, *MWR*).
- Kondrashov, Sun & Ghil (*Monthly Weather Rev.*, 2008)



Coupled O-A Model (ICM) vs. Observations

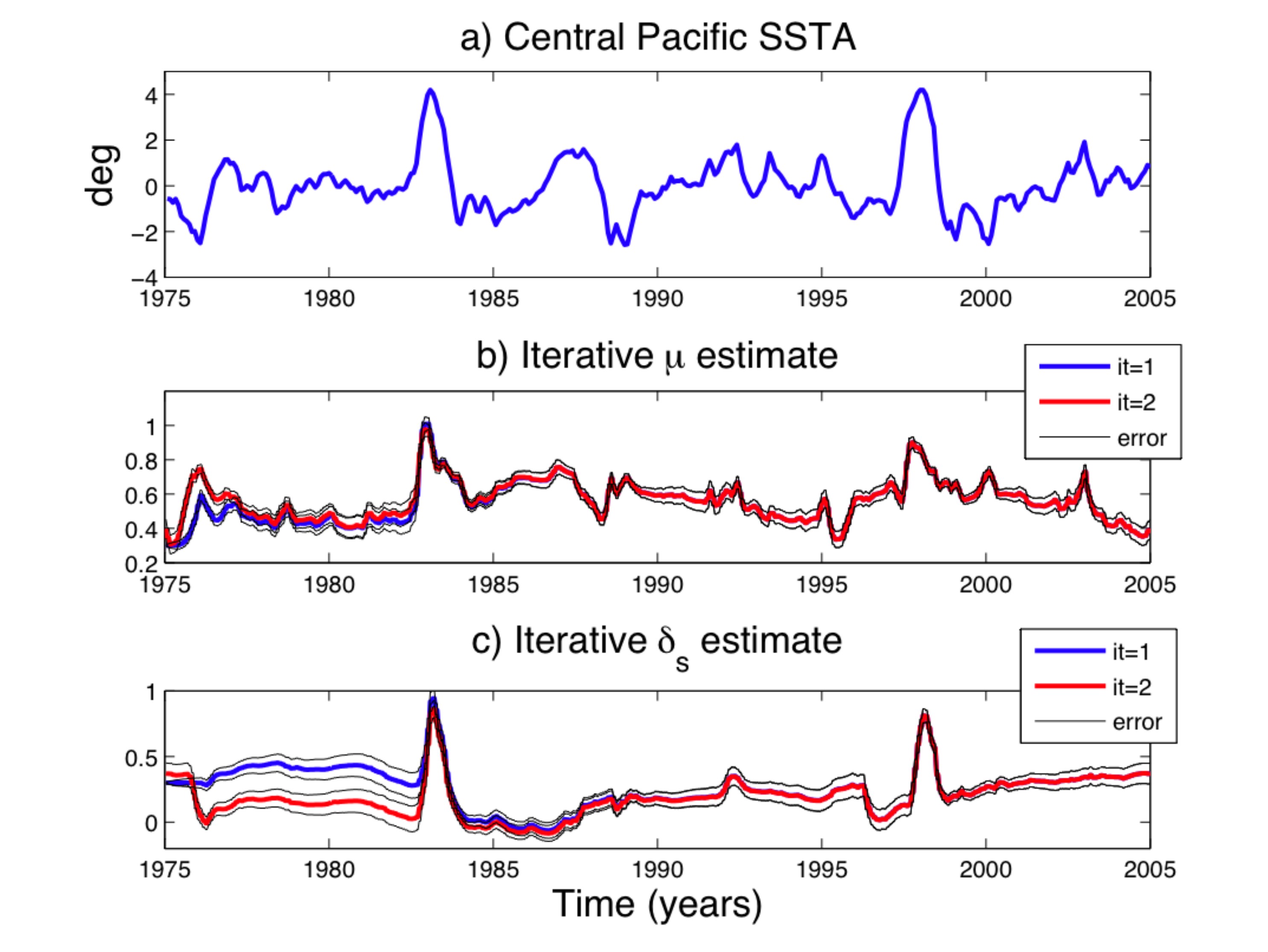


Convergence of Parameter Values – I



Identical-twin experiments

Convergence of Parameter Values – II



Real SST anomaly (SSTA) data

Outline

- ➤ Data in meteorology, oceanography and space physics
  - *in situ &* remotely sensed
- ➤ Basic ideas, data types, & issues
  - how to combine data with models
  - transfer of information
    – between variables & regions
  - filters & smoothers
  - stability of the forecast-assimilation cycle
- ➤ Parameter estimation
  - model parameters
  - noise parameters – at & below grid scale
- ➤ Novel areas of application
  - space physics
  - shock waves in solids
  - macroeconomics
  - paleoclimate
- ➤ Concluding remarks and bibliography
  - where we came from
  - where we're going

Evolution of DA – I

TABLE I. CHARACTERISTICS OF DATA ASSIMILATION SCHEMES IN OPERATIONAL USE AT THE END OF THE 1970s[a]

Organization or country	Operational analysis methods	Analysis area	Analysis/forecast
Australia	Successive correction method (SCM)	SH[d]	12 hr
	Variational blending techniques	Regional	6 hr
Canada	Multivariate 3-D statistical interpolation	NH[d] Regional	6 hr (3 hr for the surface)
France	SCM; wind-field and mass-field balance through first guess	NH	6 hr
	Multivariate 3-D statistical interpolation	Regional	
F.R. Germany	SCM. Upper-air analyses were built up, level by level, from the surface	NH	12 hr (6 hr for the surface)
	Variational height/wind adjustment		Climatology only as preliminary fields
Japan	SCM	NH	12 hr
	Height-field analyses were corrected by wind analyses	Regional	
Sweden	Univariate 3-D statistical interpolation	NH	12 hr
	Variational height/wind adjustment	Regional	3 hr
United Kingdom	Hemispheric orthogonal polynomial method		
	Univariate statistical interpolation (repeated insertion of data)	Global	6 hr
U.S.A.	Spectral 3-D analysis	Global	
	Multivariate 3-D statistical interpolation	Global	6 hr
U.S.S.R.	2-D[c] statistical interpolation	NH	12 hr
ECMWF[b]	Multivariate 3-D statistical interpolation	Global	6 hr

[a] After Gustafsson (1981).
[b] European Centre for Medium Range Weather Forecasts.
[c] 2-D is in a horizontal plane.
[d] Southern Hemisphere and Northern Hemisphere, respectively.

