Scale interactions, data-driven modeling, and uncertainty in weather and climate, TRR 165/181 Joint Conference, DFG Katholische Universität Eichstätt-Ingolstadt 28 March 2023

## Data Assimilation: From an Eventful Past to a Bright Future



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The most recent results are joint with Eviatar Bach (Caltech) and Dan Crisan (ICL)





Joint work with many people over the years Please see, for names & references https://dept.atmos.ucla.edu/tcd/ , & https://www.researchgate.net/profile/Michael\_Ghil

## 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 (i) variables & (ii) regions
  - filters & smoothers
- > Why does data assimilation work in planetary flows?
  - geostrophic adjustment
  - model & noise parameters at & below grid scale
  - stability of the forecast-assimilation (FA) process
- Machine learning
- Novel areas of application
  - space physics
  - solid Earth
  - paleoclimate
  - detection & attribution (DADA)
  - macroeconomics
- Concluding remarks and bibliography

## Main issues

- The solid earth stays put to be observed, the atmosphere, the oceans, & many other things, do not.
- Two types of information:
  - direct  $\rightarrow$  observations, and
  - indirect → dynamics (from past observations) <= ML!</li>
     both have errors.
- Combine the two in (an) optimal way(s)
- Advanced data assimilation methods provide such ways:
  - sequential estimation  $\rightarrow$  the Kalman filter(s), and
  - control theory  $\rightarrow$  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) of, as well as improvements over, currently operational methods (4-D Var, EnKF).

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## **Atmospheric data**

FGGE level II-b data Drifting 12 GMT 9 January 1979 buoys:  $P_s$  – 267 Polar-orbitius satel Cloud-drift: V -2x2259Aircraft: 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 Buovs Surface pressure observations from drifting buoys Colba Constant level balloon Drope Radiosondes dropped from aircraft Pilote Wind measurements from ascending balloons Satoma 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 radioson

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<sup>5</sup>) scalars per 12h–24h
♣ 0(10<sup>2</sup>) observations/[(significant *d-o-f*) x (significant Δ*t*)]
Nowadays 0(10<sup>7</sup>) obs. & more *d-o-f* of interest, too!

## 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  $\Rightarrow$  sea level; scatterometry  $\Rightarrow$  surface winds & sea state; acoustic tomography  $\Rightarrow$  temperature & density; etc.



#### Courtesy of Tong ("Tony") Lee, JPL

### Ocean data – past, present & future



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

- 3-D ocean obs. are still not really there: ocean tomography didn't work out but drifters are doing a better & better job.
- Two forms of DA for the coupled system:
  - weak coupling: models coupled, DA not;
  - strong coupling: both coupled; could work.

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## **Evolution of DA**

Organization or country	Operational analysis methods	Analysis area	Analysis/forecast
Australia	Successive correction method (SCM)	SH <sup>d</sup>	12 hr
	Variational blending techniques	Regional	6 hr
Canada	Multivariate 3-D statistical interpolation	NH <sup>4</sup> 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	Global	6 hr
	interpolation (repeated insertion of data)	Giobal	·
U.S.A.	Spectral 3-D analysis	Global	
	Multivariate 3-D statistical interpolation	Global	6 hr
U.S.S.R.	2-D <sup>c</sup> statistical interpolation	NH	12 hr
ECMWF <sup>6</sup>	Multivariate 3-D statistical interpolation	Global	6 hr

<sup>b</sup> European Centre for Medium Range Weather Forecasts.

<sup>c</sup> 2-D is in a horizontal plane.

<sup>4</sup> 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).

### **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)
- $T_2 = T^{\circ}$  **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,

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

then the minimum variance estimator<sup>(\*)</sup> is

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

and its accuracy is

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

(\*) BLUE = Best Linear Unbiased Estimator

### (Extended) Kalman Filter (EKF)



# Advection of information

Upper panel (NoSat): *Errors advected* off the ocean

Ф<sub>300</sub>

Lower panel (Sat): *Errors drastically reduced, as info. now comes in, off the ocean* 

Ф<sub>300</sub>

Halem, Kalnay, Baker & Atlas

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

#### {6h fcst} - {conventional (NoSat)}



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.

