Data assimilation methods based on the Kalman Filter

From theory to practical implementations (II)

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Job opportunity

- **Post-doc position available at LEGI** (Grenoble, a nice place for skiing, hiking, biking etc.), **to develop an ocean colour assimilation system in a coupled physical/biogeochemical model of the North Atlantic**

- Interested ? Contact me before Friday, or send me a CV + expression of interest (Pierre.Brasseur@hmg.inpg.fr)

1. Kalman Filter fundamentals
Assimilation cycle

$$\begin{cases} \mathbf{x}_i^a \\ \mathbf{P}_i^a \end{cases}$$

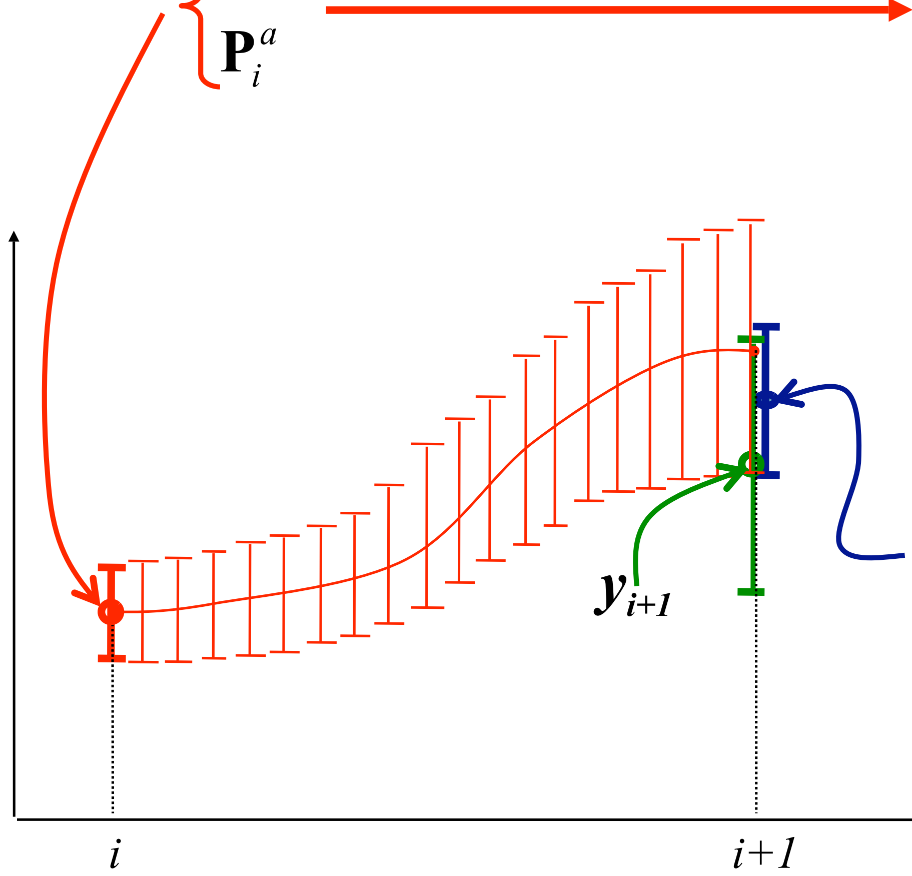
Forecast →

$$\begin{cases} \mathbf{x}_{i+1}^f = M\left(\mathbf{x}_i^a\right) \\ \mathbf{P}_{i+1}^f = \mathbf{M}\mathbf{P}_i^a\mathbf{M}^T + \mathbf{Q} \end{cases}$$

Analysis ↓

$$\mathbf{K}_{i+1} = \mathbf{P}_{i+1}^f\mathbf{H}^T(\mathbf{H}\mathbf{P}_{i+1}^f\mathbf{H}^T + \mathbf{R})^{-1}$$

$$\begin{cases} \mathbf{x}_{i+1}^a = \mathbf{x}_{i+1}^f + \mathbf{K}_{i+1}\left(\mathbf{y}_{i+1} - H\left(\mathbf{x}_{i+1}^f\right)\right) \\ \mathbf{P}_{i+1}^a = \left(\mathbf{I} - \mathbf{K}_{i+1}\mathbf{H}\right)\mathbf{P}_{i+1}^f \end{cases}$$



OUTLINE

- State-of-the-art
  1. Kalman filter: fundamentals
  2. Ocean data assimilation: specific issues
  3. Error sub-spaces
  4. Low rank filters: SEEK and EnKF

- Advanced issues
  5. Objective validation and evaluation of DA systems
  6. Error tuning and adaptive schemes
  7. Improved temporal strategies : FGAT and IAU
  8. Kalman filtering with inequality constraints

- The MERCATOR/MERSEA Assimilation Systems

3. Error sub-spaces
Why ?

Noting that :

- A full Kalman filter cannot be implemented into realistic ocean models (error forecast and analysis equations too expensive in CPU and memory requirements)
- « Optimal Interpolation » over-simplifies the propagation of errors by neglecting dynamical principles and statistical information

The concept of error sub-space is introduced, with the objectives to :

- Substantially reduce the computational burden of a full Kalman filter, but
- Preserve the essential properties of statistical estimation.

3. Error sub-spaces
Error covariance matrix decomposition

- **Properties:** covariance matrices are symetric, positive definite

$$\Rightarrow \mathbf{P} = \mathbf{L}\,\Lambda\,\mathbf{L}^T \quad \text{with} \quad \mathbf{L}: \text{ eigenvectors}$$

$$\Lambda = diag\{\lambda_i\}: \text{ eigenvalues}$$

- **Error sub-space $\mathbf{S}$** : defined as an approximation of $\mathbf{L}\sqrt{\Lambda}$, limited to the dominant eigenmodes/eigenvalues which best represent the covariance $\mathbf{P}$

<u>Low-rank approximation:</u> $\mathbf{P}_O$ **specified as a low rank matrix**

$$\mathbf{P}_O = \mathbf{S}_O \mathbf{S}_O^T \text{ , with } \mathbf{S}_O \text{ of dim } n \times r \text{ , } r \ll n = \dim(\boldsymbol{x})$$

- Accurate specification of a full-rank $\mathbf{P}_O$ is impossible !
- Approximation done at initial assimilation time only
- Drastic simplification of analysis and forecast steps : r ~ 10-100

3. Error sub-spaces
Variants

$$\mathbf{P}_0 = \mathbf{S}_0 \, \mathbf{S}_0^T$$

r ~10-100

n ~10^6-10^8

All covariance informations are contained in $\mathbf{S}_0$ *!*

Variants to build the sub-space :

- **EOFs from model variability**: large-scale modes *well suited to basin-scale problems (e.g. Tropical Pacific) ; local modes well suited to eddy-resolving ocean DA problems (Atlantic basin HR models)*
- **EOFs of prescribed covariance functions,** *using analytical models*
- **Lyapunov, singular, breeding modes** : *for non-linear models*
- **Ensemble of Monte-Carlo perturbations of model states**

- **<u>Practical recipe</u> :** to compute 3D, multivariate EOFs from a model run

  - Sampling of « historical » sequence:

$$\boldsymbol{x}^m(t_{i+1}) = M(t_i, t_{i+1})\boldsymbol{x}^m(t_i) \quad , \quad i = 0, \ldots, s-1$$

$$\Rightarrow \mathbf{X} = \left\{ \boldsymbol{x}^m(t_i) - \overline{\boldsymbol{x}^m(t_i)} \right\} \ \dim n \times s$$

