

Data Assimilation for the Atmosphere, Ocean, Climate and Space Plasmas: Some Recent Results



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Joint recent work with

D. Kondrashov, J. D. Neelin, Y. Shprits and R. M. Thorne, UCLA; C.-J. Sun, NASA Goddard; A. Carrassi, IRM, Brussels; A. Trevisan, ISAC-CNR, Bologna; F. Uboldi, Milano; and many others: please see <http://www.atmos.ucla.edu/tcd/>

Outline

- **Data in meteorology and oceanography**
 - *in situ* & remotely sensed
- **Basic ideas, data types, & issues**
 - how to combine data with models
 - transfer of information
 - between variables & regions
 - stability of the forecast–assimilation cycle
 - filters & smoothers
- **Parameter estimation**
 - model parameters
 - noise parameters – at & below grid scale
- **Subgrid-scale parameterizations**
 - deterministic (“classic”)
 - stochastic – “dynamics” & “physics”
- **Novel areas of application**
 - space physics
 - shock waves in solids
 - macroeconomics
- **Concluding remarks**

Main issues

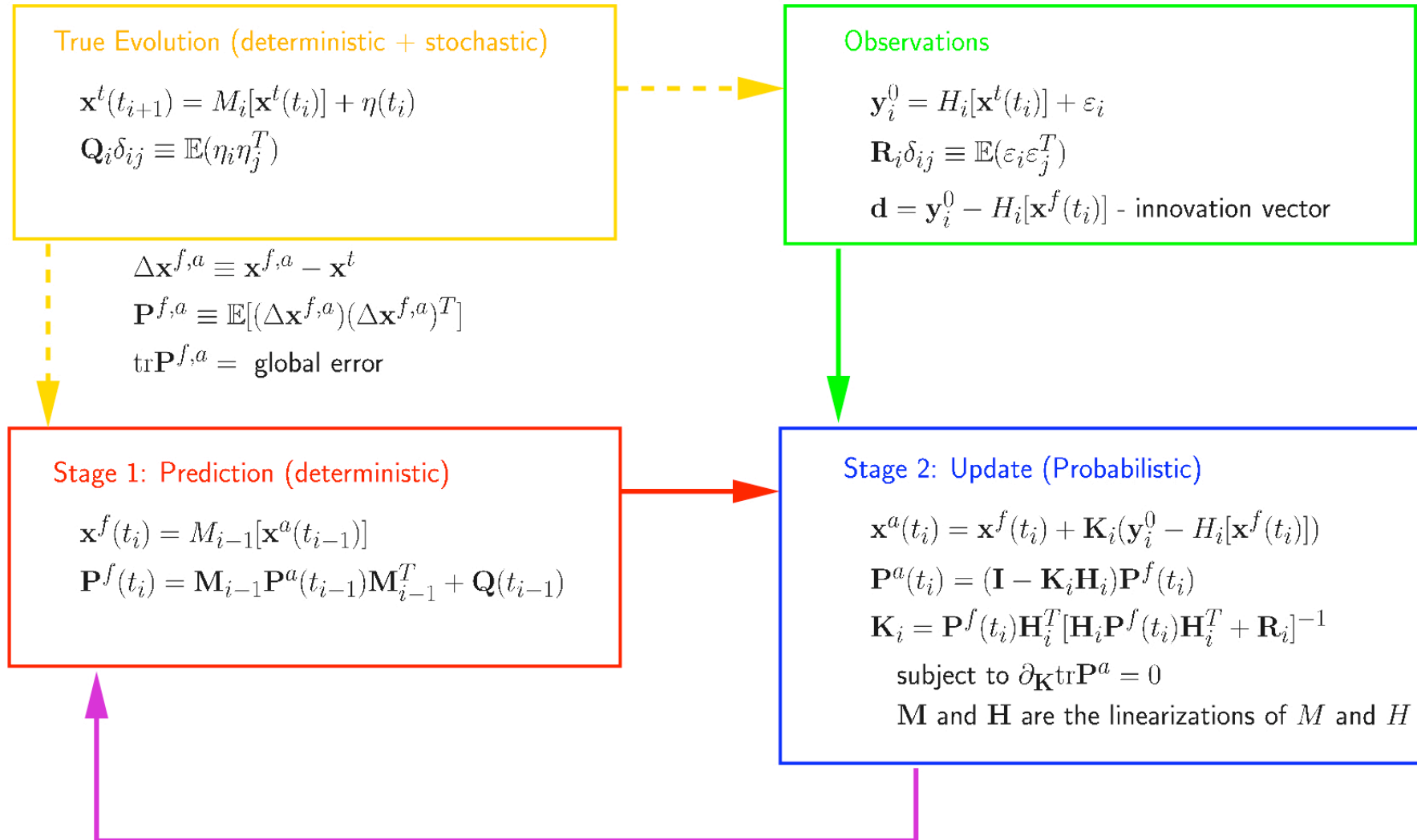
- The **solid earth stays put** to be observed, **the atmosphere, the oceans, & many other things, do not.**
- **Two types of information:**
 - **direct** → **observations**, and
 - **indirect** → **dynamics** (from past observations);
both have **errors**.
- **Combine** the two in (an) optimal way(s)
- Advanced data assimilation methods provide such ways:
 - **sequential estimation** → **the Kalman filter(s)**, and
 - **control theory** → **the adjoint method(s)**
- The two types of methods are essentially equivalent for simple linear systems (the **duality principle**)

Main issues (continued)

- 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).

The (extended) Kalman Filter (EKF)

(Extended) Kalman Filter (EKF)



Basic concepts: barotropic model

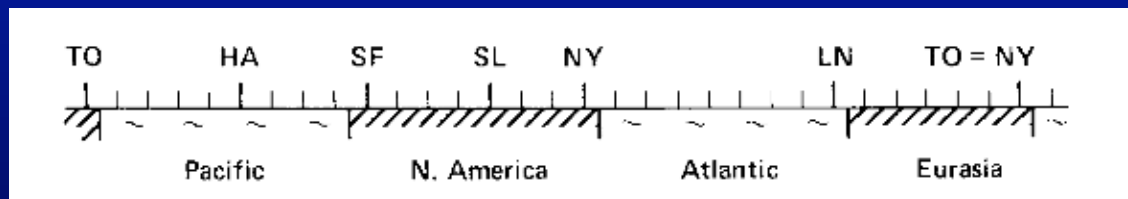
Shallow-water equations in 1-D, linearized about $(U, 0, \Phi)$, $fU = -\Phi_y$
 $U = 20 \text{ ms}^{-1}$, $f = 10^{-4} \text{ s}^{-1}$, $\Phi = gH$, $H \approx 3 \text{ km}$.

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

$$v_t + Uv_x + fu = 0$$

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

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

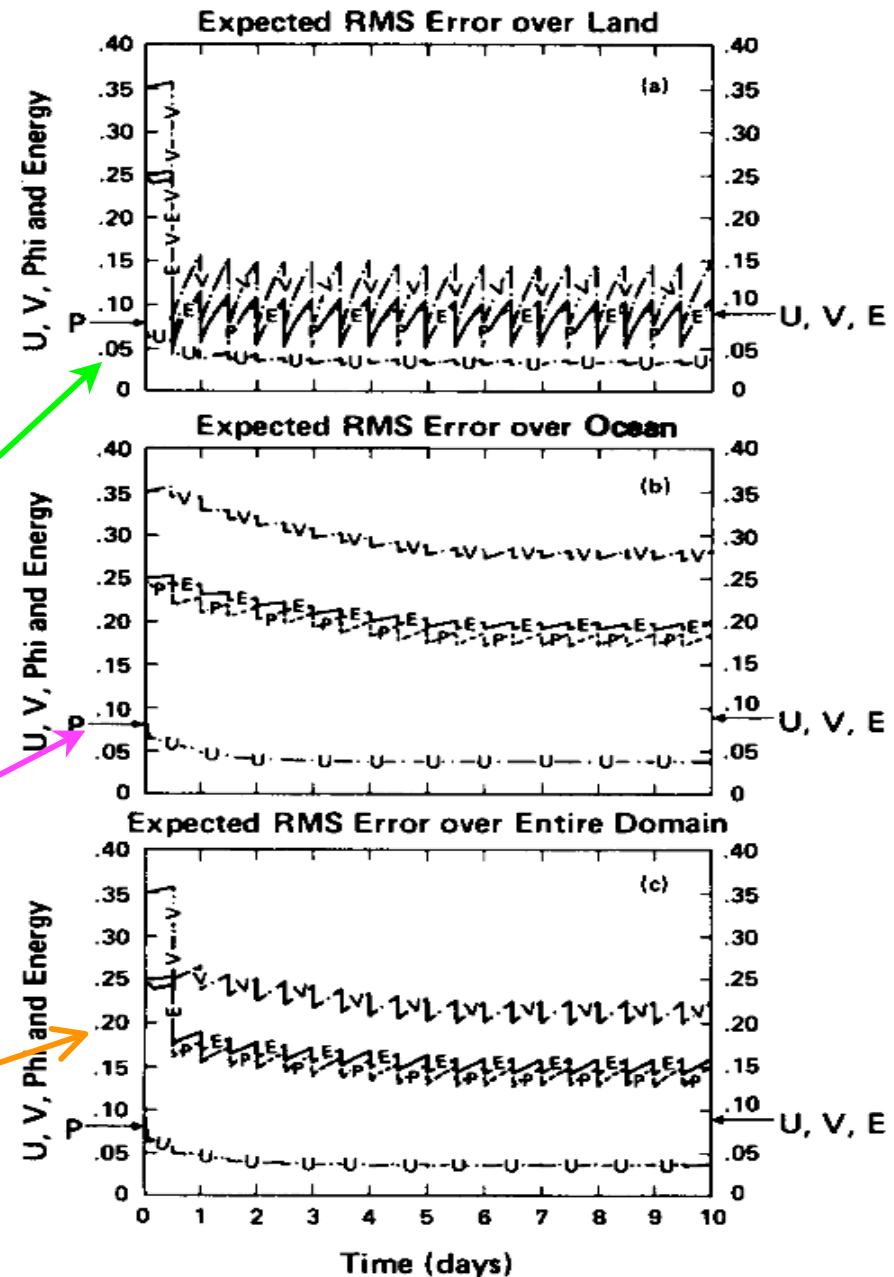
$$R \ll Q \Rightarrow P_{\infty} \approx R;$$