## The main products of estimation<sup>(\*)</sup>

- 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 to 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
 (\*\*) DA for Detection & Attribution; <sup>(†)</sup> or, these days, use machine learning (ML)

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## A little history – I

#### SVENSKA GEOFYSISKA FÖRENINGEN

VOLUME 2, NUMBER 4 Tellus NOVEMBER 1950

#### A QUARTERLY JOURNAL OF GEOPHYSICS

Numerical Integration of the Barotropic Vorticity Equation

By J. G. CHARNEY, R. FJÖRTOFT<sup>1</sup>, J. von NEUMANN The Institute for Advanced Study, Princeton, New Jersey<sup>2</sup>

(Manuscript received 1 November 1950)

#### 1. Introduction

One of the aims of the meteorological computer project at Princeton is the application of the hydrodynamic equations to forecasting. Initial conditions for this problem would be furnished by the observations at a starting time,  $t_0$ . At this time it would be required to know the meteorological variables and some of their space derivatives at certain grid points. This could be accomplished by the normal modes of analysis, that is, by subjectively drawing isopleths, and approximating the derivatives by ratios of finite differences.

#### JOURNAL OF METEOROLOGY

VOLUME 6

#### **OBJECTIVE WEATHER-MAP ANALYSIS**

#### By H. A. Panofsky

New York University<sup>1</sup>

(Manuscript received 7 February 1949)

#### ABSTRACT

Wind and pressure fields are fitted by third-degree polynomials in areas of the order of 10<sup>6</sup> square miles. Expressions involving derivatives of wind and pressure are computed and the question of computation of geostrophic deviations is re-examined. A method of connecting polynomials in separate areas is investigated. The following conclusions are drawn:

1. Isopleths and streamlines drawn from the polynomials greatly resemble subjective isopleths and streamlines. In all cases studied, the smoothing seems to be adequate.

2. Horizontal divergence and vertical velocities can be determined as well from the polynomials objectively as by other subjective methods. The errors of observation influence the magnitude of these quantities considerably, but usually do not affect the sign.

3. On the scale of these measurements, reliable pressure gradients can be obtained objectively; however, the Laplacian of pressure is very much affected by the technique of analysis and by observational errors.

4. Reliable values of the geostrophic deviations can be obtained only under favorable conditions. Hence any method of integration of the fundamental equations which requires knowledge of the geostrophic deviations is to be avoided.

## A little history – II

Use of Incomplete Historical Data to Infer the Present State of the Atmosphere

J. CHARNEY, M. HALEM<sup>1</sup> AND R. JASTROW<sup>1</sup>

Dept. of Meteorology, Massachusetts Institute of Technology, Cambridge, Mass.

22 August 1969

One of the principal objectives of the Global Atmospheric Research Program (GARP) is the acquisition of data which define the synoptic state of the atmosphere globally for use in long-range prediction. Since all pro-

<sup>1</sup>Institute for Space Studies, Goddard Space Flight Center, NASA, New York, N. Y.

posed global sounding systems suffer limitations, the concept has arisen of a combination of several such systems permitting trade-offs among the meteorological parameters and between space and time.<sup>2</sup> The system

<sup>2</sup>See preface in "Plan for U. S. Participation in the Global Atmospheric Research Program," National Academy of Sciences, Washington, D. C., 1969.

"If it should prove to be possible to obtain the large-scale wind field from temperatures alone, the time-table for the implementation of GARP might be substantially advanced."

### Time-Continuous Assimilation of Remote-Sounding Data and Its Effect on Weather Forecasting

M. GHIL<sup>1</sup>, M. HALEM AND R. ATLAS

Laboratory for Atmospheric Sciences, NASA Goddard Space Flight Center, Greenbelt, MD 20771

(Manuscript received 7 April 1978, in final form 6 October 1978)

### Stabilization of the forecast–assimilation (FA) system – I

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)



## DA as a random dynamical systems (RDS) problem

Recall the forecast–assimilation (FA) steps of sequential estimation: in continuous time, & sloppy notation, one can write

### $\hat{x}^{\cdot} = (A - KH)\hat{x} + Kz$

- Clearly Kz is a forcing by the observations z, with some weights K, optimal ("Kalman") or not nudging, variational or what not.
- > The mathematical framework of "open" dynamical systems is appropriate
  - skew-product flows (G. Sell)
  - pullback (Crauel & Flandoli, L. Arnold) or snapshot (C. Grebogi & E. Ott) attractors

#### References

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#### The sources of nonautonomous dynamics

**Physically open vs. closed systems:** fluxes of mass, momentum & energy between the system & its surroundings are present or not.

