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

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Joint work with
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and http://www.environnement.ens.fr/
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)
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: \( V - 2 \times 2259 \)

Aircraft: \( V - 2 \times 1100 \)

Ship & land surface: \( P_s, T_s, V_s - 4 \times 3446 \)

Polar orbiting satellites: \( T - 5 \times 2048 \)

Balloons: \( V - 2 \times 581 \times 10 \)

Radiosondes: \( T, V - 3 \times 749 \times 10 \)

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

\[ 0(10^2) \text{ observations/} \left[ \text{significant } d-o-f \right] \times \text{(significant } \Delta t \right] \]

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

TOPEX/POSEIDON SEA LEVEL ABOVE 1993–96 MEAN, in MM, 10 DAY AVE STARTING 19990817 (WOCE/PO–DAAC v1.1b)

Courtesy of Tong (“Tony”) Lee, JPL
Space physics data

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
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

$$\hat{T} = T_1 + [A_2 / (A_2 + A_1)] (T_2 - T_1)$$

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)

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

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

Stage 1: Prediction (deterministic)

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

Stage 2: Update (Probabilistic)

\[ x^a(t_i) = x^f(t_i) + K_i(y_i^0 - H_i[x^f(t_i)]) \]
\[ P^a(t_i) = (I - K_i H_i)P^f(t_i) \]
\[ K_i = P^f(t_i)H_i^T[H_i P^f(t_i) H_i^T + R_i]^{-1} \]
subject to \( \partial_K \text{tr} P^a = 0 \)
\( M \) and \( H \) are the linearizations of \( M \) and \( H \)

Observations

\[ y_i^0 = H_i[x^t(t_i)] + \epsilon_i \]
\[ R_i \delta_{ij} = \mathbb{E}(\epsilon_i \epsilon_j^T) \]
\[ d = y_i^0 - H_i[x^f(t_i)] - \text{innovation vector} \]
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Basic concepts: barotropic model

Shallow-water equations in 1-D, linearized about \((U, 0, \Phi)\), \(fU = -\Phi_y\)

\[ U = 20 \text{ ms}^{-1}, \ f = 10^{-4} \text{s}^{-1}, \ \Phi = gH, \ H \approx 3 \text{ km}. \]

\[
\begin{align*}
    u_t + Uu_x + \phi_x - fv &= 0 \\
    v_t + Uv_x + fu &= 0 \\
    \phi_t + U\phi_x + \Phi u_x - fuv &= 0
\end{align*}
\]

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

\[ P_\infty = \frac{QR}{Q + (1 - \Psi^2)R} \]

(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

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

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Error components in forecast–analysis cycle

\[
P^f \approx P^a + \Delta t (2AP^a + Q)
\]

The relative contributions to error growth of

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

\[
\Psi = e^{A\Delta t} \approx 1 + A\Delta t
\]
Assimilation of observations: Stability considerations

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

Forecast state: model integration from a previous analysis

\[
x_{n+1}^f = M(x_n^a)
\]

Corresponding perturbative (tangent linear) equation

\[
\delta x_{n+1}^f = M \delta x_n^a
\]

**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

\[
x_{n+1}^a = \left[I - KH \circ \right] M(x_n^a) + Ky_{n+1}^o
\]

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

\[
\delta x_{n+1}^a = \left[I - KH \right] M \delta x_n^a
\]

- 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)*
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 \textbf{BDAS} and assimilated by \textbf{AUS} (Trevisan & Uboldi, 2004).

\textbf{BDAS}: Breeding on the Data Assimilation System
\textbf{AUS}: Assimilation in the Unstable Subspace
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:
\[ \lambda_{\text{max}} \approx 0.31 \text{ days}^{-1}; \]
Doubling time \( \approx 2.2 \) days;
Number of positive exponents:
\( N^+ = 24; \)
Kaplan-Yorke dimension \( \approx 65.02. \)

3-DVar–BDAS
Leading exponent:
\[ \lambda_{\text{max}} \approx 0.002 \text{ days}^{-1}; \]
Kaplan-Yorke dimension \( \approx 1.1 \)

AUS–BDAS
Leading exponent:
\[ \lambda_{\text{max}} \approx -0.52 \times 10^{-3} \text{ days}^{-1} \]
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Parameter Estimation

a) Dynamical model

\[ \frac{dx}{dt} = M(x, \mu) + \eta(t) \]
\[ y^o = H(x) + \varepsilon(t) \]