(ii) “poor” observations

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

(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):

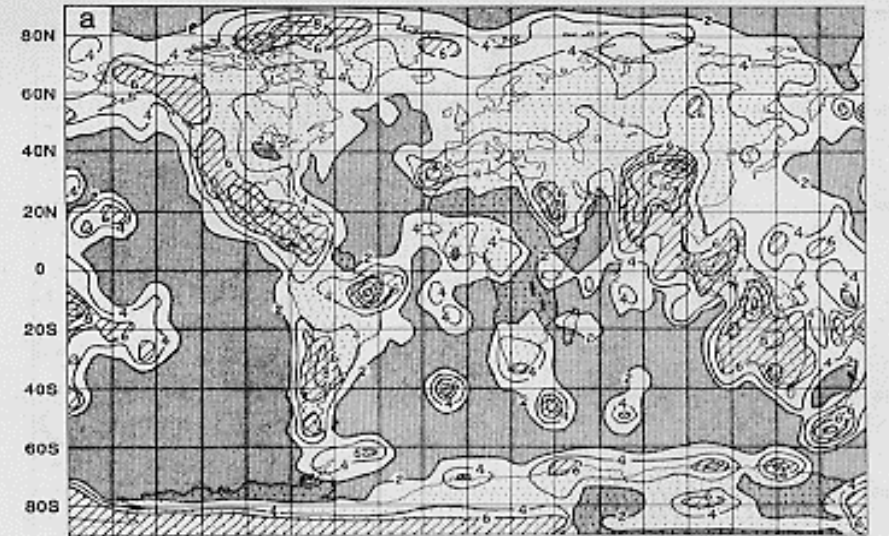
*Errors drastically reduced,
as info. now comes in,
off the ocean*

ϕ_{300}

Halem, Kalnay, Baker & Atlas

(BAMS, 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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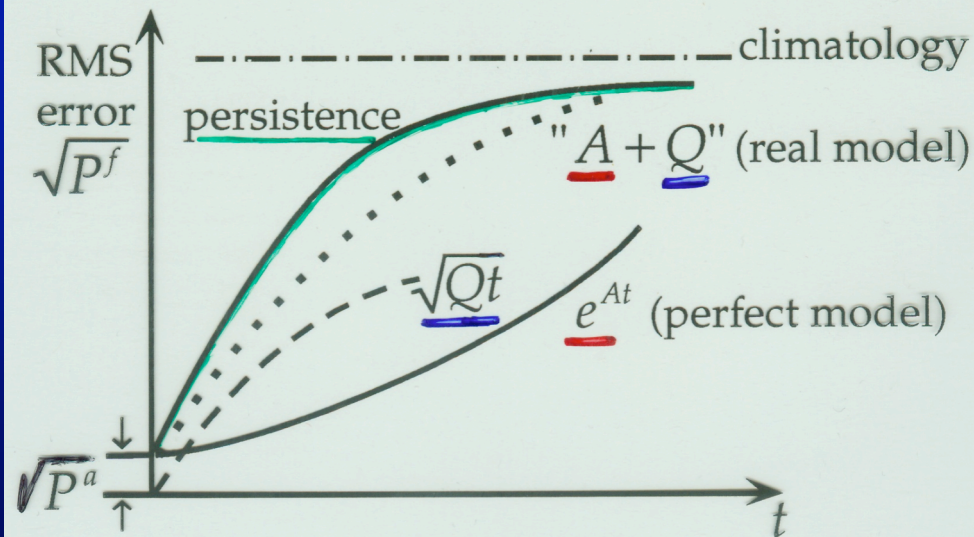
Error components in forecast–analysis cycle

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

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

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

$$\mathbf{x}_{n+1}^f = M(\mathbf{x}_n^a)$$

Corresponding perturbative (tangent linear) equation

$$\delta\mathbf{x}_{n+1}^f = \mathbf{M}\delta\mathbf{x}_n^a$$

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

If observations are available and we assimilate them:

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

$$\mathbf{x}_{n+1}^a = [\mathbf{I} - \mathbf{K}\mathbf{H} \ \mathbf{0}]M(\mathbf{x}_n^a) + \mathbf{K}\mathbf{y}_{n+1}^o$$

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

$$\delta\mathbf{x}_{n+1}^a = [\mathbf{I} - \mathbf{K}\mathbf{H}]M\delta\mathbf{x}_n^a$$

- The matrix $(\mathbf{I} - \mathbf{K}\mathbf{H})$ is expected, in general, to have a **stabilizing effect**;
- the free-system instabilities, which dominate the forecast step error growth, can be reduced during the analysis step.

Joint work with A. Carrassi, A. Trevisan & F. Uboldi

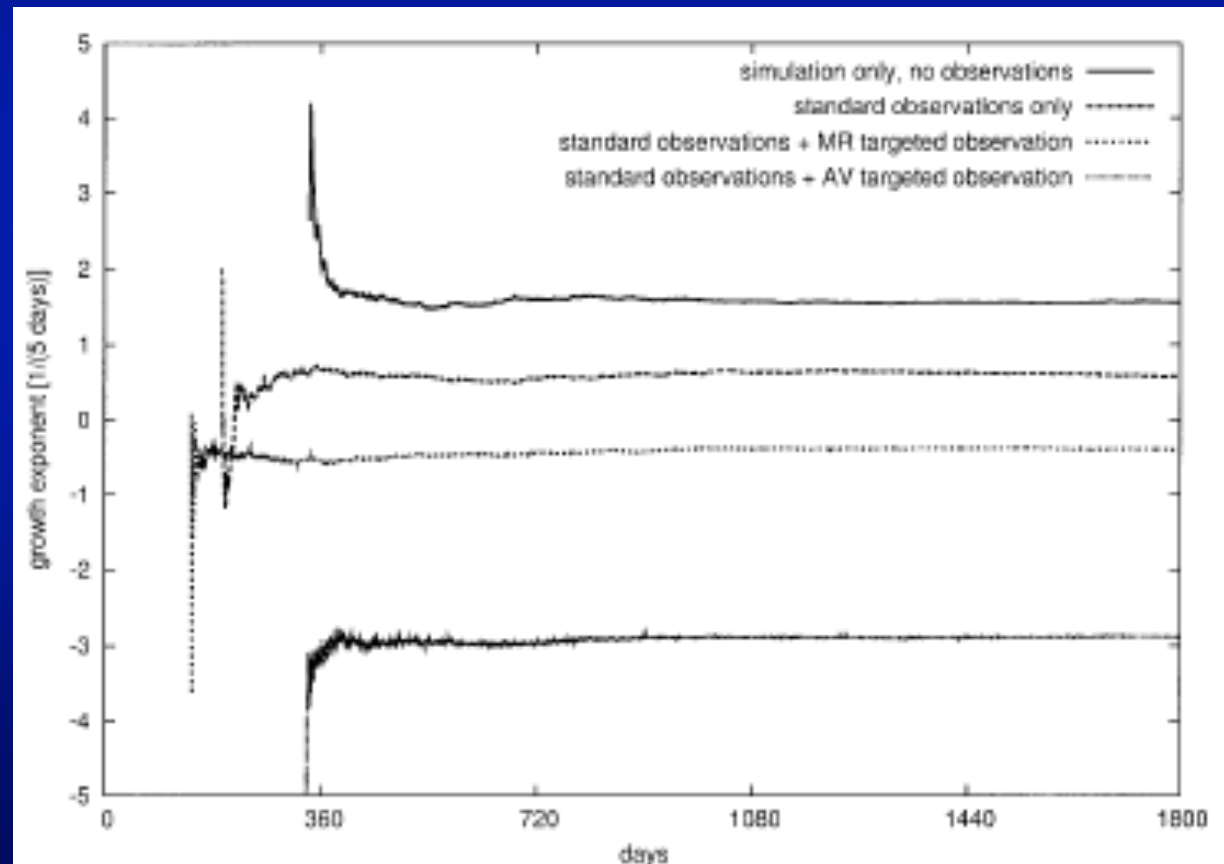
Stabilization of the forecast–assimilation system – I