Transition from "early" to "mature" phase of DA in NWP:

- no Kalman filter (Ghil *et al.*, 1981 (*))
- no adjoint (Lewis & Derber, *Tellus,* 1985); Le Dimet & Talagrand (*Tellus,* 1986)

(*) Bengtsson, Ghil & Källén (Eds., 1981), *Dynamic Meteorology: Data Assimilation Methods.*

M. Ghil & P. M.-Rizzoli (*Adv. Geophys.,* 1991).

3D-Var

$$J = \min \frac{1}{2}[(\mathbf{x}^a - \mathbf{x}^b)^{\mathrm{T}} \mathbf{B}^{-1} (\mathbf{x}^a - \mathbf{x}^b) + (H\mathbf{x}^a - \mathbf{y})^{\mathrm{T}} \mathbf{R}^{-1} (H\mathbf{x}^a - \mathbf{y})]$$

Distance to forecast — Distance to observations

at the analysis time

4D-Var

$$J = \min \frac{1}{2}[(\mathbf{x}_0 - \mathbf{x}_0^b)^{\mathrm{T}} \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}_0^b) + \sum_{i=1}^{s} (H\mathbf{x}_i - \mathbf{y}_i)^{\mathrm{T}} \mathbf{R}_i^{-1} (H\mathbf{x}_i - \mathbf{y}_i)]$$

Distance to background at the initial time

Distance to observations in a **time window interval t_0-t_1**

Control variable $\mathbf{x}(t_0)$

Analysis $\mathbf{x}(t_1) = M[\mathbf{x}(t_0)]$

It seems like a simple change, but it is not! (e.g., adjoint)

What is B? It should be tuned…

Courtesy of E. Kalnay (2006)

Extended Kalman Filter (EKF) (Ghil 1980's)

Forecast step:

$$\mathbf{x}_n^b = M_n\left(\mathbf{x}_{n-1}^a\right)$$

$$\mathbf{B}_n = \mathbf{M}_n \mathbf{A}_{n-1} \mathbf{M}_n^T + \mathbf{Q}_n$$

Analysis step:

$$\mathbf{x}_n^a = \mathbf{x}_n^b + \mathbf{K}_n(\mathbf{y}_n - H\mathbf{x}_n^b)$$

where the optimal weight matrix is given by

$$\mathbf{K}_n = \mathbf{B}_n(\mathbf{R} + \mathbf{H}\mathbf{B}_n\mathbf{H}^T)^{-1}$$

and the new analysis error covariance by

$$\mathbf{A}_n = (\mathbf{I} - \mathbf{K}_n\mathbf{H})_n\mathbf{B}_n$$

Still requires adjoint of model *M* and obs. operator *H*

Ensemble Kalman Filter (EnKF)

Forecast step:

$$\mathbf{x}^{b}_{n,k} = M_n\left(\mathbf{x}^{a}_{n-1,k}\right)$$

$$\mathbf{B}_n = \frac{1}{K-1}\mathbf{E}^b_n\mathbf{E}^{bT}_n, \textit{ where } \mathbf{E}^b_n = \left[\mathbf{x}^b_{n,1} - \overline{\mathbf{x}}^b_n; \ldots, \mathbf{x}^b_{n,K} - \overline{\mathbf{x}}^b_n\right]$$

Analysis step:

$$\mathbf{x}^a_n = \mathbf{x}^b_n + \mathbf{K}_n(\mathbf{y}_n - H\overline{\mathbf{x}}^b_n)$$

The new analysis error covariance in the ensemble space is (Hunt 2005)

$$\hat{\mathbf{A}}_n = \left[\left(K-1\right)\mathbf{I} + (\mathbf{H}\mathbf{E}^b_n)^T\mathbf{R}^{-1}(\mathbf{H}\mathbf{E}^b_n)\right]^{-1}$$

And the new ensemble perturbations are given by

$$\mathbf{E}^a_n = \mathbf{E}^b_n\left[\left(K-1\right)\hat{\mathbf{A}}_n\right]^{1/2}$$

Evolution of DA – II

TABLE IV. DUALITY RELATIONSHIPS BETWEEN STOCHASTIC ESTIMATION AND DETERMINISTIC CONTROL[a]

A. Continuous (linear) Kalman Filter

System Model	$\dot{\mathbf{w}}^{t}(t) = F(t)\mathbf{w}^{t}(t) + G(t)\mathbf{b}^{t}(t), \quad \mathbf{b}^{t}(t) \sim \mathrm{N}[0, Q(t)]$
Measurement Model	$\mathbf{w}^{0}(t) = H(t)\mathbf{w}^{t}(t) + \mathbf{b}^{0}(t), \quad \mathbf{b}^{0}(t) \sim \mathrm{N}[0, R(t)]$
State estimation	$\dot{\mathbf{w}}^{a}(t) = F(t)\mathbf{w}^{a}(t) + K(t)[\mathbf{w}^{0}(t) - H(t)\mathbf{w}^{a}(t)], \quad \mathbf{w}^{a}(0) = \mathbf{w}^{a}_{0}$
Error covariance propagation (Riccati Equation)	$\dot{P}(t) = F(t)P(t) + P(t)F^{T}(t) + G(t)Q(t)G^{T}(t) - K(t)R(t)K^{T}(t), \quad P(0) = P_0$
Kalman Gain	$K(t) = P(t)H^{T}(t)R^{-1}(t)$
Initial conditions	$E[\mathbf{w}^{t}(0)] = \mathbf{w}^{a}_{0}, \quad E\{[\mathbf{w}^{t}(0) - \mathbf{w}^{a}_{0}][\mathbf{w}^{t}(0) - \mathbf{w}^{a}_{0}]^{T}\} = P_0$
Assumptions	$R^{-1}(t)$ exists $E\{\mathbf{b}^{t}(t)[\mathbf{b}^{0}(t')]^{T}\} = 0$
Performance Index	$p^{f,a}(t) = E\{[\mathbf{w}^{f,a} - \mathbf{w}^{t}][\mathbf{w}^{f,a} - \mathbf{w}^{t}]^{T}\}$