Simple (EKF) idea – augmented state vector
\[ \frac{d\mu}{dt} = 0, \quad X = (x^T, \mu^T)^T \]

b) Statistical model

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

Examples:
1) Dee et al. (IEEE, 1985) – estimate a few parameters in the covariance matrix \( Q = E(\eta, \eta^T) \); also the bias \( <\eta> = E\eta \);
3) \( \frac{dx}{dt} = M(x, \mu) + \eta \): 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 $\mu$

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

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

\[
\bar{x}^a_k = \bar{x}^f_k + \bar{K}(y_k^0 - \bar{H}\bar{x}^f_k); \quad \bar{K} = \bar{P}^f\bar{H}^T(\bar{H}\bar{P}^f\bar{H}^T + R)^{-1}
\]

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

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

- 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 $\mu$ and surface-layer coefficient $\delta_s$ 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.
- Kondrashov, Sun & Ghil (Monthly Weather Rev., 2008)
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

**a) Ocean–atmosphere coupling coefficient**

- **Estimate**
- **True**
- **Error**

**b) Surface–layer coefficient**

- **Estimate**
- **True**
- **Error**

Identical-twin experiments
Convergence of Parameter Values – II

Real SST anomaly (SSTA) data
EKF results with and w/o parameter estimation

a) SSTA from EKF with $\mu$ and $\delta_s$ estimation

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

c) SSTA from model forced with estimated $\mu(t), \delta_s(t)$
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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 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.
Aiming for Better Prediction: The Data Assimilation Research Testbed

DA Research Testbed (DART)

Data assimilation combines observations with model forecasts to estimate the state of a physical system. Developed in the 1960s (Dafer 1995; Kalnay 2001) to provide initial conditions for numerical weather prediction (NWP; Lyons 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 (Moure 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 (Bodzek et al. 1996; Aksoy et al. 2004). Assimilation is now used also for the ocean (Keppenne and Rieckers 2002; Zhang et al. 2005), land surface (Rakob et al. 2002), cryosphere (Masson 2008), biosphere (Williams et al. 2006a), and chemical constituents (Constantinou 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.
General references


“Miss Peterson, may I go home? I can’t assimilate any more data today.”
Reserve slides
Estimating noise – I

\[ Q_1 = Q_{\text{slow}}, \quad Q_2 = Q_{\text{fast}}, \quad Q_3 = 0; \]
\[ R_1 = 0, \quad R_2 = 0, \quad R_3 = R; \]
\[ Q = \sum \alpha_i Q_i; \quad R = \sum \alpha_i R_i; \]
\[ \alpha(0) = (6.0, 4.0, 4.5)^T; \]
\[ Q(0) = 25*I. \]


Poor convergence for \( Q_{\text{fast}} \)?
Estimating noise – II

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

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


Good convergence for $Q_{\text{fast}}$!
Evolution of DA – I

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.
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
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 observations) in – direct insertion, nudging.

• Advanced DA:
  • Plenty of data, fine models.
  • E(n)KF, 4-D Var (2nd duality).

• Post-industrial DA:
  (Satellite) images --> (weather) forecasts, climate “movies” …
  (Ihler, Kirshner, Ghil, Robertson & Smyth, Physica D, 2007)
Overall Conclusion

• No **observing system** without **data assimilation** and no assimilation without **dynamics**

• Quote of the day: “You cannot step into the same river twice”

---

$^a$ 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 ρέει = Everything flows
Daily fluxes of 1 MeV relativistic electrons in Earth’s outer radiation belt (CRRES observations from 28 August 1990) $K_p$ - index of solar activity (external forcing) – used to determine the position of the plasmapause $L_{pp}$ (black) in the observations.

Kondrashov, Shprits, Ghil & Thorne (J. Geophys. Res., 2007)
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:

\( \tau_{L_0} = \zeta/K_p(t) \); \( \tau_{L_i} = \text{const.} \).

What are the optimal lifetimes to match the observations best?
Daily observations from the “truth” —

\[ \tau_{Lo} = \zeta/K_p, \ zeta = 3, \ \text{and} \ \tau_{LI} = 20 \] — are used to correct the model’s “wrong” parameters, \( \zeta = 10 \) and \( \tau_{LI} = 10 \).

The estimated error \( \text{tr}(P_f) \rightarrow \text{actual} \). When the parameters’ assumed uncertainty is large enough, their EKF estimates converge rapidly to the “truth.”