  - Eigenmodes of « sample » matrix $\mathbf{X}\mathbf{X}^T$ $(\dim n \times n)$ can be easily computed from the eigenmodes of $\mathbf{X}^T\mathbf{X}$ $(\dim s \times s)$ because

$$\mathbf{X}\mathbf{X}^T\mathbf{L} = \mathbf{L}\Lambda \Leftrightarrow \mathbf{X}^T\mathbf{X}\mathbf{X}^T\mathbf{L} = \mathbf{X}^T\mathbf{L}\Lambda = \mathbf{V}\Lambda$$

$$\Rightarrow \mathbf{L} = \mathbf{X}\mathbf{V}\Lambda^{-1}$$

  - Truncation to r dominant modes

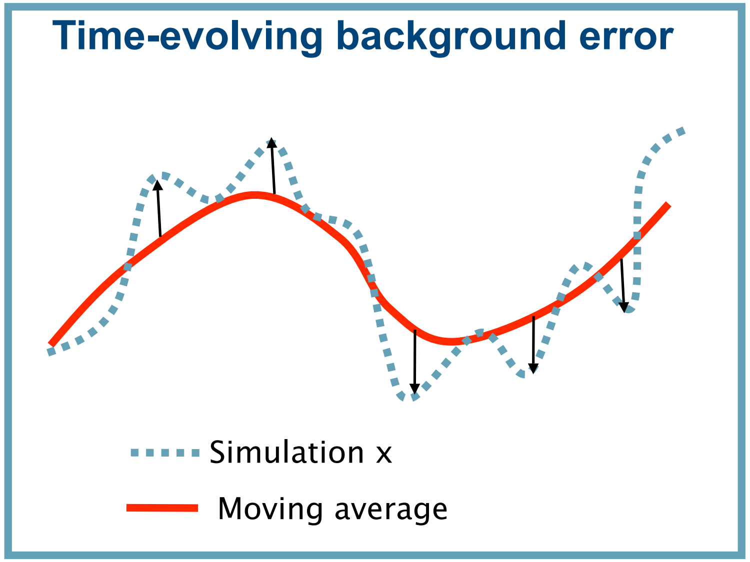
$$\Rightarrow \mathbf{S}_0 \quad \text{and} \quad \mathbf{P}_0 \approx \mathbf{S}_0\mathbf{S}_0^T$$

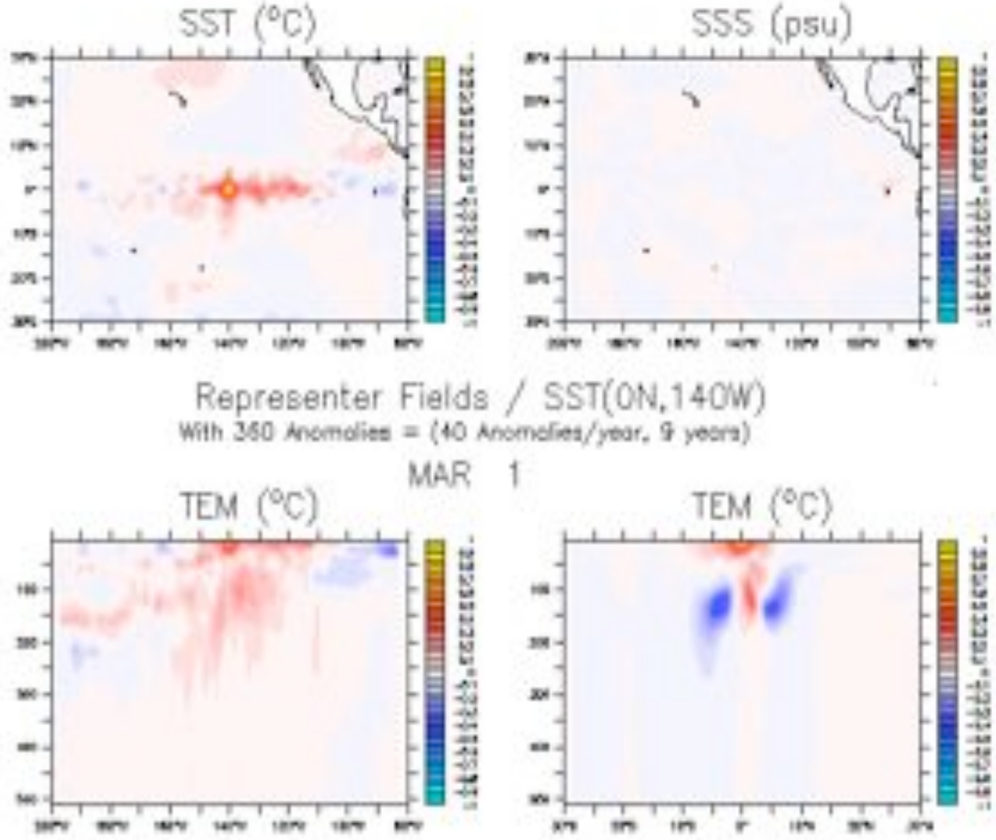
Time-evolving background error

Testut *et al.*, 2005

Objective: improve the representation of high-frequency processes

SST / température and salinity representers (ORCA2)





4. Low rank Kalman filters
Forecast equation - SEEK filter

Concept:

Use order reduction $\mathbf{P}_i^a = \mathbf{S}_i^a \mathbf{S}_i^{aT}$ **to compute** $\mathbf{P}_{i+1}^f = \mathbf{M}\,\mathbf{P}_i^a \mathbf{M}^T + \mathbf{Q}$

$$\Rightarrow \quad \mathbf{P}_{i+1}^f = \left(\mathbf{M}\mathbf{S}_i^a\right)\left(\mathbf{M}\mathbf{S}_i^a\right)^T + \mathbf{Q}$$

- Time-evolving sub-space at moderate cost (max r model integrations)
- Model error parameterized in the evolving sub-space $\mathbf{Q} \propto \mathbf{M}\,\mathbf{P}_i^a \mathbf{M}^T$ to preserve low rank

Variants to evolve the sub-space $\mathbf{S}_i^a \rightarrow \mathbf{S}_{i+1}^f$

- **« Extended » evolutive :** $\mathbf{S}_{i+1}^f = \mathbf{M}\mathbf{S}_i^a$ *(apply linear tangent model : Pham et al., 1998)*
- **« Interpolated » evolutive :** $\mathbf{S}_{i+1}^f \approx M\left(\boldsymbol{x}_i^a + \alpha\, \mathbf{S}_i^a\right) - M\left(\boldsymbol{x}_i^a\right)$ *(use non- linear model to update the error modes dynamically : Brasseur et al., 1999; Ballabrera et al., 2001)*
- **« Fixed basis » :** $\mathbf{S}_{i+1}^f = \mathbf{I}\,\mathbf{S}_i^a$ *(assume persistence or dominant model error to update the sub-space: Verron et al., 1999)*

4. Low rank Kalman filters
Analysis equation - SEEK filter

Concept: **Use order reduction** $\mathbf{P}^f_{i+1} = \mathbf{S}^f_{i+1}\mathbf{S}^{f\ T}_{i+1}$ **to compute the** $\mathbf{K}$ **gain**

$$\mathbf{K}_{i+1} = \mathbf{P}^f_{i+1}\mathbf{H}^T(\mathbf{H}\mathbf{P}^f_{i+1}\mathbf{H}^T + \mathbf{R})^{-1}$$