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 (JAS, 2004)

Stabilization of the forecast–assimilation system – II

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

Spectrum of Lyapunov exponents:

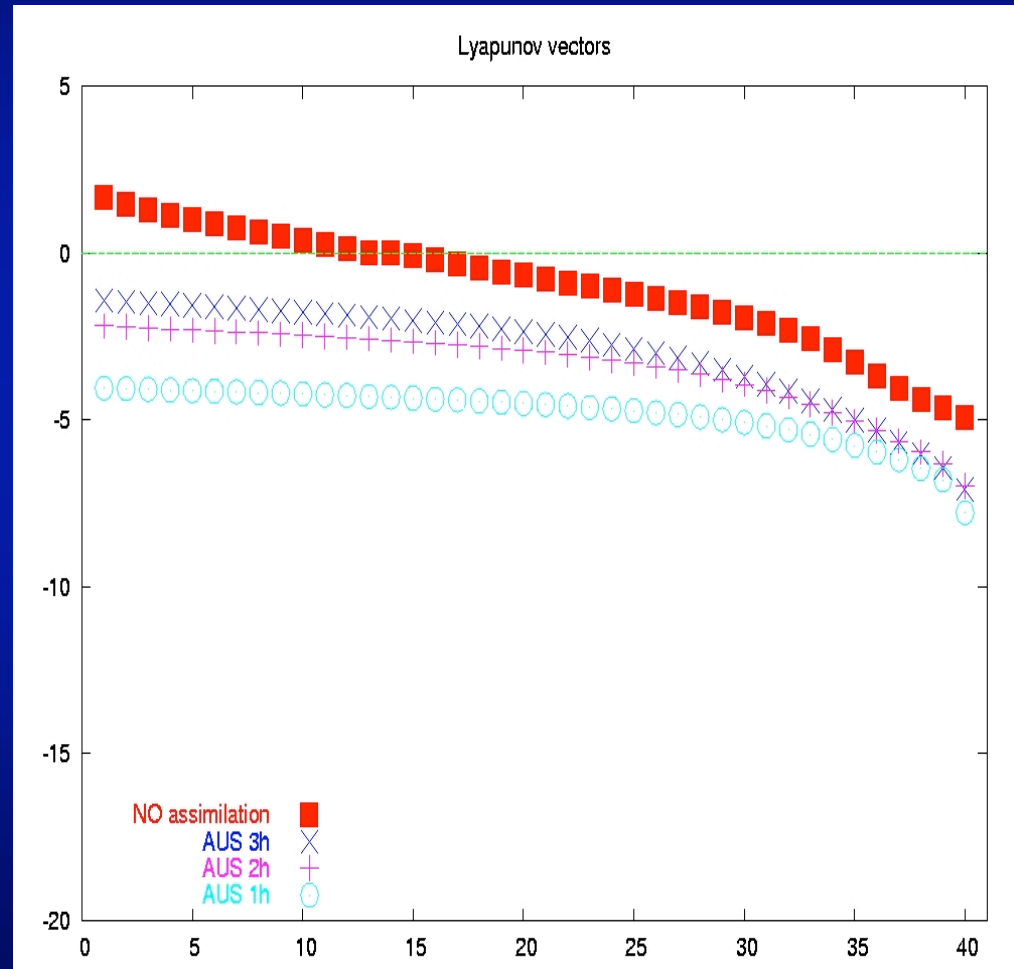
Red: free system

Dark blue: AUS with 3-hr updates

Purple: AUS with 2-hr updates

Light blue: AUS with 1-hr updates

Carrassi, Ghil, Trevisan & Uboldi,
2007, *sub judice*

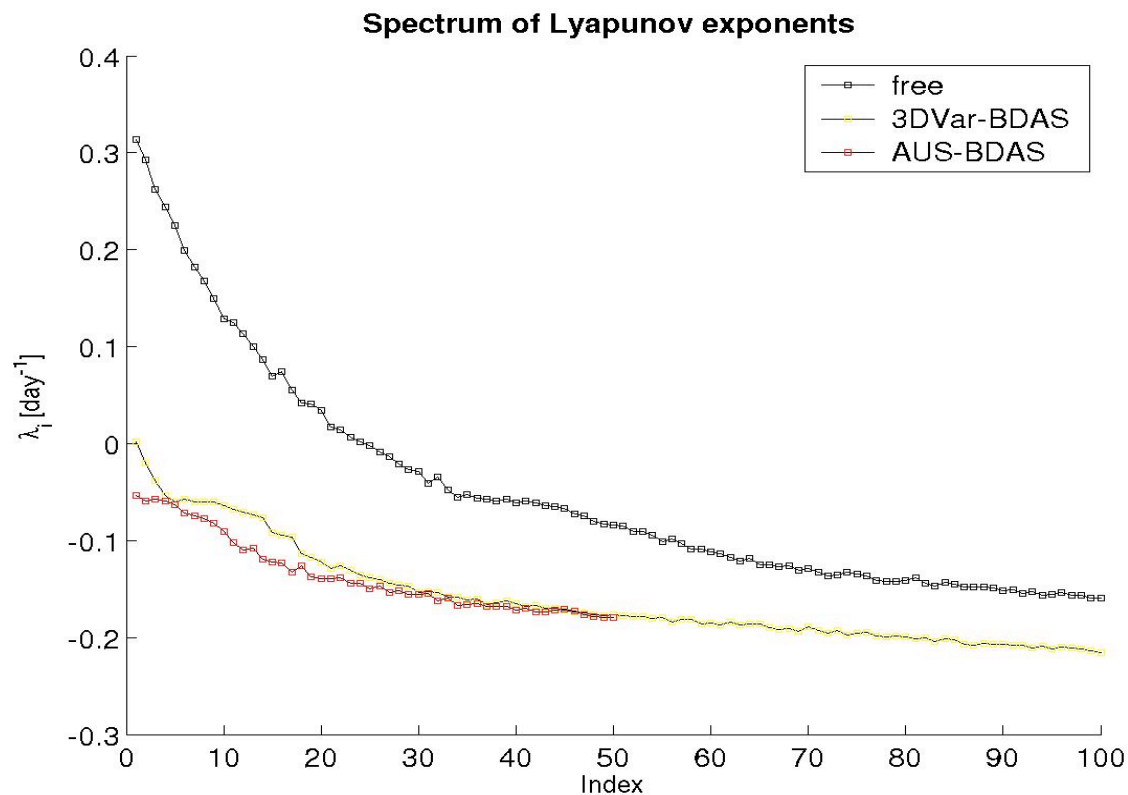


Stabilization of the forecast–assimilation system – III

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 \Rightarrow Unstable subspace reduction



► Free System

Leading exponent:

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

Doubling time ≈ 2.2 days;

Number of positive exponents:

$$N^+ = 24;$$

Kaplan-Yorke dimension ≈ 65.02 .