B. Continuous (linear) Optimal Control

System Model	$\dot{\mathbf{w}}^{t}(t) = \tilde{F}(t)\mathbf{w}(t) + \tilde{H}(t)\mathbf{u}(t)$
Measurement Model	$\mathbf{w}^{0}(t) = \mathbf{w}(t)$ (all system variables are measured)
Performing control	$\mathbf{u}(t) = -\tilde{K}(t)\mathbf{w}(t)$
Performance propagation (Riccati Equation)	$\dot{\tilde{P}}(t) = -\tilde{F}^{T}(t)\tilde{P}(t) - \tilde{P}(t)\tilde{F}(t) - \tilde{Q}(t) + \tilde{P}(t)\tilde{H}(t)\tilde{K}(t)$
Control Gain	$\tilde{K}(t) = \tilde{R}^{-1}(t)\tilde{H}(t)\tilde{P}(t)$
Terminal conditions	$\mathbf{w}(t_f) = 0$ $\mathbf{P}(t_f) = \tilde{Q}_f$
Cost function	$J[\mathbf{w}, \mathbf{u}] = \mathbf{w}_f^{T}\tilde{Q}_f\mathbf{w}_f + \int_0^{t_f} [\mathbf{w}^{T}(t)\tilde{Q}(t)\mathbf{w}(t) + \mathbf{u}^{T}(t)\tilde{R}(t)\mathbf{u}(t)]\, dt$

C. Estimation-Control Duality

Estimation	Control
t_0 initial time	t_f final time
$\mathbf{w}(t)$ unobservable state variable of random process	$\mathbf{w}(t)$ observable state variable to be controlled
$\mathbf{w}^{0}(t)$ random observations	$\mathbf{u}(t)$ deterministic control
$F(t)$ dynamic matrix	$\tilde{F}^{T}(t)$ dynamic matrix
$Q(t)$ covariance matrix for the model errors	$\tilde{Q}(t)$ quadratic matrix defining acceptable errors on model variables
$H(t)$ effect of observations on state variables	$\tilde{H}(t)$ effect of control on state variables
$P(t)$ covariance of estimation error under optimization	$\tilde{P}(t)$ quadratic performance under optimization
$K(t)$ weighting on observation for optimal estimation	$\tilde{K}(t)$ weighting on state for optimal control

[a] (A), Kalman filter as the optimal solution for the former problem; (B), optimal solution for the latter problem; (C), equivalences between the two (after Kalman, 1960, and Gelb, 1974, Section 9.5; courtesy of R. Todling).

Cautionary note:

"Pantheistic" view of DA:

- variational ~ KF;
- 3- & 4-D Var ~ 3- & 4-D PSAS or EnKF.

Fashionable to claim it's all the same but it's not:

- **God** is in **everything,**
- **but the devil is in the details.**

M. Ghil & P. M.-Rizzoli (*Adv. Geophys.*, 1991).

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Computational advances

a) Hardware

- more computing power (CPU throughput)
- larger & faster memory (3-tier)

b) Software

- better numerical implementations of algorithms
- automatic adjoints
- block-banded, reduced-rank & other sparse-matrix algorithms
- better ensemble & particle filters
- efficient parallelization, ….

How much DA *vs*. forecast?

- Design integrated observing–forecast–assimilation systems!

Observing system design

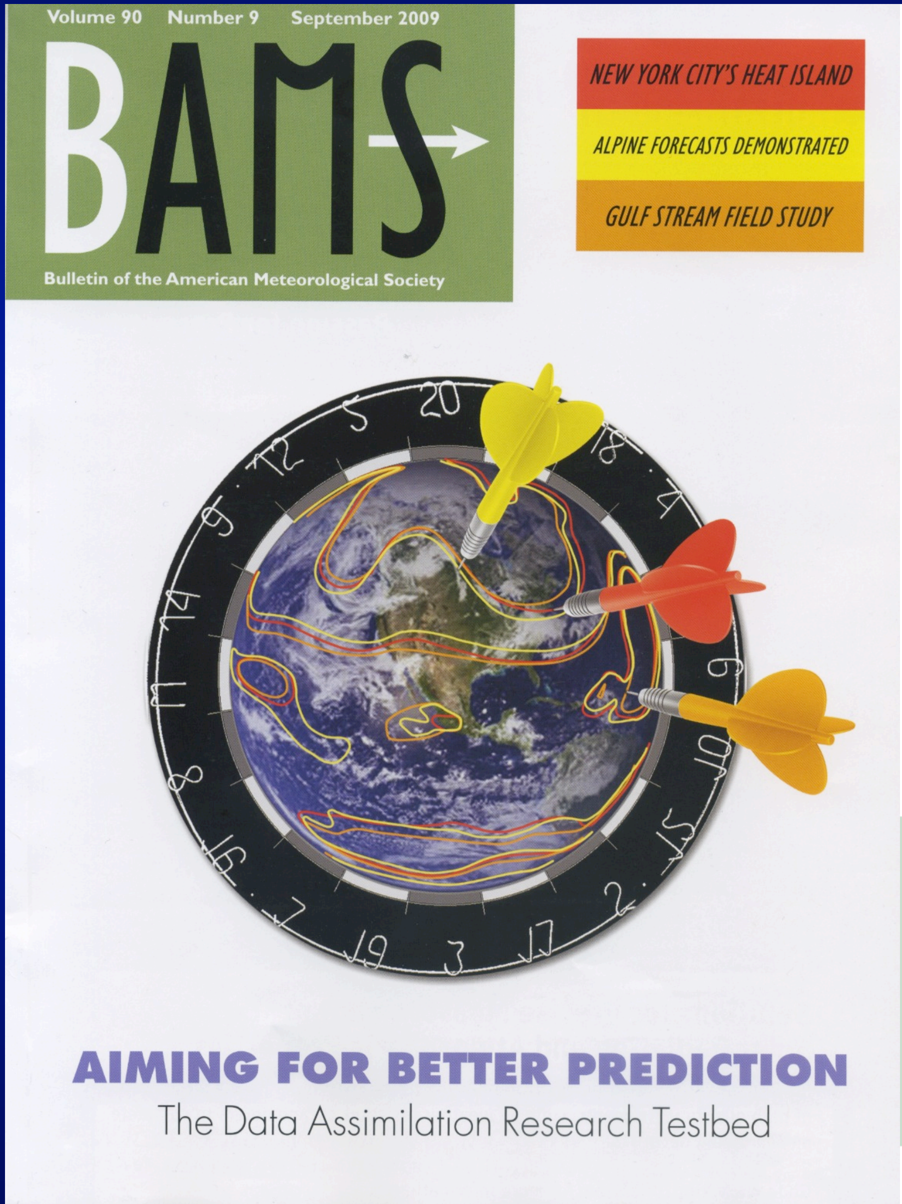
- **Need no more (independent) observations than *d-o-f* to be tracked:**
  - "features" (Ide & Ghil, *Dyn. Atmos. Oceans,* 1997a, b);
  - instabilities (Todling & Ghil, 1994 + Ghil & Todling, 1996, *MWR*);
  - trade-off between mass & velocity field (Jiang & Ghil, *JPO*, 1993).
- The cost of **advanced** DA is **much less** than that of instruments & platforms:
  - at best use DA **instead** of instruments & platforms.
  - at worst use DA to determine which instruments & platforms (**advanced** OSSE)
- **Use any** observations, if forward modeling is possible (observing operator H)
  - satellite images, 4-D observations;
  - pattern recognition in observations and in phase-space statistics.