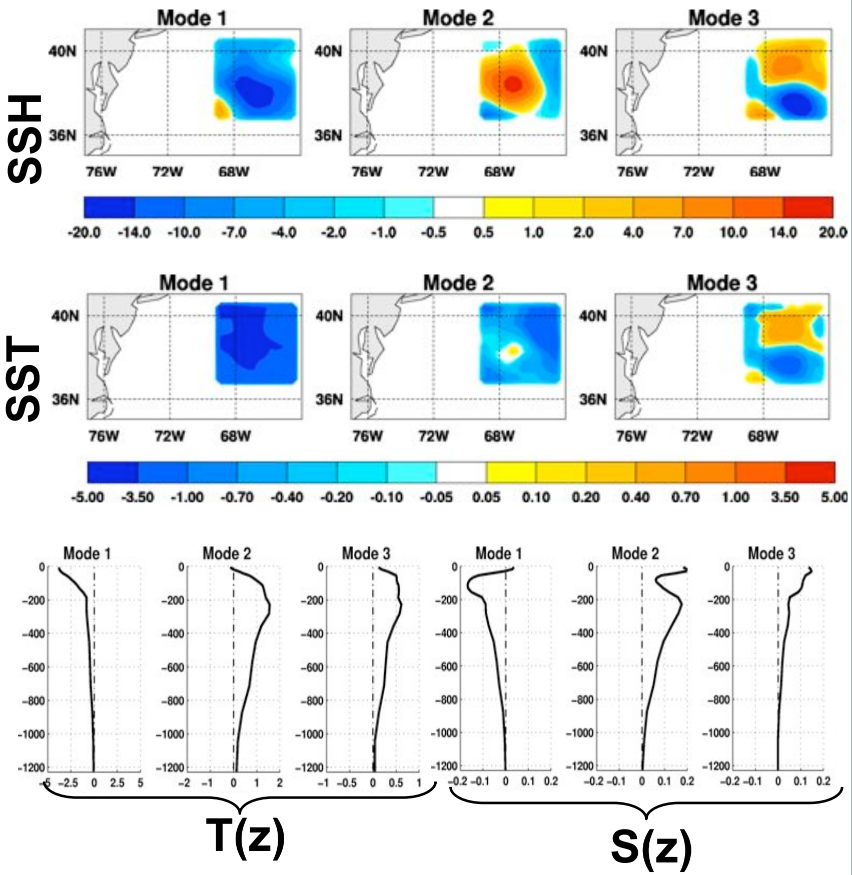
$$\rightarrow \quad = \ldots = \mathbf{S}^f_{i+1}\left[\mathbf{I} + \left(\mathbf{H}\mathbf{S}^f_{i+1}\right)^T \mathbf{R}^{-1}\left(\mathbf{H}\mathbf{S}^f_{i+1}\right)\right]^{-1}\left(\mathbf{H}\mathbf{S}^f_{i+1}\right)^T \mathbf{R}^{-1}$$

- More efficient inversion: in **reduced space** instead of **observation space**, with r often much smaller than dim ($\mathbf{y}$)
- Updates are combinations of modes: $\mathbf{x}^a_{i+1} - \mathbf{x}^f_{i+1} = \mathbf{K}_i\left(\mathbf{y}_i - \mathbf{H}\mathbf{x}^f_{i+1}\right) = \mathbf{S}^f_{i+1}\mathbf{c}$

Variants to compute updates

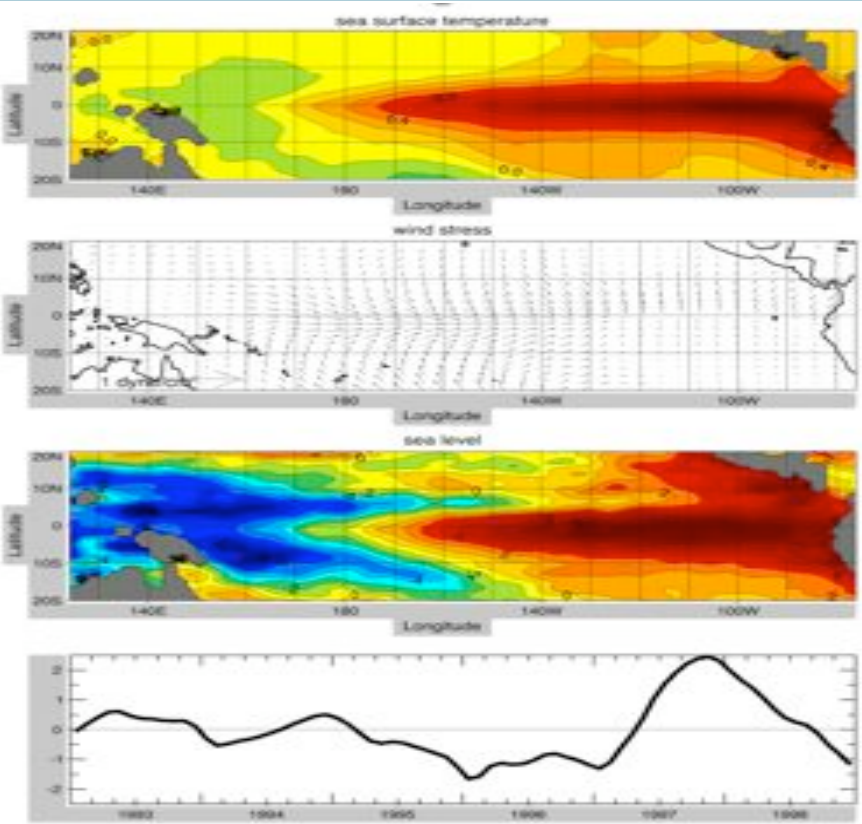
- **« Global » analysis : the standard formulation ,** *requires regular data distributions in space to avoid spurious corrections at large distances*
- **« Local » analysis : define $\mathbf{H}$ as a « local » operator** to compensate for truncation errors and eliminate remote influence of data *(Brankart et al., 2003)*

Examples of error modes



(from Testut et al., 2001)

Local EOFs



(from Picaut et al., 2001)

Global EOFs

Concept:

Use an ensemble of r model states $x_i^{a,j}$ to specify the spread of possible initial conditions around the mean $\overline{x_i^{a,j}}$ and propagate each member individually (Evensen 1994).

Forecast equation:

$$x_{i+1}^{f,j} = M\left(x_i^{a,j}\right) + ç^j \quad \text{with} \quad \overline{ç^j ç^{jT}} = \mathbf{Q} \quad , \quad j = 1,\ldots,r$$

This provides automatically: $$\mathbf{P}_{i+1}^f = \frac{1}{r-1}\left(x_{i+1}^{f,j} - \overline{x_{i+1}^{f,j}}\right)\left(x_{i+1}^{f,j} - \overline{x_{i+1}^{f,j}}\right)^T$$

Analysis equation:

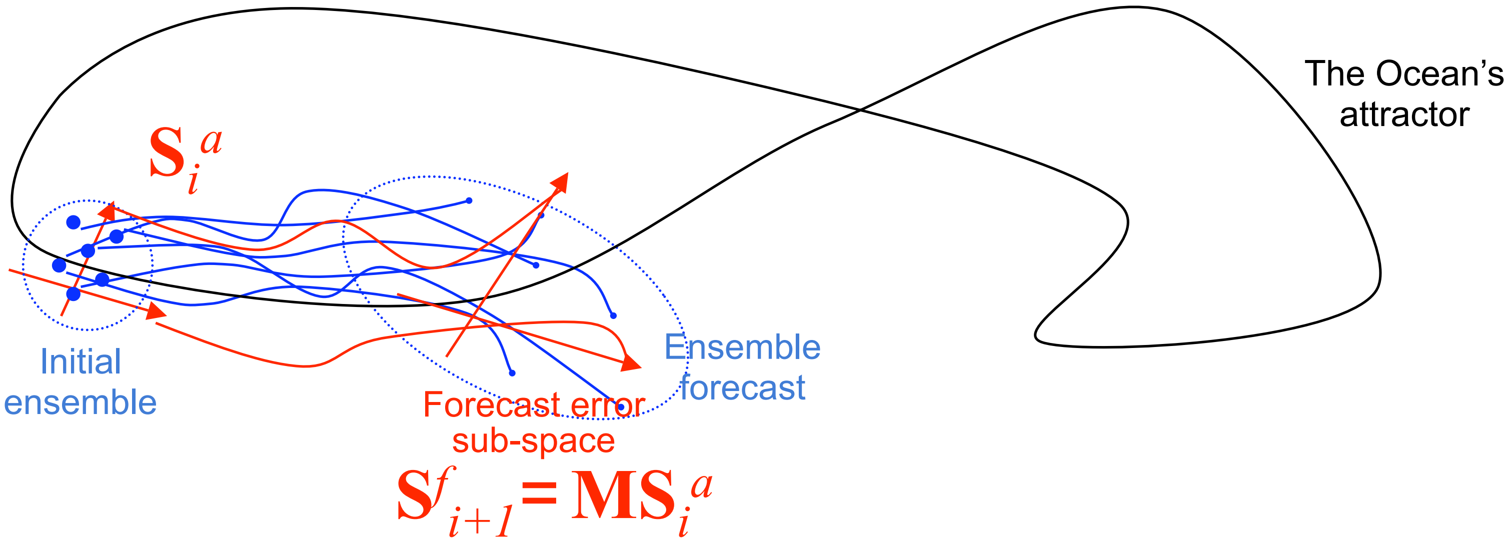
$$x_{i+1}^{a,j} = x_{i+1}^{f,j} + \mathbf{K}_{i+1}\left(\tilde{y}_{i+1} - H\left(x_{i+1}^{f,j}\right)\right) \quad , \quad j = 1,\ldots,r$$

This provides automatically: $$\mathbf{P}_{i+1}^a = \frac{1}{r-1}\left(x_{i+1}^{a,j} - \overline{x_{i+1}^{a,j}}\right)\left(x_{i+1}^{a,j} - \overline{x_{i+1}^{a,j}}\right)^T$$

4. Low rank Kalman filters
EnKF vs. SEEK

Same philosophy :

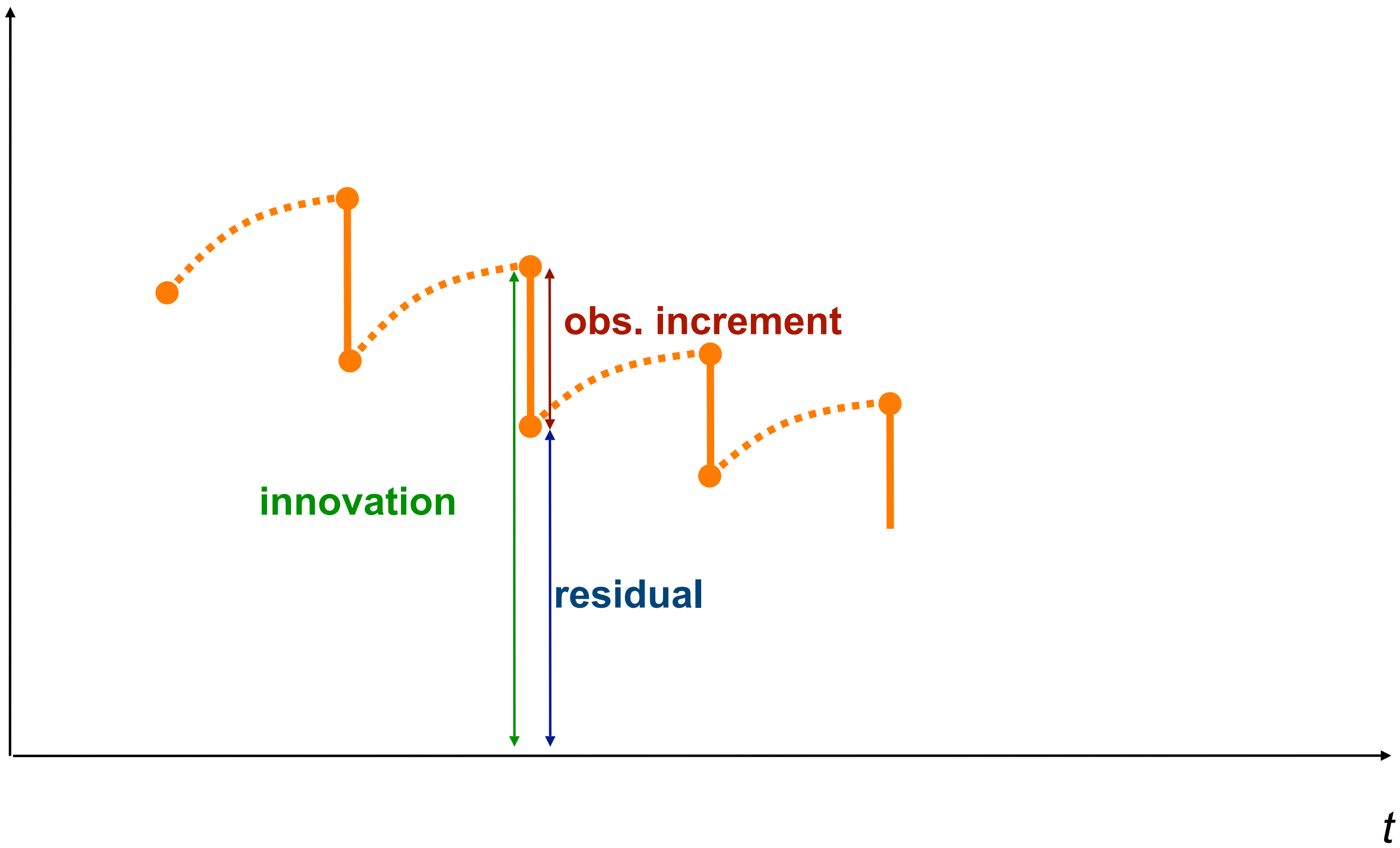
Sequential corrections along privileged directions of error growth



Differences between SEEK, EnKF, EnKS : Nerger *et al.*, Tellus, 2005

5. Validation and evaluation of DA systems
Innovation statistics

observation misfit



5. Validation and evaluation of DA systems
Innovation statistics

§ **A major difficulty with DA schemes is the specification of background and observation error statistics, which are critical to the analysis step.**

§ **During the assimilation process, « anomalies » can be detected between the innovation sequence and the prior statistical assumptions (in a KF context).**

q **Error statistics :** $\overline{\boldsymbol{\varepsilon}^{o}} = 0 \quad \overline{\boldsymbol{\varepsilon}^{f}} = 0 \quad \mathbf{R} = \overline{\boldsymbol{\varepsilon}^{o}\boldsymbol{\varepsilon}^{o\,T}} \quad \mathbf{P}^{f} = \overline{\boldsymbol{\varepsilon}^{f}\boldsymbol{\varepsilon}^{f\,T}}$

q **Innovation « seen » by the filter:**

$$\mathbf{d}^{\mathbf{f}}_{\mathbf{i+1}} = \mathbf{H}\mathbf{x}^{\mathbf{f}}_{\mathbf{i+1}} - \mathbf{y}_{\mathbf{i+1}} = \mathbf{H}\mathbf{x}^{\mathbf{f}}_{\mathbf{i+1}} - (\mathbf{H}\mathbf{x}^{\mathbf{t}}_{\mathbf{i+1}} + \boldsymbol{\varepsilon}^{\mathbf{o}}_{\mathbf{i+1}}) = \mathbf{H}\boldsymbol{\varepsilon}^{\mathbf{f}}_{\mathbf{i+1}} - \boldsymbol{\varepsilon}^{\mathbf{o}}_{\mathbf{i+1}}$$