► 3-DVar–BDAS

Leading exponent:

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

Kaplan-Yorke dimension ≈ 1.1

► AUS–BDAS

Leading exponent:

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

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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

$$L(\rho)\eta = w(t), \quad L - \text{AR(MA) model, } \rho = (\rho_1, \rho_2, \dots, \rho_M)$$

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

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** (Kravtsov *et al.*, 2005, Kondrashov *et al.*, 2005)

Estimating noise – I

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

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

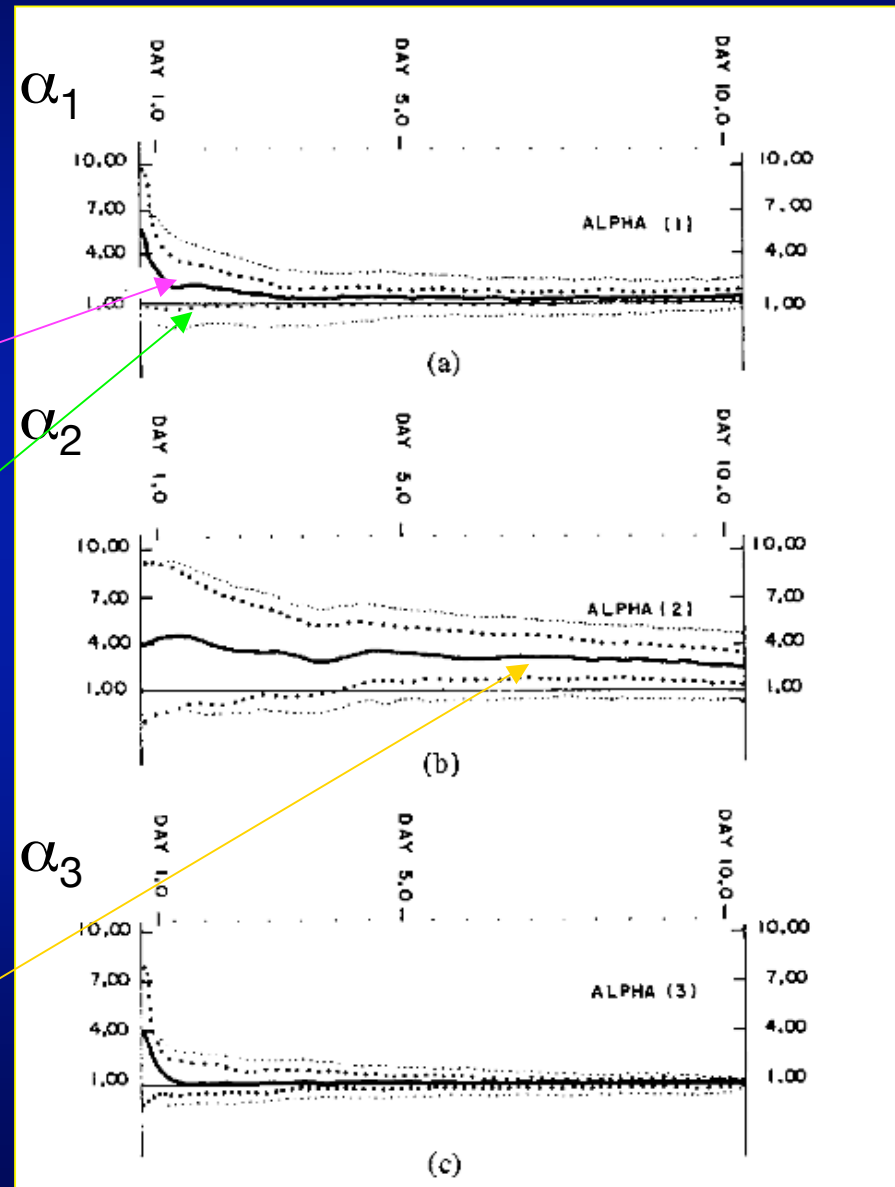
$$Q = \sum \alpha_j Q_j; \quad R = \sum \alpha_j R_j;$$

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

$$Q(0) = 25 * I.$$

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

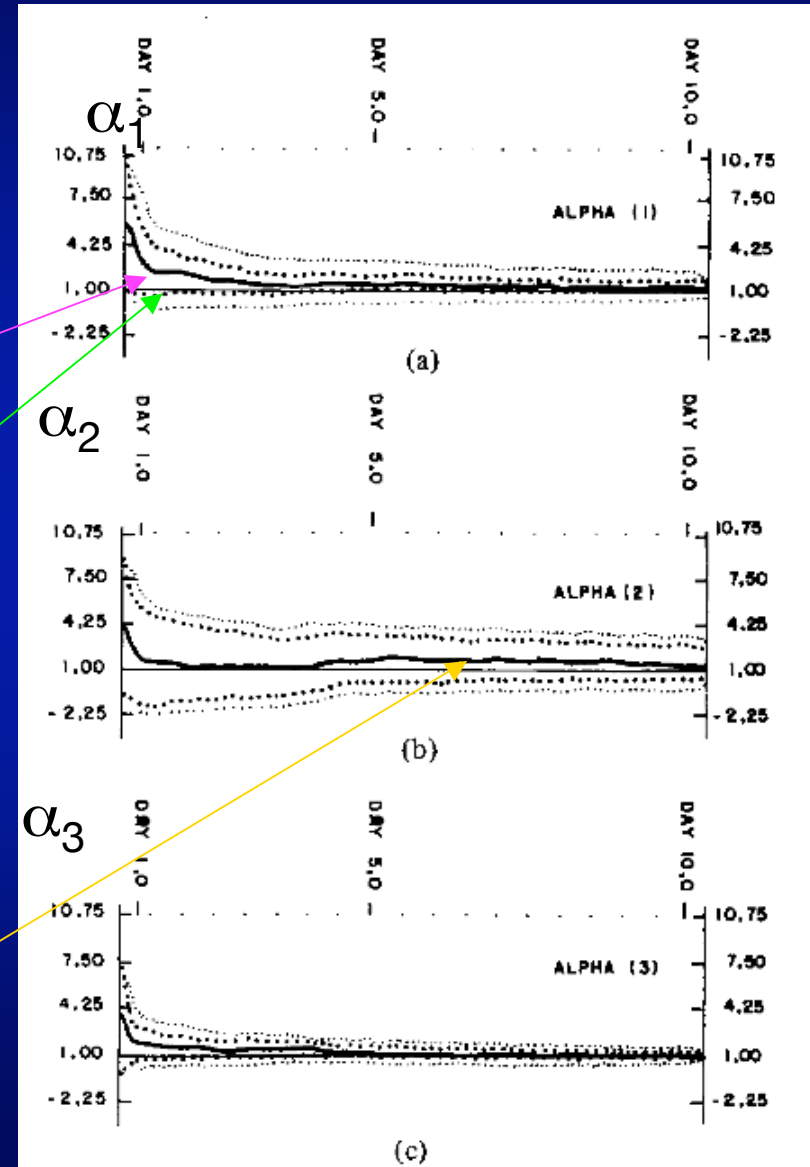
$$\Theta(0) = 25 * \begin{bmatrix} 1 & 0.8 & 0 \\ 0.8 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

estimated

true ($\alpha = 1$)

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

Good convergence for Q_{fast} !



Parameter Estimation

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Nonlinear approach: Empirical mode reduction (Kravtsov *et al.*, 2005, Kondrashov *et al.*, 2005)

Sequential parameter estimation

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

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

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

$$\bar{x}_k^a = \bar{x}_k^f + \bar{K} (y_k^o - \bar{H} \bar{x}_k^f); \quad \bar{K} = \bar{P}^f \bar{H}^T (\bar{H} \bar{P}^f \bar{H}^T + R)^{-1}$$