Conclusions

- **Theoretical concepts** can play a useful role in devising better **practical algorithms**, and vice-versa.
- Judicious choices of observations and method can **stabilize the forecast-assimilation cycle**.
- **Trade-off** between cost of **observations** and of **data assimilation**.

- *Assimilation of ocean data in the coupled O–A system is useful.*
- *They help estimate both ocean and coupling parameters.*
- *Changes in estimated parameters compensate for model imperfections.*

DA Research Testbed (DART)



ARTICLES

THE DATA ASSIMILATION RESEARCH TESTBED

A Community Facility

BY JEFFREY ANDERSON, TIM HOAR, KEVIN RAEDER, HUI LIU, NANCY COLLINS, RYAN TORN, AND AVELINO AVELLANO

DART, developed and maintained at the National Center for Atmospheric Research, provides well-documented software tools for data assimilation education, research, and development.

Data assimilation combines observations with model forecasts to estimate the state of a physical system. Developed in the 1960s (Daley 1991; Kalnay 2003) to provide initial conditions for numerical weather prediction (NWP; Lynch 2006), data assimilation can do much more than initialize forecasts. Repeating the NWP process after the fact using all available observations and state-of-the-art data assimilation produces reanalyses, the best available estimate of the atmospheric state (Kistler et al. 2001; Uppala et al. 2005; Compo et al. 2006). Data assimilation can estimate the value of existing or hypothetical observations (Khare and Anderson 2006a; Zhang et al. 2004). Applications include predicting efficient flight paths for planes that release dropsondes (Bishop et al. 2001) and assessing the potential impact of a new satellite instrument before it is built or launched (Mourre et al. 2006). Data assimilation tools can also be used to evaluate forecast models, identifying quantities that are poorly predicted and comparing models to assess relative strengths and weaknesses. Data assimilation can guide model development by estimating values for model parameters that are most consistent with observations (Houtekamer et al. 1996; Aksoy et al. 2006). Assimilation is now used also for the ocean (Keppene and Rienecker 2002; Zhang et al. 2005), land surface (Reichle et al. 2002), cryosphere (Stark et al. 2008), biosphere (Williams et al. 2004), and chemical constituents (Constantinescu et al. 2007). Assimilation tools under different names are used in other areas of geophysics, engineering, economics, and social sciences.

The Data Assimilation Research Testbed (DART) is an open-source community facility that provides software tools for data assimilation research,

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*The National Center for Atmospheric Research is sponsored by the National Science Foundation

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The abstract for this article can be found in this issue, following the table of contents.

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In final form 8 April 2009

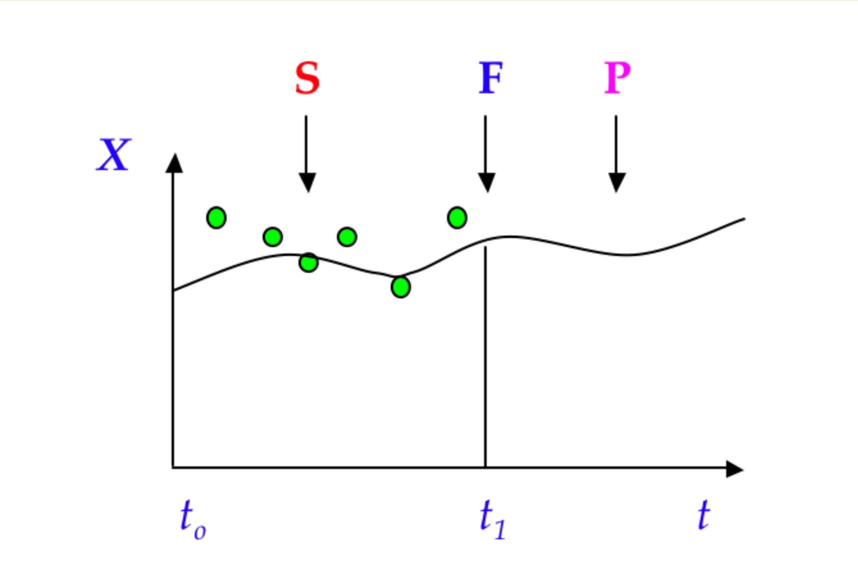
The DA Maturity Index of a Field

- **Pre-DA:** few data, poor models
  - The theoretician: Science is truth, don't bother me with the facts!
  - The observer/experimentalist: Don't ruin my beautiful data with your lousy model!!
- **Early DA:**
  - Better data, so-so models.
  - Stick it (the obs'ns) in – direct insertion, nudging.
- **Advanced DA:**
  - Plenty of data, fine models.
  - E(n)KF, 4-D Var (2nd duality); UKF, particle filters, etc.
- **Post-industrial DA:**

  (Satellite) images → (weather) forecasts, climate "movies" …

The main products of estimation(*)

- Filtering (F) – "video loops"
- Smoothing (S) – full-length feature "movies"
- Prediction (Pr) – NWP, ENSO
- Parameter estimates (Pe) – all of the above + DADA



Distribute all of this over the Web to scientists, and the "person in the street" (or on the information superhighway).

In a general way: Have fun!!!

(*) F + S + P: N. Wiener (1949, MIT Press); Pe – a lot recently

Concluding remarks

We've come a long way in 30 years — some advances are laborious and incremental (e.g., sequential vs. control-theoretical methods), but others are fresh and exciting.

The latter include new areas of application
- – biology, geomagnetism, paleoclimate, space physics, …, DADA, as well as novel methodological challenges
- – multi-scale and multi-model problems
- – inverse problems for evolution equations, including climate simulation & sensitivity studies, & uncertainty quantification

Technological advances both pose new problems (massive data sets, higher resolution, …) and help solve them.