Ø **Examples of statistical “anomalies”:**

1. biases in innovation sequence : $\overline{\mathbf{d}^{f}_{i+1}} \neq 0$
2. inconsistencies in innovation amplitudes :

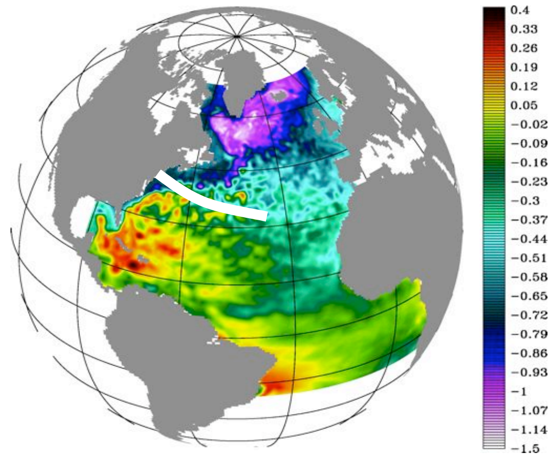
$$tr(\overline{\mathbf{d}^{f}_{i+1}\mathbf{d}^{f\,T}_{i+1}}) \neq tr(\mathbf{H}\mathbf{P}^{f}_{i+1}\mathbf{H}^{T}) + tr(\mathbf{R})$$

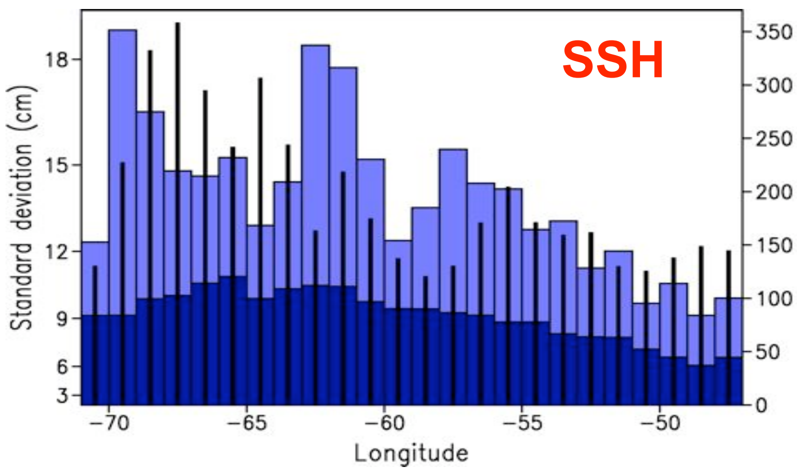
5. Validation and evaluation of DA systems
Example

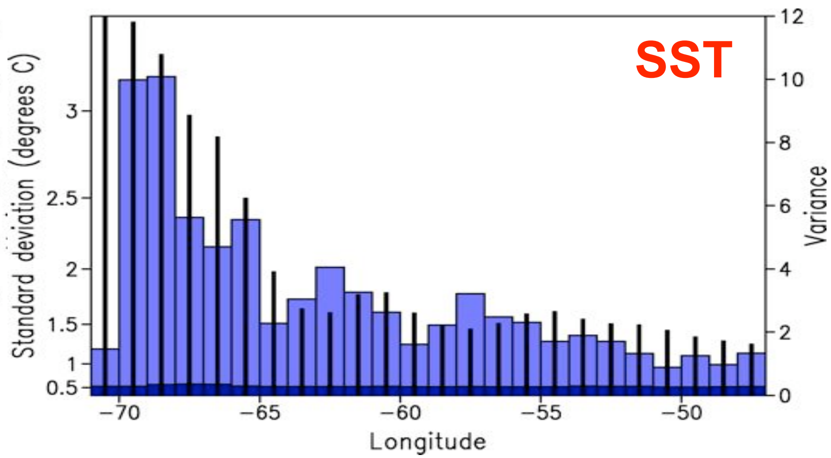
Comparison between 2 estimations of the forecast error variance in a zonal section crossing the Gulf Stream (HYCOM model, Brankart et al., 2003):

(i) from the filter (blue histograms) and
(ii) from innovation sequence (black bars).

$$tr(\overline{\mathbf{d}_i^f \mathbf{d}_i^{f^T}}) \approx tr(\mathbf{H}\mathbf{P}^f\mathbf{H}^T) + tr(\mathbf{R})$$



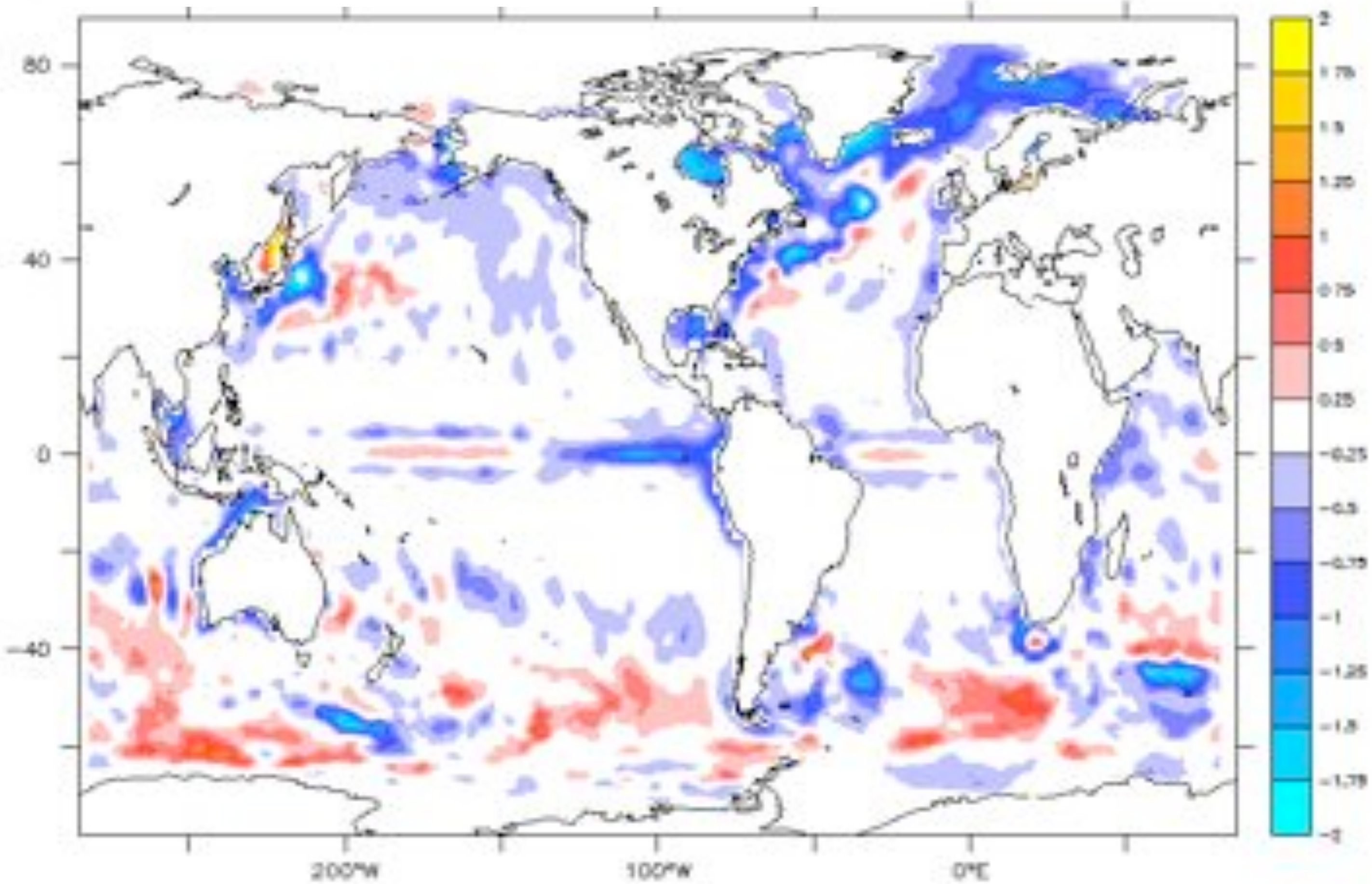




| $diag\,(\overline{\mathbf{d}_i^f \mathbf{d}_i^{f^T}})$ | diag $\mathbf{R}$ | diag $\mathbf{P}^f$ |