The mathematical framework of **nonautonomous dynamical systems (NDSs)** is appropriate for physically open ones, in which **the fluxes depend explicitly on time**:

- skew-product flows (G. Sell)
  - $\dot{x} = f(x,q), \ \dot{q} = g(q), \ x \in \mathbb{R}^d, \ q \in \mathbb{R}^n$ , with q the driving force for x.
- pullback (Flandoli, L. Arnold) or snapshot (C. Grebogi & E. Ott) attractors  $dX_t = f(X,q) dt + \sigma(X) dW_t$ ,

where  $W_t$  is a Brownian motion in  $\mathbb{R}^d$  and  $dt \sim (dW)^2$ .

More generally, studying explicit time dependence in forcing or coefficients requires NDSs.

The term **nonautonomous** is used both for the deterministic case and for a unified perspective on the deterministic & the random case.

The commonality between the two cases is (i) the independence & (ii) the semi-group property of the driving force, whether q(t) or  $W_t$ .

Likewise, pullback attractor (PBA) is used both for the deterministic & the random case, while in the latter case uses more specifically the phrase random attractor (RA).

## **Time-dependent forcing**, I

- Much of the theoretical work on the intrinsic variability of the wind-driven ocean circulation has been done with time-independent wind stress.
- To address truly coupled ocean—atmosphere behavior and climate change an important step is to examine time-dependent wind stress.
- The proper framework for doing so is the theory of non-autonomous and random dynamical systems (NDS and RDS).
- We do so here with a "toy" model given by the low-order truncation of the QG, equivalent-barotropic potential vorticity equation (PVE).

The forcing is deterministic, aperiodic, and dominated by multi-decadal variability. *x(s, t; x\_0), with x\_0 varying* 

The pullback attractor of a linear, scalar ODE,

$$\dot{x} = -\alpha x + \sigma t, \ \alpha > 0, \ \sigma > 0,$$

is given by

$$a(t) = \frac{\sigma}{\alpha}(t - \frac{1}{\alpha}).$$



Formally, the indexed family  $\mathscr{A}$  of all pullback attracting sets  $\mathcal{A}_t$  is termed the *pullback attractor* (PBA) of the NDS, if the following two conditions are fulfilled:

(i) each snapshot  $A_t$  is compact and the family  $\mathscr{A} = \{A(t)\}_{t \in R}$  is invariant with respect to the dynamics

$$X(t,s;X_0) \in \mathcal{A}_t \quad \forall s \le t \text{ and } X_0 \in \mathcal{A}_s; \text{ and}$$
(1)

(ii) the pullback attraction occurs for all times:

$$\lim_{s \to -\infty} |X(t,s;X_0) - \mathcal{A}_t| \to 0 \quad \forall t.$$
<sup>(2)</sup>



Figure: Schematic diagram of an RA  $\mathscr{A}(\omega)$ . From Ghil, Chekroun & Simonnet (2008).

#### Stabilization of the forecast-assimilation (FA) system - II

The rigorous proof of the FA process stabilizing the unstable, chaotic dynamics of planetary flows — based on the above ideas, along with other methods from stochastic calculus and nonlinear filtering — is given by Theorems I and II below:

**Theorem I (nonlinear).** If the coefficients f, h and  $\sigma$  and the measures  $\pi_0$  and  $\mu \in \mathcal{P}_2(\mathbb{R}^d)$  satisfy suitable conditions, then there exists  $R = R(\pi_0, \mu)$  such that

 $\sup_{t\geq 0} \mathbb{E}[W_2(\pi_t^{\mu},\pi_t)] \leq R.$ 

**Theorem II (linear).** If the coefficients f, h and  $\sigma$  and the measures  $\pi_0$  and  $\mu \in \mathcal{P}_2(\mathbb{R}^d)$  satisfy suitable conditions, then we have that

 $\lim_{t\to\infty}W_2(\pi_t^\mu,\pi_t)=0.$ 

Here, the Wasserstein distance is defined by

$$W_{2}(\mu,\nu) = \left(\inf \mathbb{E}\left[|X-Y|^{2}\right]\right)^{1/2},$$
(3)

where  $\mathbb{E}[Z]$  denotes the expected value of Z and the infimum is taken over all joint distributions of the random variables X and Y with marginals  $\mu$  and  $\nu$ , respectively.