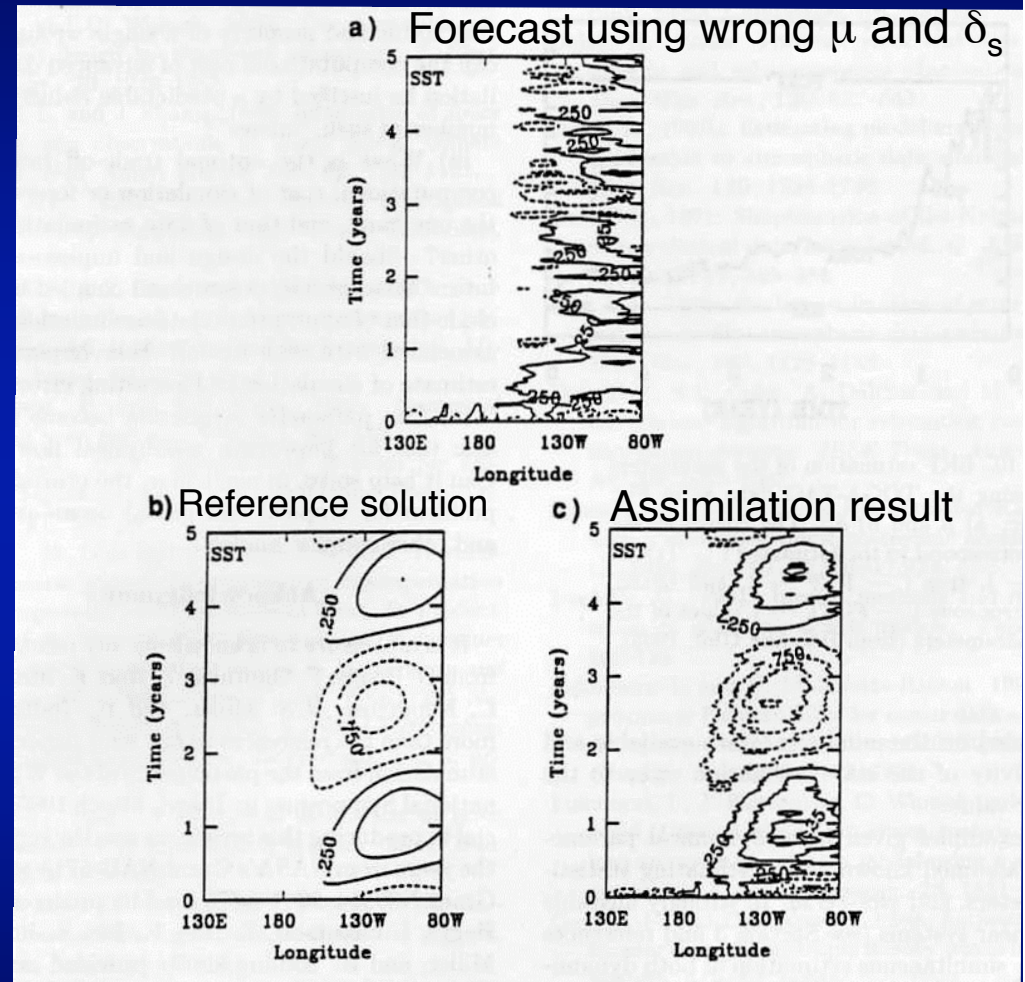
- **The parameters are not directly observable, but** the **cross-covariances** drive parameter changes from innovations of the state:

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

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

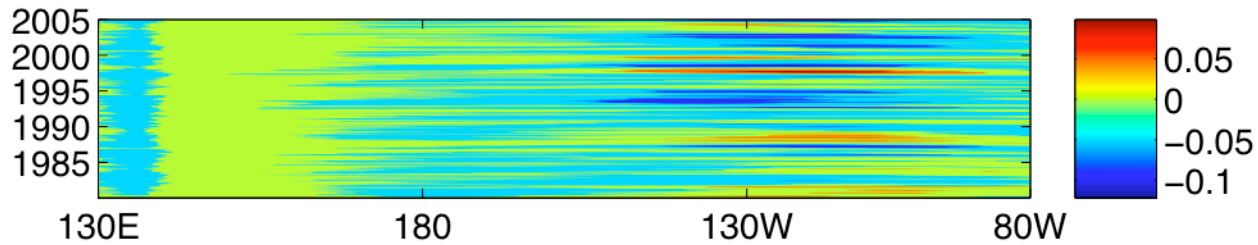
Parameter estimation for coupled O-A system

- 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.
- M. Ghil (1997, *JMSJ*); Hao & Ghil (1995, *Proc. WMO Symp. DA Tokyo*); Sun *et al.* (2002, *MWR*).
- *Current work with D. Kondrashov, J.D. Neelin, & C.-j. Sun.*

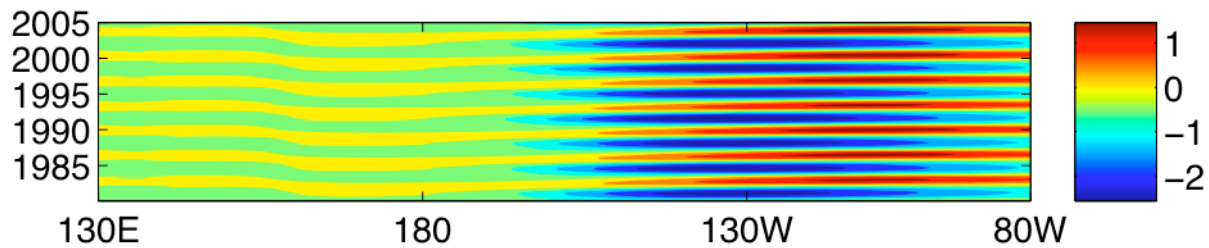


Coupled O-A Model (ICM) vs. Observations

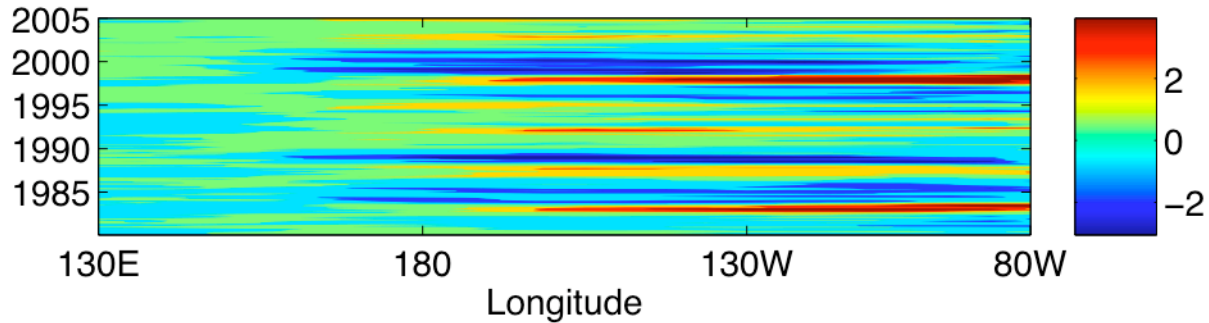
SSTA for westward-propagating regime: $\delta_s = 0.8, \mu = 0.56$



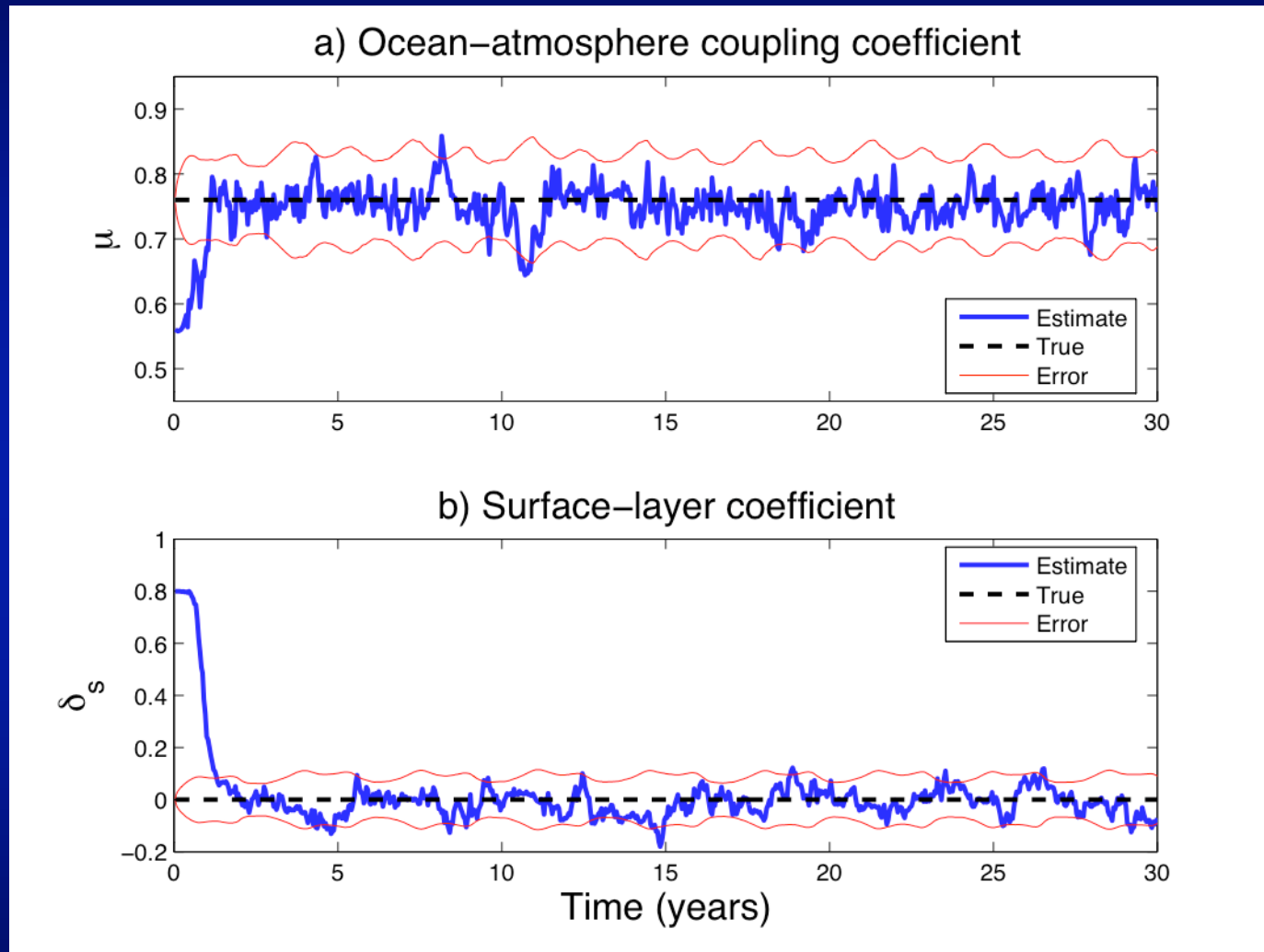
SSTA for delayed-oscillator regime: $\delta_s = 0, \mu = 0.76$