Overall, it's a brave new world, in which data and models actively speak to each other, and we do so to both: enjoy!

"Miss Peterson, may I go home? I can't assimilate any more data today."

J.B. Handelsman (5/31/1969)

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Reserve slides

Overall Conclusion

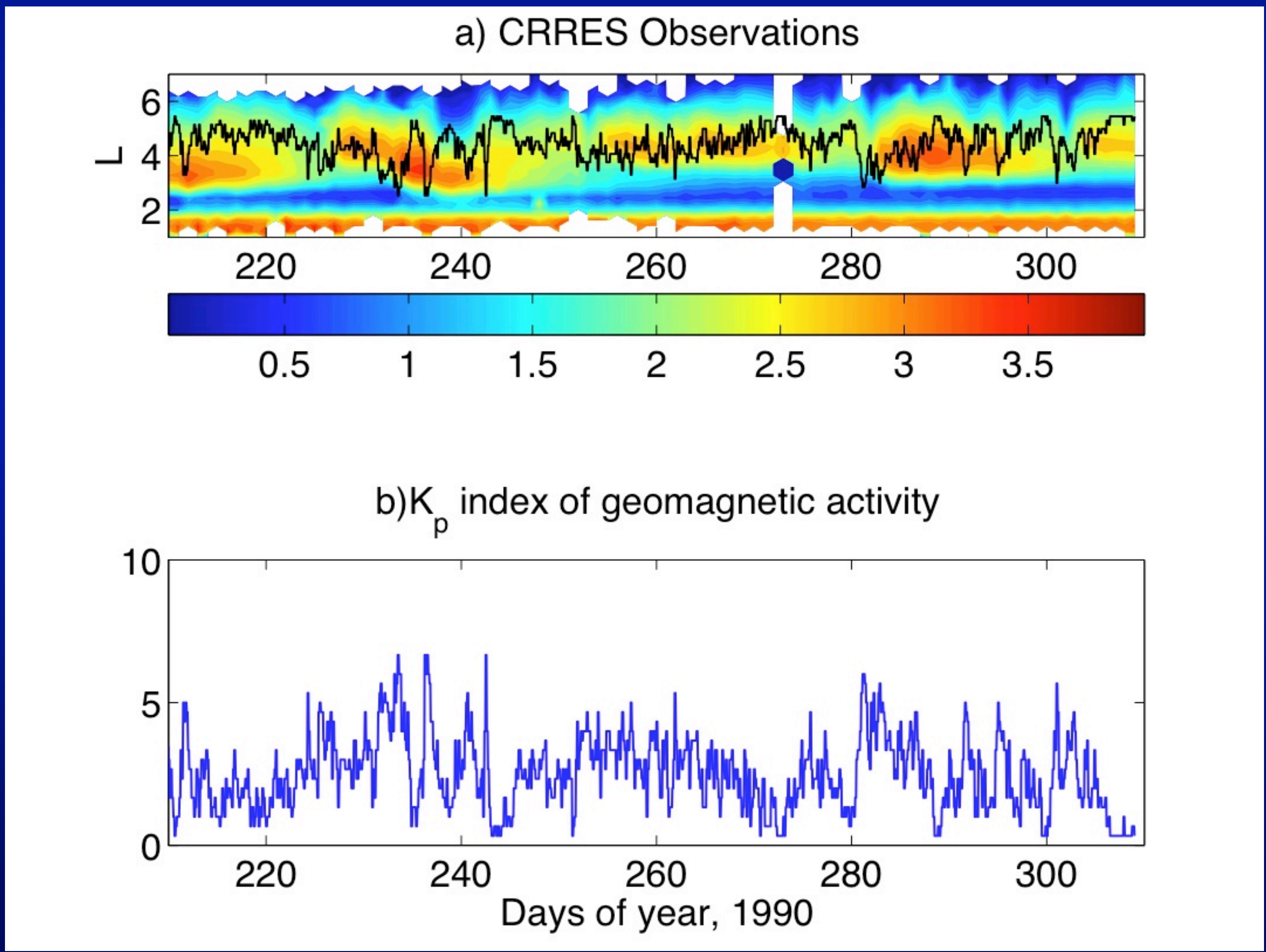
- No observing system without data assimilation and no assimilation without dynamics[a]
- Quote of the day: "You cannot step into the same river[b] twice[c]" (Heracleitus, *Trans. Basil. Phil. Soc. Miletus*, *cca.* 500 B.C.)

[a] of state and errors
[B] Meandros
[c] "You cannot do so even once" (subsequent development of "flux" theory by Plato, *cca.* 400 B.C.)

Τα πάντα ρεί = Everything flows

Parameter Estimation for Space Physics – I

Daily fluxes of relativistic (1 MeV) electrons in Earth's outer radiation belt
(CRRES observations starting on August 28, 1990)
***K_p* - index of geomagnetic activity (external forcing)**



Joint work with
D. Kondrashov, Y. Shprits,
& R. Thorne, UCLA;
R. Friedel & G. Reeves,
LANL