**D.** Crisan and M. Ghil, 2022: Asymptotic behavior of the forecast-assimilation process with unstable dynamics, *Chaos* **33**(2), doi:10.1063/5.0105590.

Michael Ghil (ENS & UCLA)

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### Machine learning

- > Novel areas of application
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The applications of ML to DA have proliferated in recent years:

- For model error correction (Farchi et al., 2021).
- As the forecast model itself (Chattopadhyay et al., 2021).
  - Can be implemented as an online process, where DA is used to provide better training data for ML, and ML is used to forecast (Brajard et al., 2020).
- To emulate unresolved scales (Brajard et al., 2021).
- For learning the assimilation process directly (McCabe and Brown, 2021).

In forecasting, due to the high dimensionality of the atmosphere and its models, hybrid methods that combine ML forecasts with physical models are necessary (Pathak et al., 2018).

#### Multi-model data assimilation (MM-DA) - I

- Can we optimally combine ML, physical models, and observations for state estimation?
- Idea: use multi-model DA.



Consider a generalization of the Kalman filter cost function: from

$$(x - x^{f})^{T} (P^{f})^{-1} (x - x^{f}) + (Hx - y)^{T} R^{-1} (Hx - y),$$
 (1)

to

$$\sum_{m=1}^{M} (G_m x - x_m^f)^T (P_m^f)^{-1} (G_m x - x_m^f) + (H x - y)^T R^{-1} (H x - y),$$
(2)

where each model *m* has its own forecast state  $x_m^f$  with forecast error covariance matrix  $P_m^f$  and operator  $G_m$ .

- MM-DA is also a generalization of the Bayesian formulation of the KF and is the best linear unbiased estimator.
- In Bach and Ghil (2022), we develop a multi-model EnKF and show that
  - it can outperform a multi-model ensemble,
  - as well as the best model in the ensemble.

■ Future: test as a hybrid DA and forecasting method with physical and ML models. Eviatar Bach and Michael Ghil. A multi-model ensemble Kalman filter for data assimilation and forecasting. *arXiv:2202.02272* [physics, stat], February 2022.

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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 (i) variables & (ii) regions
  - filters & smoothers
- > Why does data assimilation work in planetary flows?
  - geostrophic adjustment
  - model & noise parameters at & below grid scale
  - stability of the forecast-assimilation (FA) process
- Machine learning
- Novel areas of application
  - space physics
  - solid Earth
  - paleoclimate
  - detection & attribution (DADA)
  - macroeconomics
- Concluding remarks and bibliography

## Space physics data



Two decades ago ...

... and now



Space platforms in Earth's magnetosphere



## Outline

- > Data in meteorology, oceanography and space physics
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Concluding remarks and bibliography

## **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, including localization
- 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);
- AUS (Trevisan & colleagues) + rigorous math results (Crisan & Ghil).

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 => ML;
- pattern recognition in observations and in phase-space statistics => ML.

## 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.

## 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 (2<sup>nd</sup> duality); UKF, particle filters, etc.

### Post-industrial DA:

(Satellite) images  $\rightarrow$  (weather) forecasts, climate "movies" ...

## **Concluding remarks**

We've come a long way in 60 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 (MM-DA)
- various forms of machine learning,
- inverse problems for evolution equations,
   including climate simulation & sensitivity studies,
   & uncertainty quantification (UQ)

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!



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## **Reserve slides**

## A little history – III

Charney et al., JAS, 1969: "If it [were] possible to obtain the large-scale wind field from temperatures alone, the time-table for the implementation of GARP might be substantially advanced."