SSTA in NCAR-NCEP Reanalysis

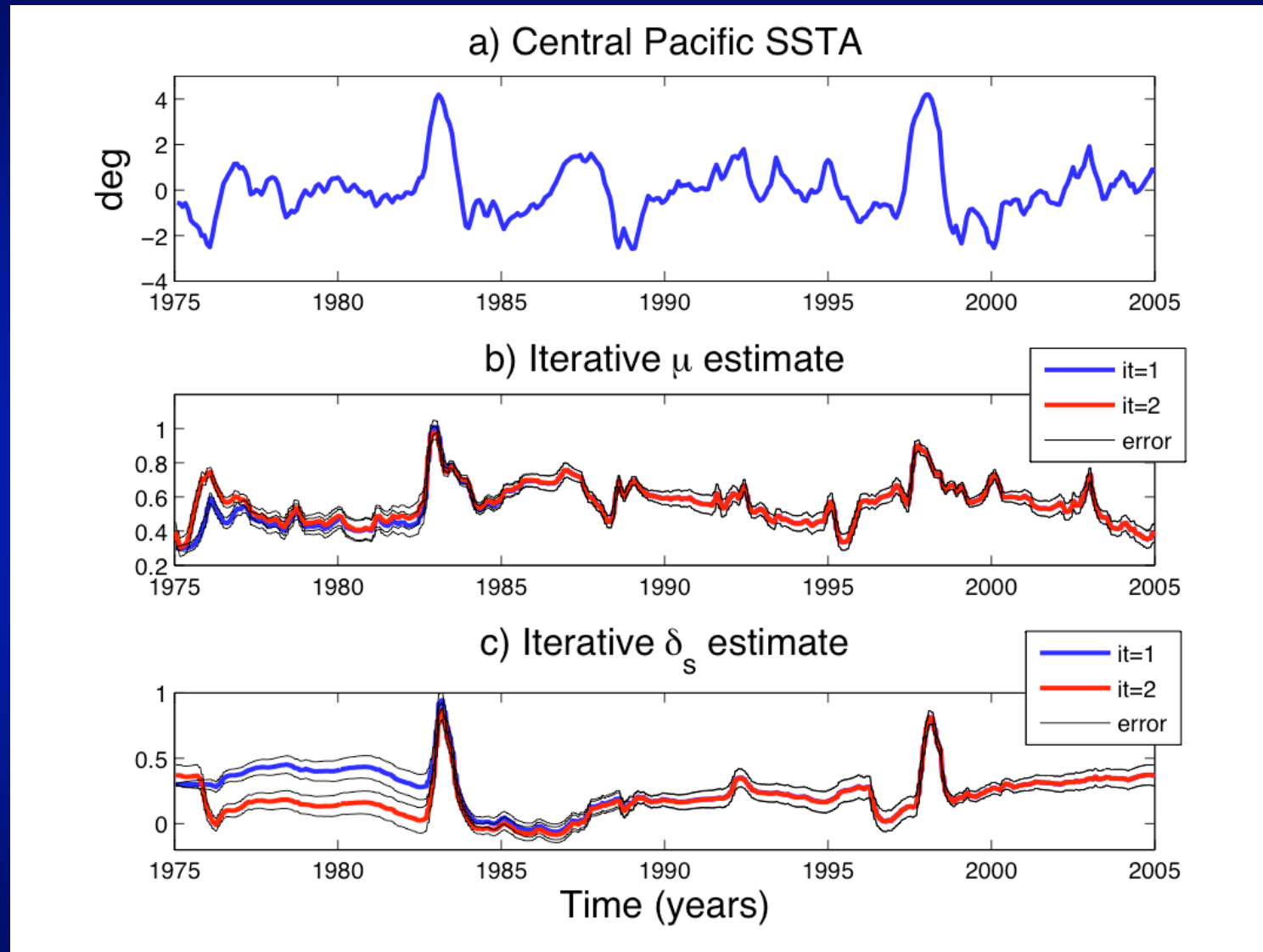


Convergence of Parameter Values – I



Identical-twin experiments

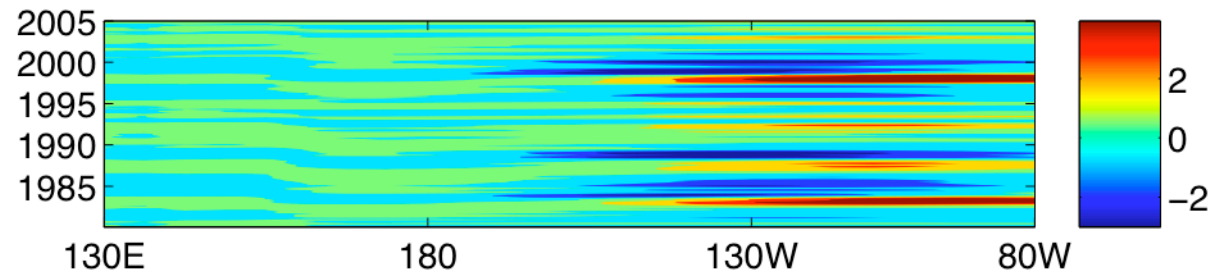
Convergence of Parameter Values – II



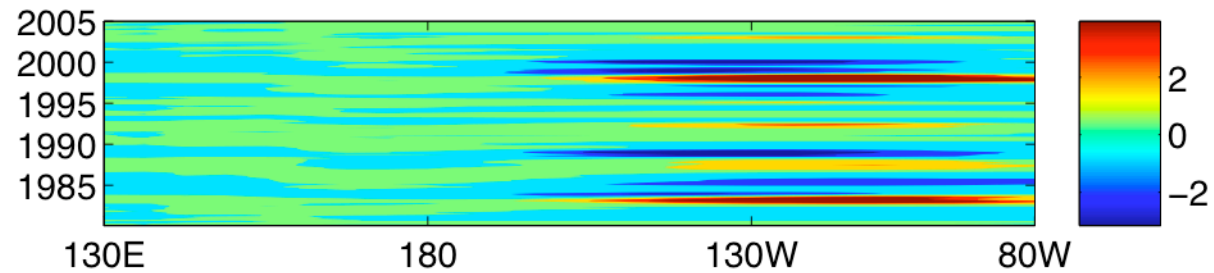
Real SSTA data

EKF results with and w/o parameter estimation

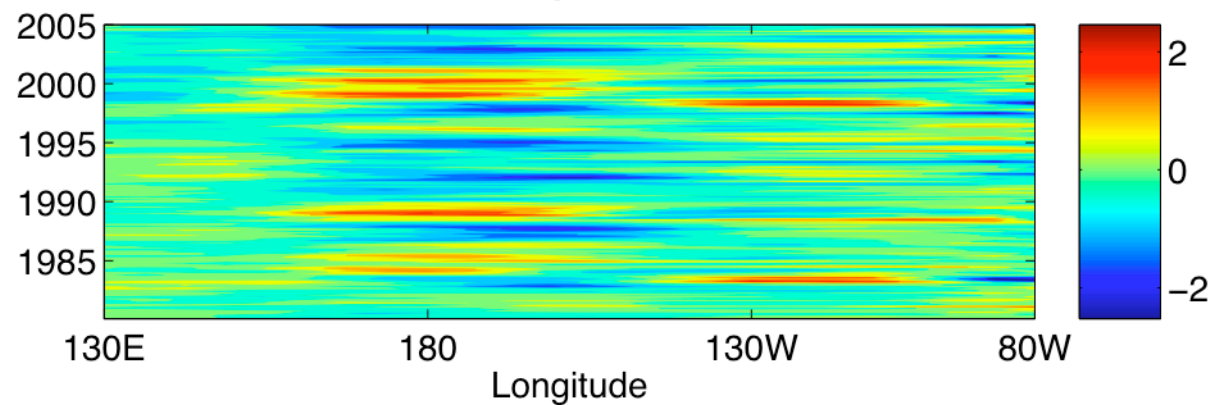
SSTA from EKF with fixed $\mu = 0.76$, $\delta_s = 0$