Estimating noise – I

$Q_1 = Q_{slow}\,,\;\; Q_2 = Q_{fast}\,,\;\; Q_3 = 0;$

$R_1 = 0,\;\; R_2 = 0,\;\; R_3 = R;$

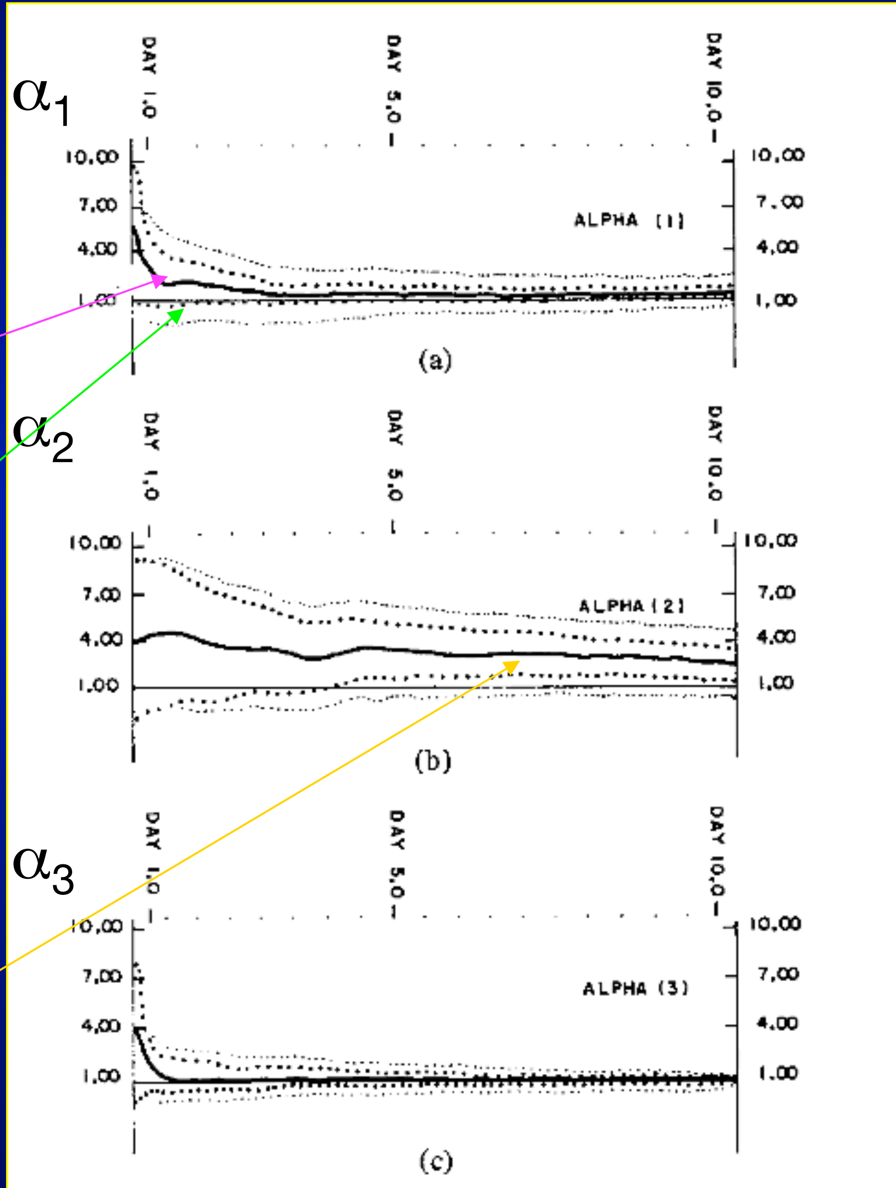
$Q = \sum \alpha_i Q_i;\; R = \sum \alpha_i R_i\,;$

$\alpha(0) = (6.0,\, 4.0,\, 4.5)^T;$

$Q(0) = 25 * I.$

estimated

true (α =1)



Dee *et al*. (1985, *IEEE Trans. Autom. Control*, **AC-30**)

Poor convergence for Q_{fast}?

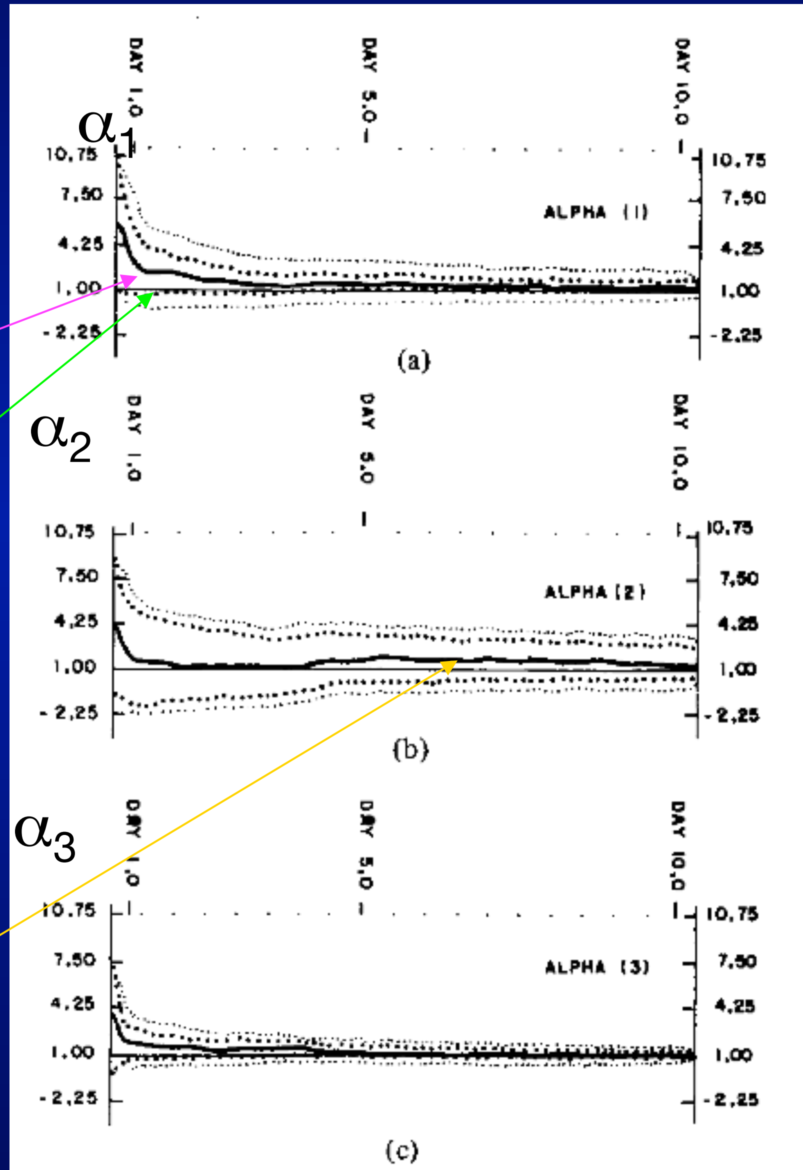
Estimating noise – II

Same choice of $\alpha(0)$, Q_i, and R_i but

$$\Theta(0) = 25 * \begin{bmatrix} 1 & 0.8 & 0 \\ 0.8 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