Ghil et al., *MWR*, 1979: "Satellite-sounding data, though promising, provide only one of the basic variables, viz., temperature. Moreover, while the conventional data sets are available simultaneously over the entire globe, temperature sounding data are obtained only in asynoptic, time-continuous fashion. In one of the earliest efforts at using remote-sounding temperatures for NWP, Charney et al. (1969) put forward the conjecture that a complete knowledge of the continuous temperature history of the atmosphere will determine other initial state variables, in particular the winds.

Tellus (1980), 32, 198-206

## The compatible balancing approach to initialization, and four-dimensional data assimilation

By MICHAEL GHIL, Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, N.Y. 10012, U.S.A. and Laboratory for Atmospheric Sciences, NASA Goddard Space Flight Center, Greenbelt, MD. 20771, U.S.A.

## A little history – IV

Charney et al., JAS, 1969: "If it [where] possible to obtain the large-scale wind field from temperatures alone, the time-table for the implementation of GARP might be substantially advanced."

In a rotating Cartesian (x, y)-coordinate system the linearized shallow-water equations (SWEs) are

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

$$v_t + \phi_y + fu = 0,$$
  

$$\phi_t + \Phi(u_x + v_y) = 0,$$

with (u,v) the velocity,  $\varphi$  the geopotential, and f the Coriolis parameter. In this model, knowing the history of the mass field means knowing  $\phi(x, y, t)$  and hence  $(\phi_t, \phi_{tt})$  at any given instant.

Differentiating the three equations above w.r.t. x, y and t, respectively, and substituting the mixed derivatives  $u_{xt}$  and  $v_{yt}$  from the first two into the third one, yields:

$$\Phi f(v_x - u_y) - \Phi(\phi_{xx} + \phi_{yy}) + \phi_{tt} = 0.$$

This equation, together with the continuity equation above, leads to the Cauchy-Riemann system for the velocity components below:

$$u_x + v_y = -\phi_t/\Phi,$$
  
$$u_y - v_x = -f^{-1}(\Delta \phi - \phi_{tt}/\Phi),$$

where ⊿ is the Laplacian. Similar diagnostic relations for the velocities were obtained for nonlinear SWEs and baroclinic models. E. Titi & colleagues obtained recently rigorous & more general results.

#### The sources of nonautonomous dynamics

**Physically open vs. closed systems:** fluxes of mass, momentum & energy between the system & its surroundings are present or not.

The mathematical framework of **nonautonomous dynamical systems** (NDSs) is appropriate for physically open ones, in which **the fluxes depend explicitly on time**:

- skew-product flows (G. Sell)
  - $\dot{x} = f(x,q), \ \dot{q} = g(q), \ x \in \mathbb{R}^d, \ q \in \mathbb{R}^n$ , with q the driving force for x.
- pullback (Flandoli, L. Arnold) or snapshot (C. Grebogi & E. Ott) attractors  $dX_t = f(X,q) dt + \sigma(X) dW_t$ ,

where  $W_t$  is a Brownian motion in  $\mathbb{R}^d$  and  $dt \sim (dW)^2$ .

More generally, studying explicit time dependence in forcing or coefficients requires NDSs.

The term **nonautonomous** is used both for the deterministic case and for a unified perspective on the deterministic & the random case.

The commonality between the two cases is (i) the independence & (ii) the semi-group property of the driving force, whether q(t) or  $W_t$ .

Likewise, pullback attractor (PBA) is used both for the deterministic & the random case, while in the latter case uses more specifically the phrase random attractor (RA).

## **Parameter Estimation**

#### a) Dynamical model

 $\begin{aligned} dx/dt &= M(x, \mu) + \eta(t) \\ y^{o} &= H(x) + \varepsilon(t) \\ \text{Simple (EKF) idea - augmented state vector} \\ d\mu/dt &= 0, \ X = (x^{T}, \mu^{T})^{T} \end{aligned}$ 

#### b) Statistical model

 $L(\rho)\eta = w(t),$   $L - AR(MA) \mod \rho = (\rho_1, \rho_2, \dots, \rho_M)$ 

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 (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)

## Parameter estimation for space physics – II

HERRB-1D code (Y. Shprits) – estimating phase-space density f and electron lifetime  $\tau_L$ :

$$\frac{\partial f}{\partial t} = L^2 \frac{\partial}{\partial L} \left( L^{-2} D_{LL} \frac{\partial f}{\partial L} \right) - \frac{f}{\tau_L}$$

Different lifetime parameterizations for plasmasphere – out/in:

 $τ_{Lo} = ζ/K_p(t); τ_{Li} = const.$ What are the **optimal** lifetimes to match the observations best?