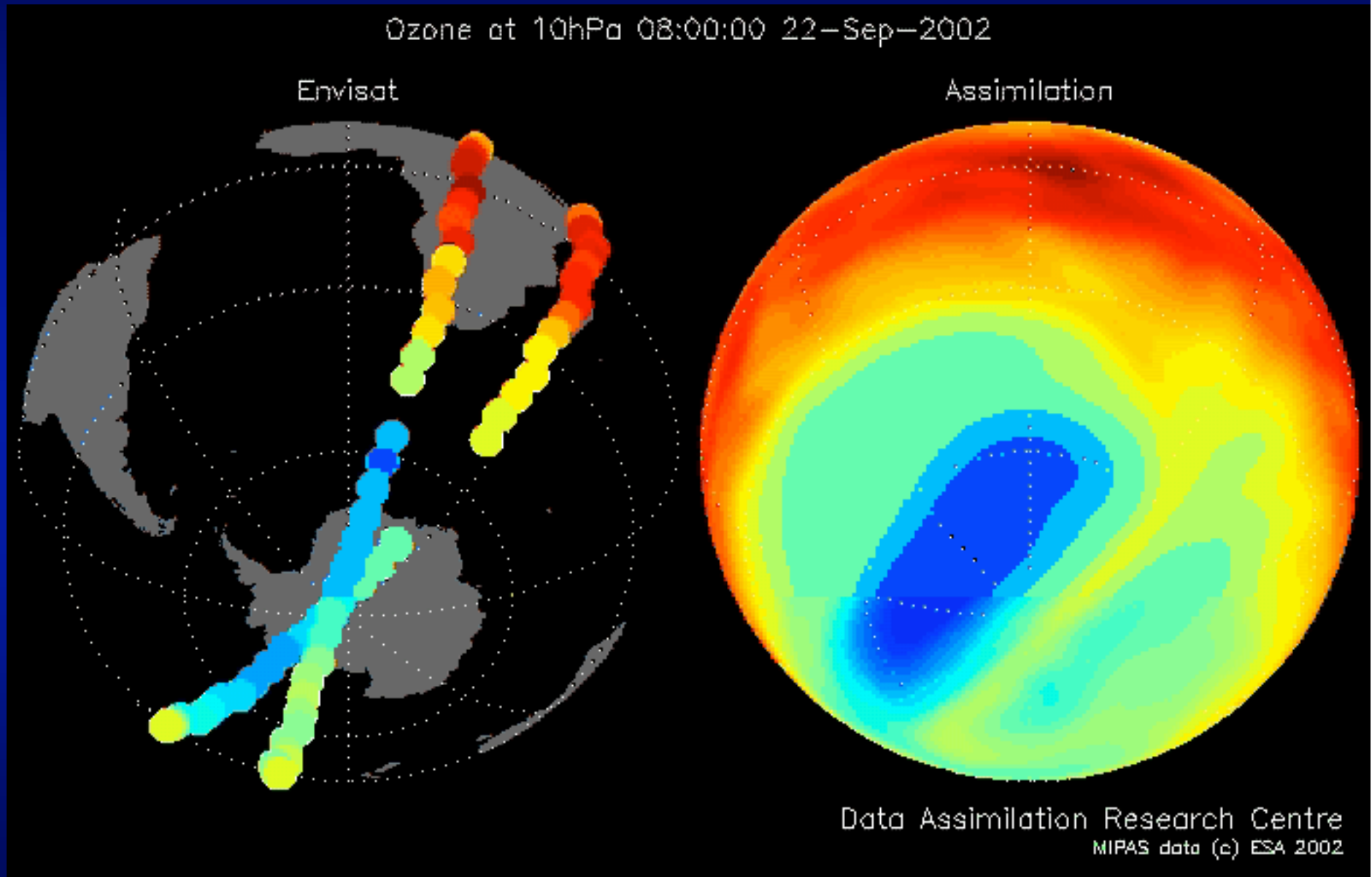
SSTA from EKF with μ and δ_s estimation



SSTA difference of EKF (μ , δ_s) estimation and NCEP-NCAR

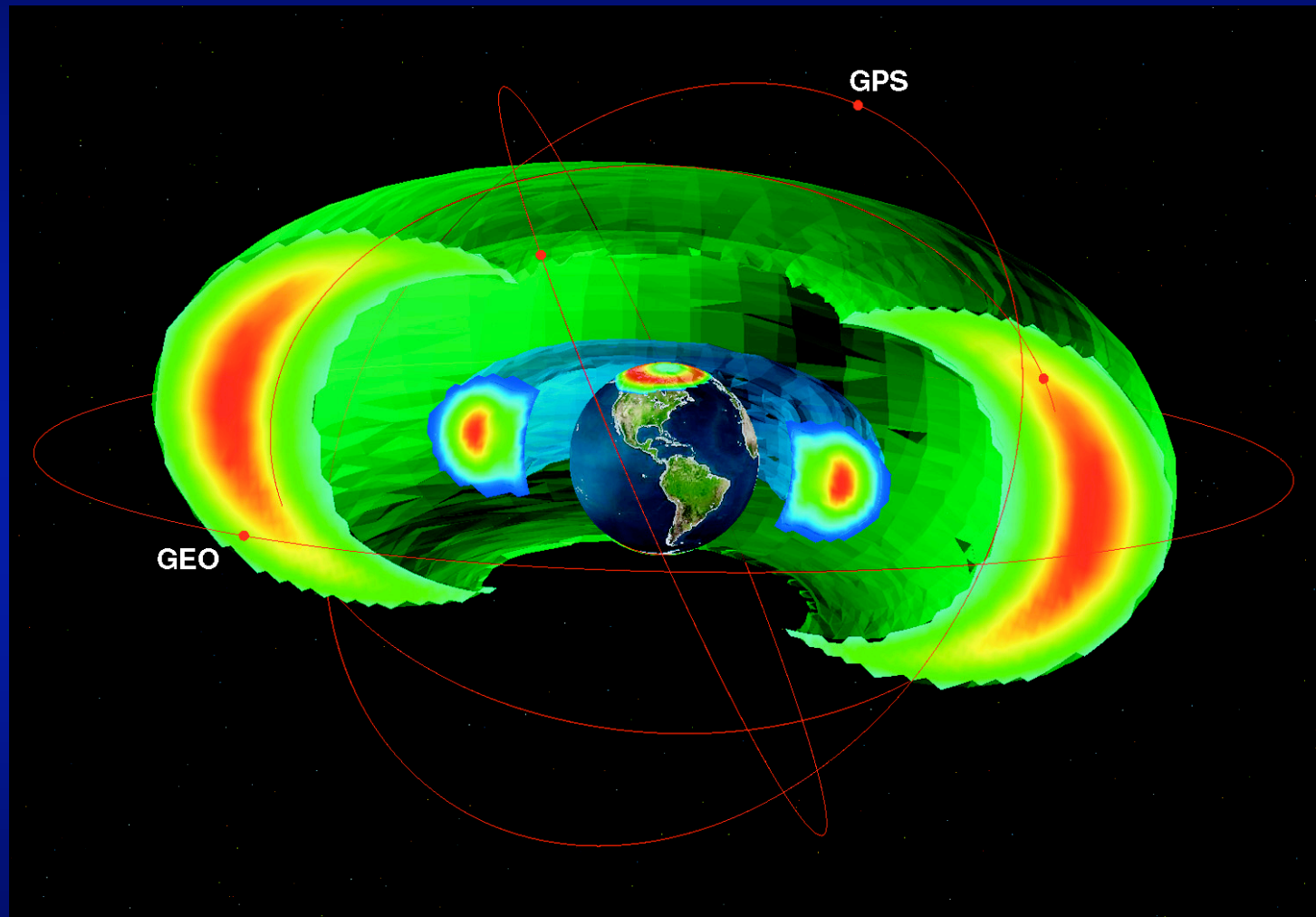


How data assimilation fills the ozone hole: Model information fills in the gaps in stratospheric ozone concentration levels between satellite tracks