5. Validation and evaluation of DA systems
Detection of system biases

average SLA increment, 1993-2002, (cm)



Mercator global ocean prototype (Ferry *et al.*, 2006)

6. Error tuning
Adaptive schemes

Concept: **« on line » modification of prior statistics ($\mathbf{P}^f$, $\mathbf{R}$, $\mathbf{Q}$, …) in order to better match the statistics of the innovation sequence**

- Simple adaptive schemes can be implemented *easily*, and *at low cost*, into operational systems

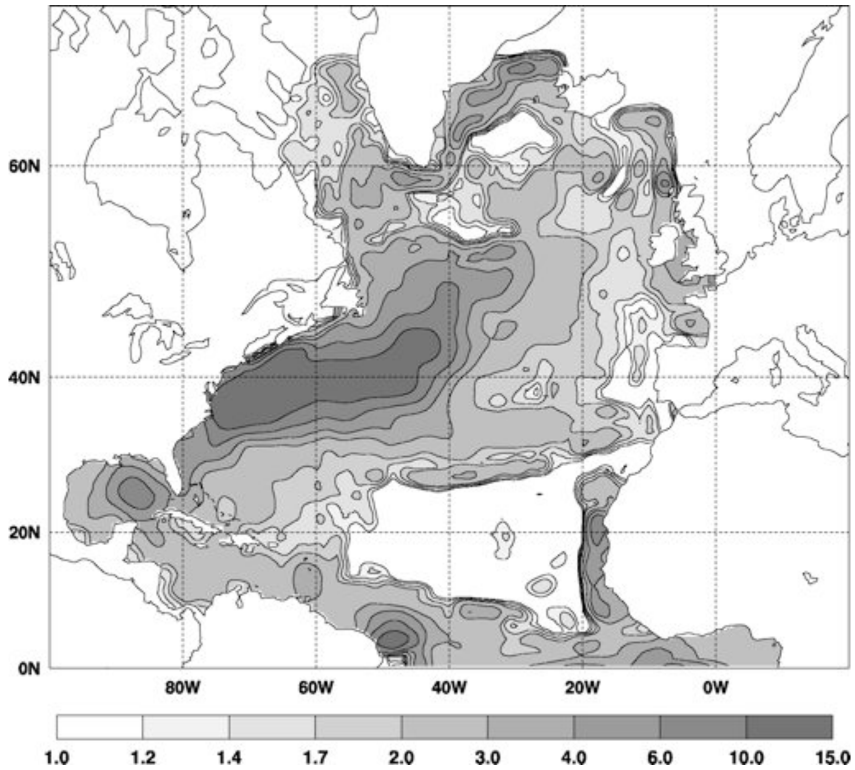
Adaptivity variants

- **« Adaptive basis » :** use residual innovation to generate new modes and refresh the sub-space intermittently (Brasseur et al., 1999; Durand et al., 2003)
- **« Adaptive variance » :** tune model error parameterization to improve the fit between innovation and filter statistics *(Brankart et al., 2003)*

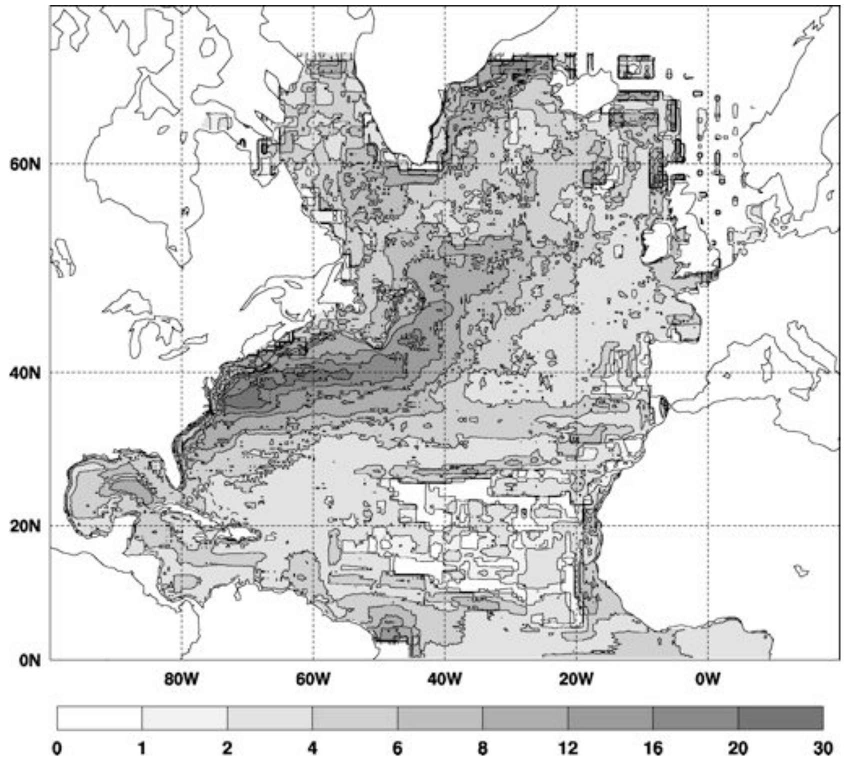
Parameterization example : $\mathbf{P}_{i+1}^{f} \approx \alpha\, \mathbf{P}_{i}^{a}$

α → determined using innovation statistics history

6. Error tuning
Example



Model error amplification α



Forecast error estimates

7. Improved temporal strategies
Distributed observations

- Ocean observations are continuously distributed in time during the assimilation period; however, it is impossible to rigorously incorporate the data at their exact acquisition time. Therefore, **intermittent data assimilation schemes are *approximate*.**

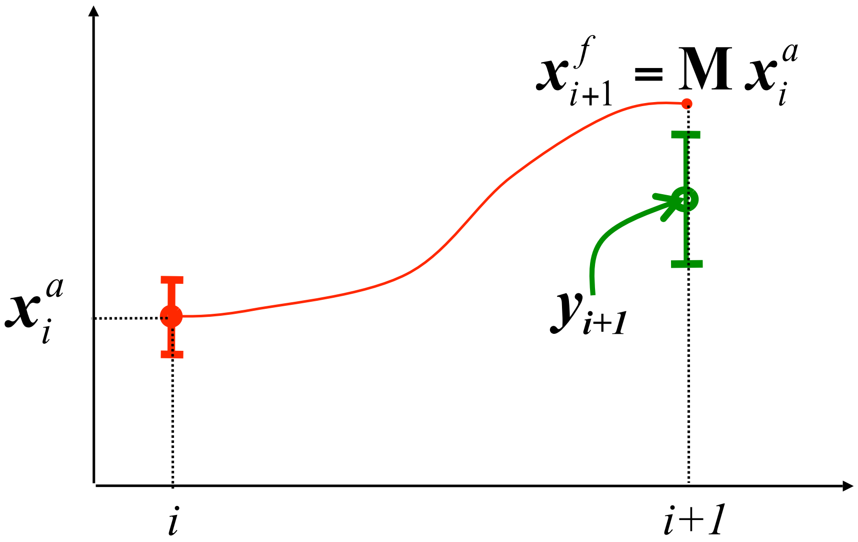
- Typical length of assimilation periods:
  - 3-7 days for mesoscale ocean current predictions;
  - 30 days for initialisation of seasonal climate predictions.