estimated

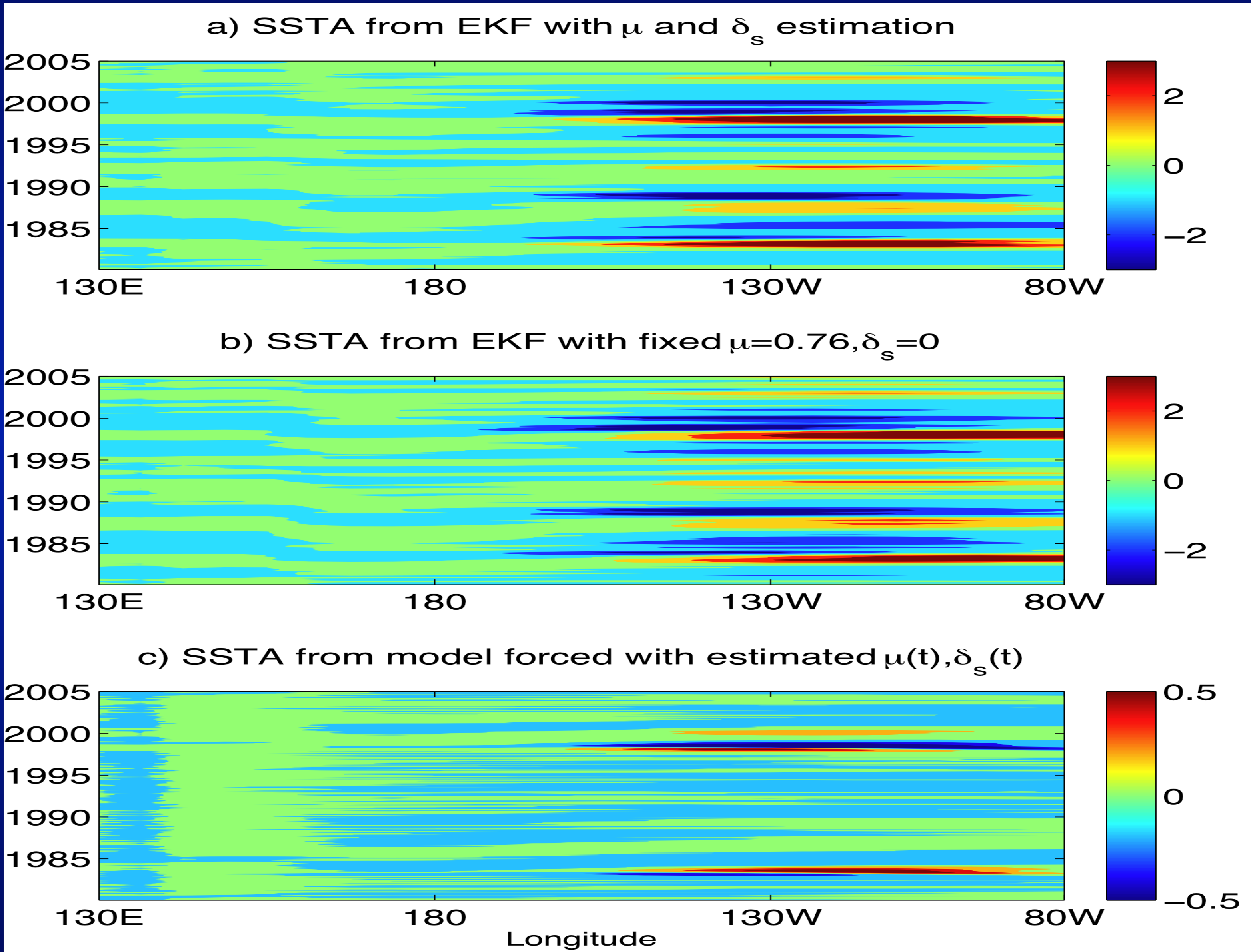
true ($\alpha = 1$)



Dee *et al.* (1985, *IEEE Trans. Autom. Control*, **AC-30**)

Good convergence for Q_{fast}!

EKF results with and w/o parameter estimation



Parameter estimation for space physics – III

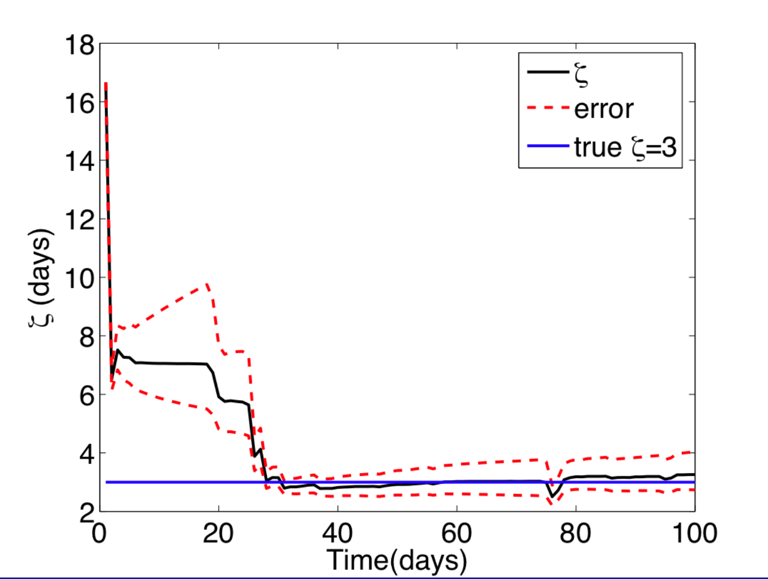
Daily observations from the "truth" —

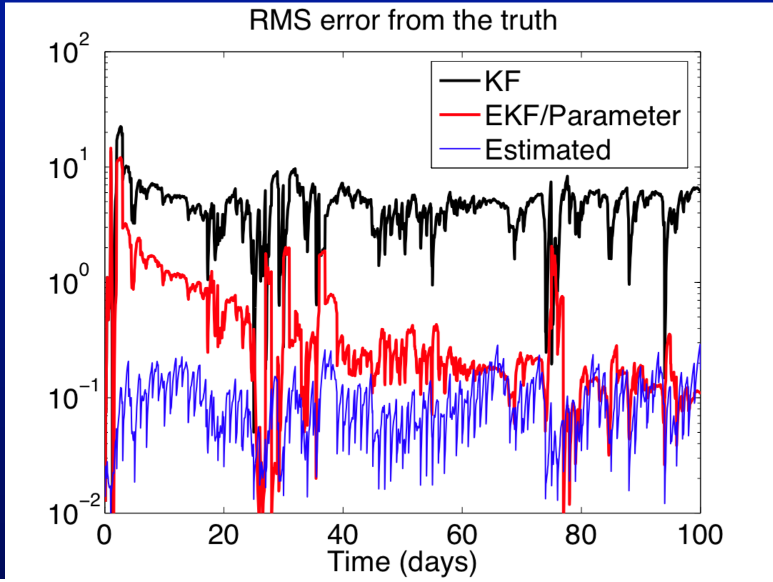
$\tau_{Lo} = \zeta / K_p$, $\zeta = 3$, and $\tau_{LI} = 20$ —