## 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<sup>f</sup>)  $\approx$  actual. When the parameters' assumed uncertainty is large enough, their EKF estimates converge rapidly to the "truth".





Black – actual errors for state estimation only Red – actual errors for state and parameter estimation Blue – EKF-estimated error (tr  $P_k^{f}$ )

## Parameter estimation for energy balance models with memory (EBMMs) – I

One considers a 1-D paleoclimate model governed by an EBM for zonally averaged surface air temperatures T(t, x):

 $c(x)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k(x)\frac{\partial T}{\partial x}\right) + \mu Q(x)[1 - a(x,T)] - g(x,T);$ 

here  $R_i = \mu Q(x)[1 - a(x, T)]$  is the absorbed solar radiation, with a = a(x, T) the planetary albedo, and  $R_o = g(x, T)$  is the terrestrial radiation, modified by the greenhouse effect, while  $0 \le x \le 1$  is a meridional variable. The albedo depends on past temperatures, because of the long time needed to build up and melt ice sheets.

Ghil (*JAS*, 1976), Bhattacharya, Ghil & Vulis (*JAS*, 1983), Roques, Chekroun *et al.* (*PRS-A*, 2014)



Zonal belt with heat capacity C(x) and temperature T(t, x), subject to incoming radiation  $R_{i}$ , outgoing radiation  $R_{o}$ , and meridional diffusion D.

## **Evolution of DA – II**

TABLE IV. DUALITY RELATIONSHIPS BETWEEN STOCHASTIC ESTIMATION AND DETERMINISTIC CONTROL<sup>®</sup>

$\begin{split} \dot{\mathbf{w}}^{\mathbf{a}}(t) &= F(t)\mathbf{w}^{\mathbf{a}}(t) + K(t)[\mathbf{w}^{0}(t) - H(t)\mathbf{w}^{\mathbf{a}}(t)], \qquad \mathbf{w}^{\mathbf{a}}(0) = \mathbf{w}_{0}^{\mathbf{a}}\\ \dot{P}(t) &= F(t)P(t) + P(t)F^{T}(t) + G(t)Q(t)G^{T}(t)\\ &- K(t)R(t)K^{T}(t), \qquad P(0) = P_{0} \end{split}$	
$K(t) = P(t)H^{T}(t)R^{-1}(t)$	
$E[\mathbf{w}^{t}(0)] = \mathbf{w}_{0}^{a}, \qquad E\{[\mathbf{w}^{t}(0) - \mathbf{w}_{0}^{a}][\mathbf{w}^{t}(0) - \mathbf{w}_{0}^{a}]^{T}\} = P_{0}$ $R^{-1}(t) \text{ exists}$ $E\{\mathbf{b}^{t}(t)[\mathbf{b}^{0}(t')]^{T}\} = 0$ $f^{t}(t) \in E\{[\mathbf{w}^{t}(0) - \mathbf{w}_{0}^{t}]^{T}\}$	
$p^{(n)}(t) = E\{ [\mathbf{w}^{(n)} - \mathbf{w}^{(n)}] \}$	
nal Control	

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

C. Estimation-Control Duality

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

<sup>a</sup> (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).

## **DA Research Testbed (DART)**







#### **AIMING FOR BETTER PREDICTION**

The Data Assimilation Research Testbed

### 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.

D ata 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

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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 ©2009 American Meteorological Society 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,

AMERICAN METEOROLOGICAL SOCIETY

## **Overall Conclusion**

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

<sup>a</sup> of state and errors
 <sup>B</sup> Meandros
 <sup>c</sup> "You cannot do so even once" (subsequent development of "flux" theory by Plato, *cca.* 400 B.C.)
 Τα πάντα ρεί = Everything flows