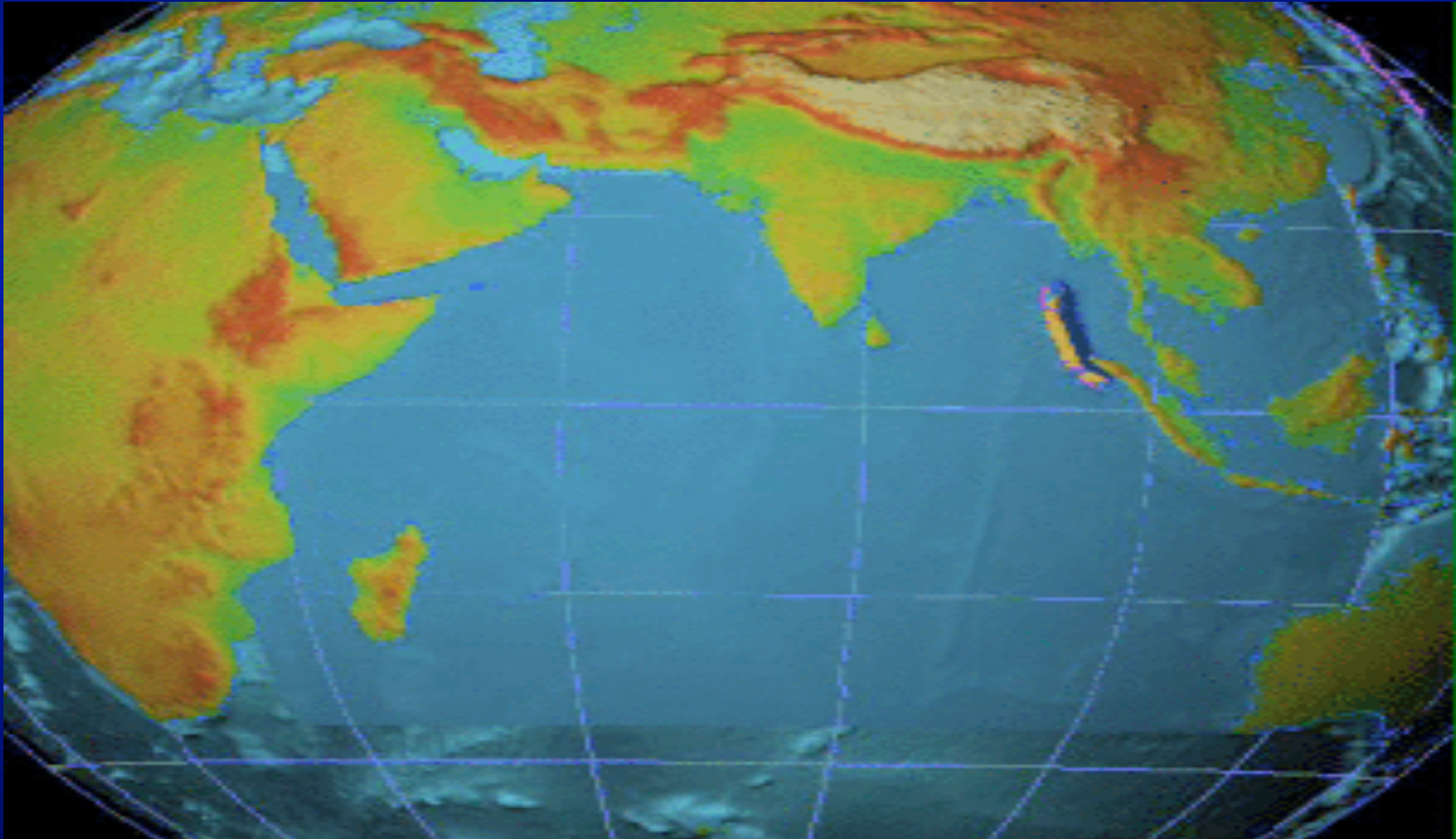
DARC, Reading, UK (courtesy Bill Lahoz)

Space physics data



Space platforms in Earth's magnetosphere

The December 2004 Sumatra–Indian Ocean Tsunami



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 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, 1997a, b, *DAO*);
 - 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.

Concluding remarks

- **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**.
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 - *They help **estimate** both **ocean and coupling parameters**.*
 - *Changes in estimated parameters compensate for **model imperfections**.*
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 - *Changes in estimated parameters compensate for **model imperfections**.*
-
- **Novel areas of application**: space physics, **shock waves** in solids, laboratory experiments in fluids, **tsunamis**, **macroeconomics**
 - **Novel approaches and methods**: hard- and software, **data-adaptive observations**
 - **Next decade** in data assimilation **should be interesting!**
- <http://www.atmos.ucla.edu/tcd/>



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

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

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General references

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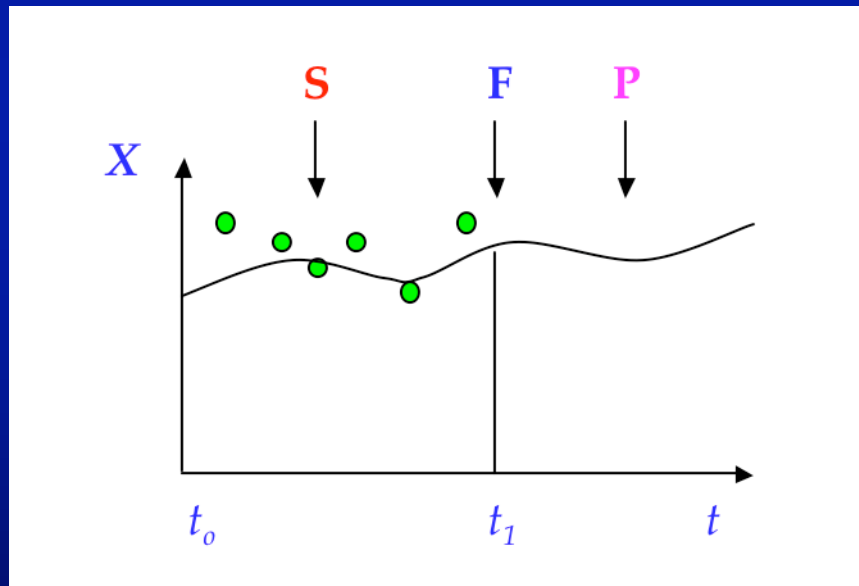
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Reserve slides

The main products of estimation^(*)

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



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!!!**

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

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).

Evolution of DA – II

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

A. Continuous (linear) Kalman Filter	
System Model	$\dot{\mathbf{w}}^s(t) = F(t)\mathbf{w}^s(t) + G(t)\mathbf{b}^s(t), \quad \mathbf{b}^s(t) \sim N[0, Q(t)]$
Measurement Model	$\mathbf{w}^o(t) = H(t)\mathbf{w}^s(t) + \mathbf{b}^o(t), \quad \mathbf{b}^o(t) \sim N[0, R(t)]$
State estimation	$\dot{\mathbf{w}}^a(t) = F(t)\mathbf{w}^a(t) + K(t)[\mathbf{w}^o(t) - H(t)\mathbf{w}^a(t)], \quad \mathbf{w}^a(0) = \mathbf{w}_0^a$
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	$E\{\mathbf{w}^s(0)\} = \mathbf{w}_0^s, \quad E\{[\mathbf{w}^s(0) - \mathbf{w}_0^s][\mathbf{w}^s(0) - \mathbf{w}_0^s]^T\} = P_0$
Assumptions	$R^{-1}(t)$ exists $E\{\mathbf{b}^s(t)[\mathbf{b}^o(t')^T]\} = 0$
Performance Index	$J^{f,s}(t) = E\{[\mathbf{w}^{f,s} - \mathbf{w}^s][\mathbf{w}^{f,s} - \mathbf{w}^s]^T\}$
B. Continuous (linear) Optimal Control	
System Model	$\dot{\mathbf{w}}(t) = \tilde{F}(t)\mathbf{w}(t) + \tilde{H}(t)\mathbf{u}(t)$
Measurement Model	$\mathbf{w}^o(t) = \mathbf{w}(t)$ (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	$\mathbf{w}(t_f) = 0$ $\tilde{P}(t_f) = \tilde{Q}_f$
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
$\mathbf{w}^o(t)$ 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.

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).

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.
 - EKF, 4-D Var (2nd duality).
- **Post-industrial DA:**

(Satellite) images --> (weather) forecasts, climate “movies” ...

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.)

^aof state and errors

^bMeandros

^c “You cannot do so even once” (subsequent development of “flux” theory by Plato, cca. 400 B.C.)

Τα πάντα ρει = Everything flows