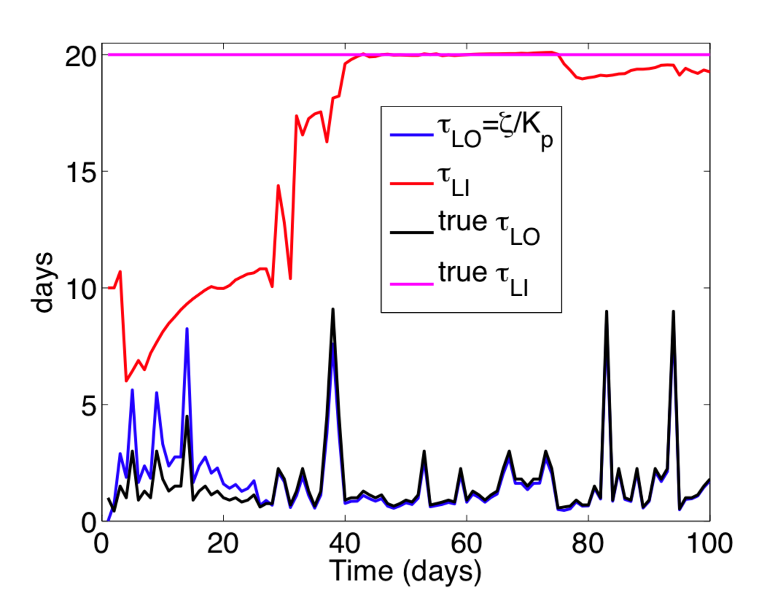
are used to correct the model's "wrong" parameters, $\zeta = 10$ and $\tau_{LI} = 10$.

The estimated error $tr(P_f)$ —> actual.

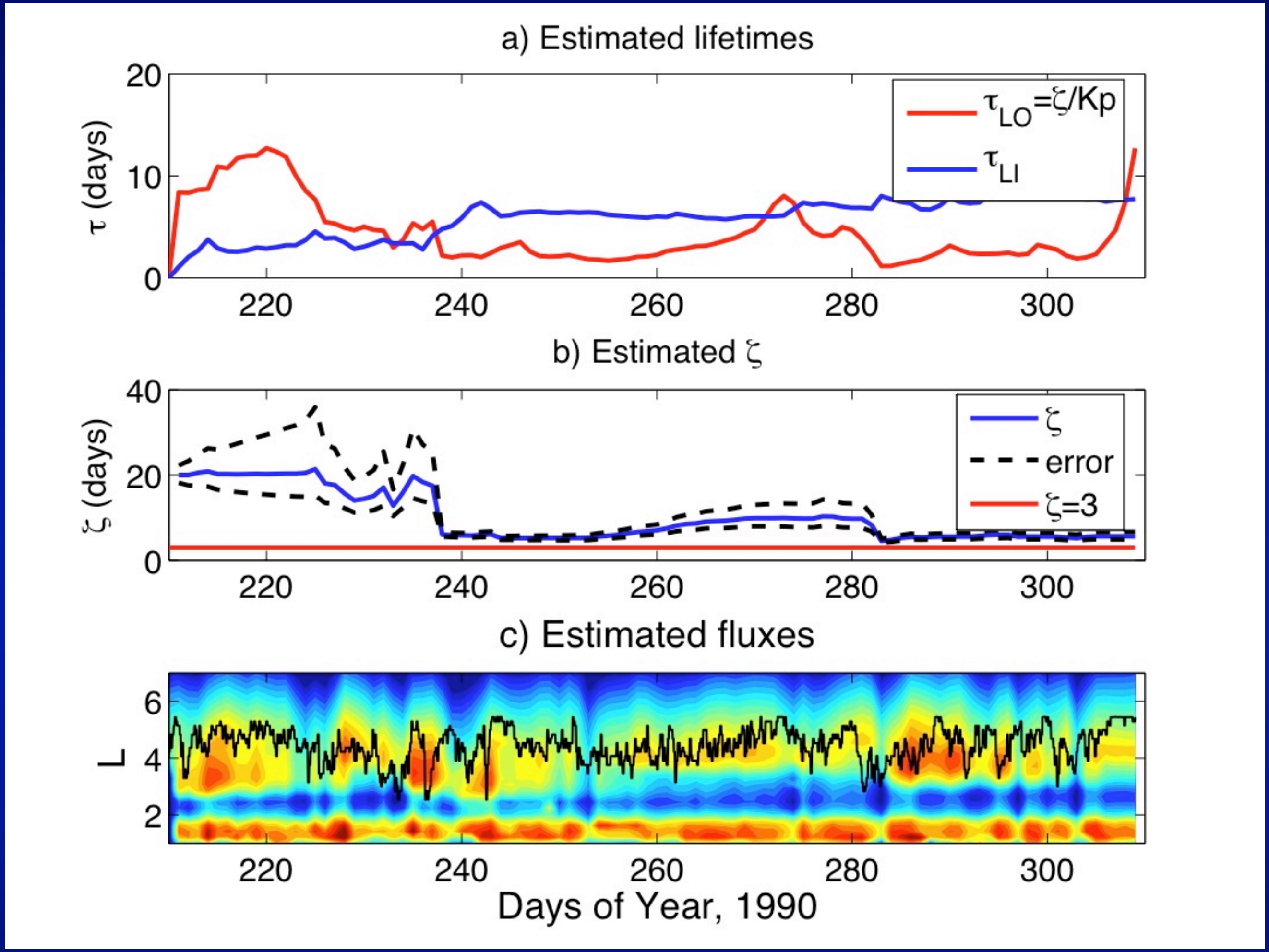
When the parameters' assumed uncertainty is large enough, their EKF estimates converge rapidly to the "truth."







Parameter estimation for space physics – IV



- Daily observations from the CRRES are used to estimate parameters ζ and τ_{LI}.
- Losses and sources are different for CIR-driven (September 11, 1990; DOY 260–280) and CME-driven (October 9, 1990; DOY 285–300) storms.