- Two related problems arise with intermittent corrections: shocks to the model, and data rejection.

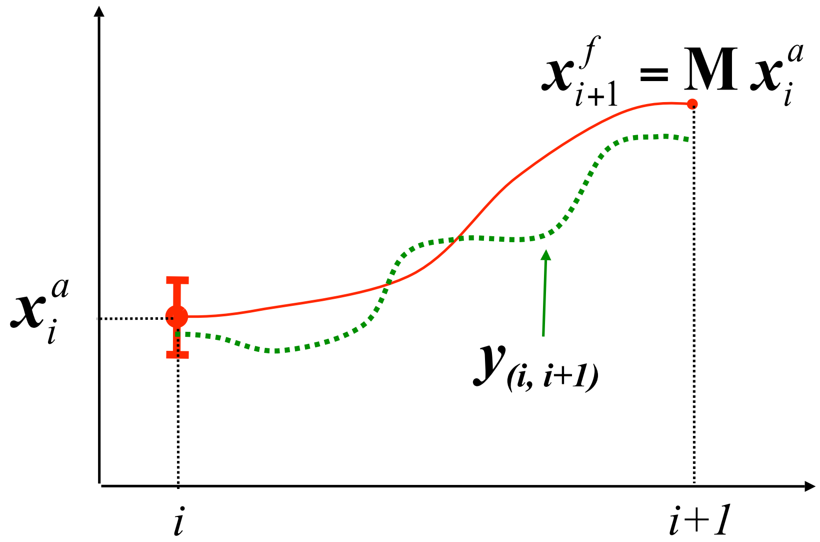
Strategies to avoid these problems ?

7. Improved temporal strategies
Distributed observations

- **Discrete DA problem**

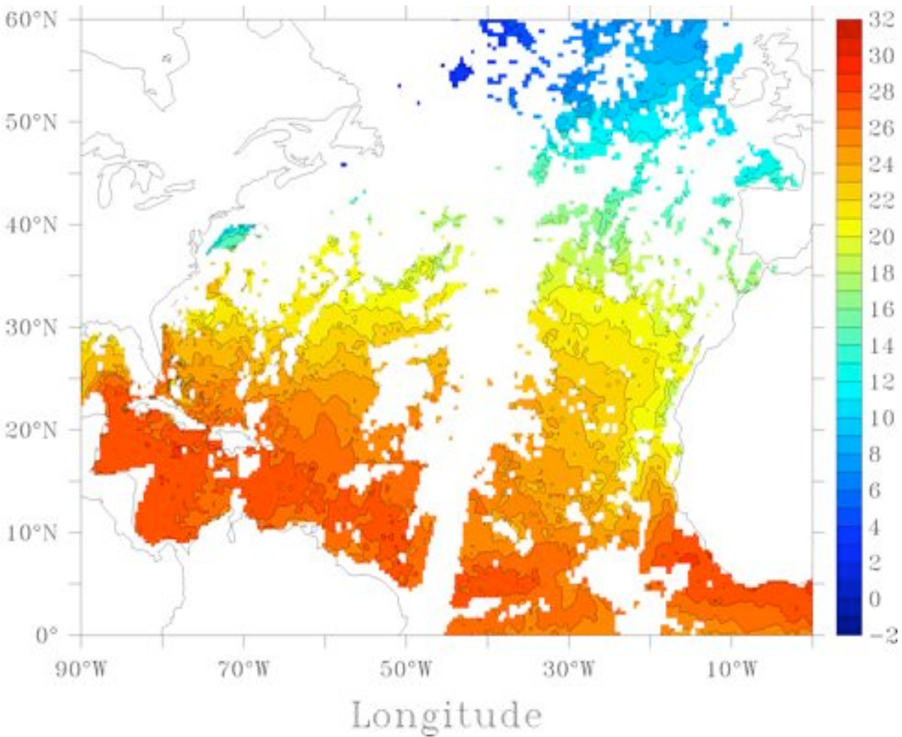


- **Continuous DA problem**

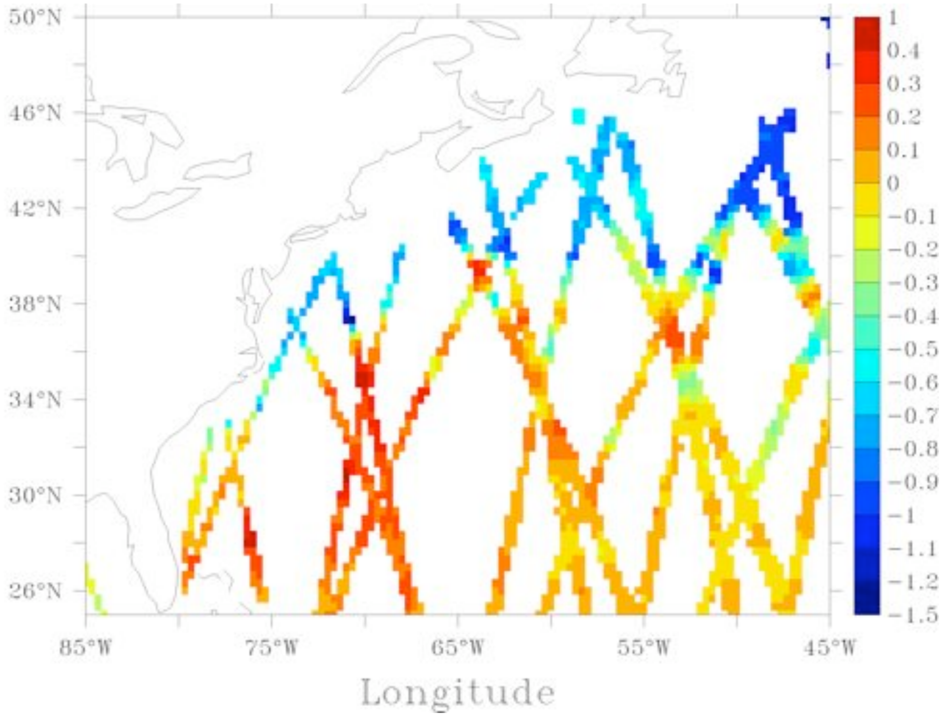


7. Improved temporal strategies
Example: composite data sets

3-day composite AVHRR SST
December 20-21-22,1992



3-day composite SLA
December 20-21-22,1992



- The observation vector $\boldsymbol{y}_{i+1}$ contains informations related to different instants.

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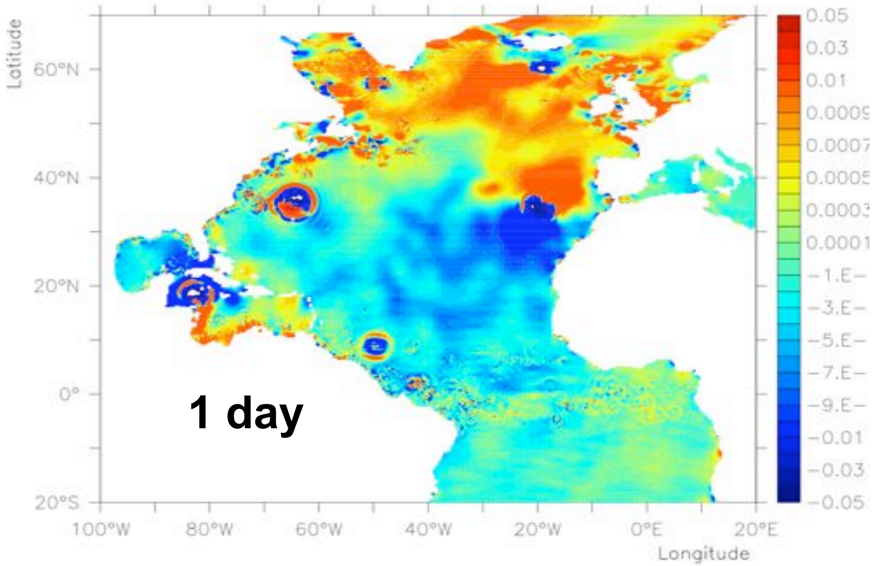
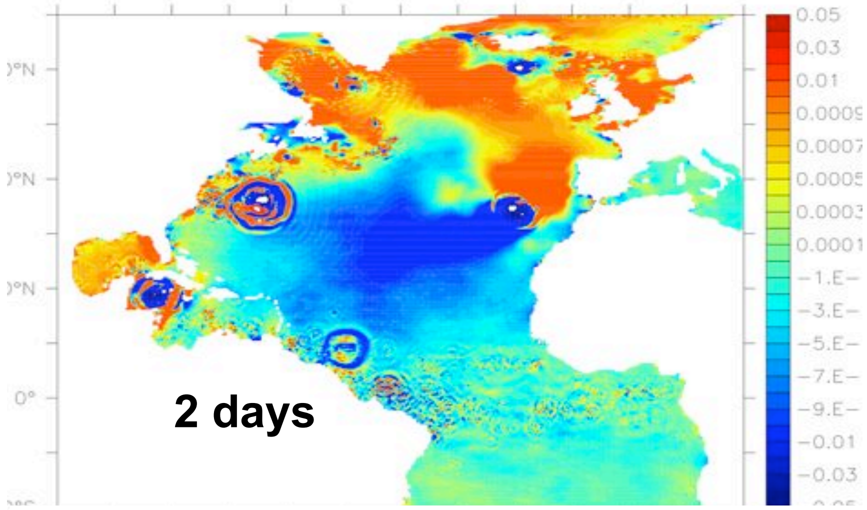
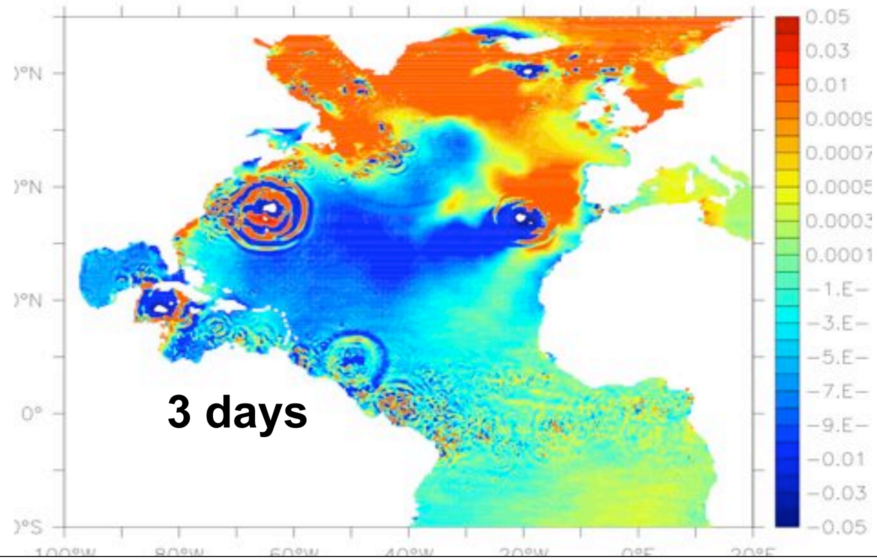
7. Improved temporal strategies
« Shocks » to model forecasts

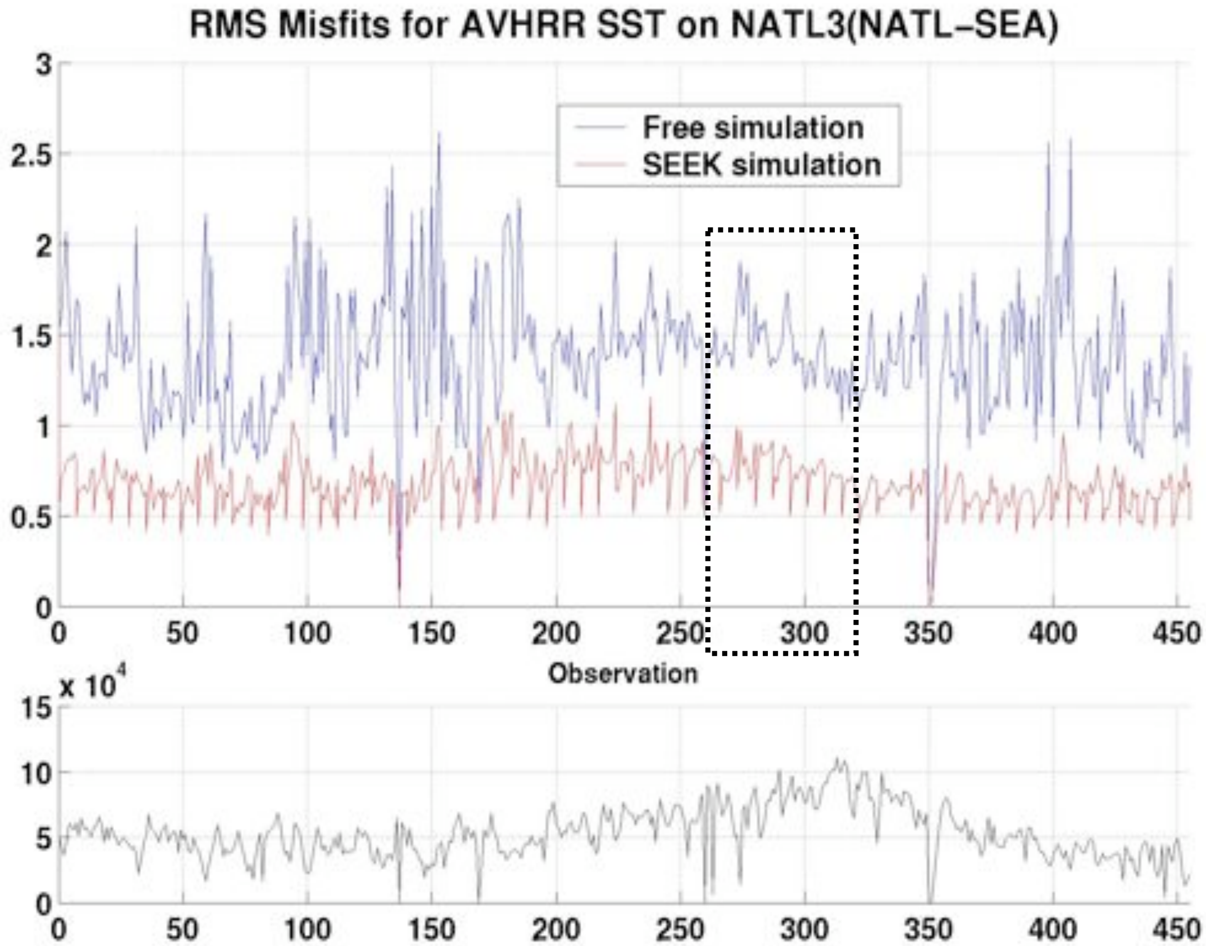


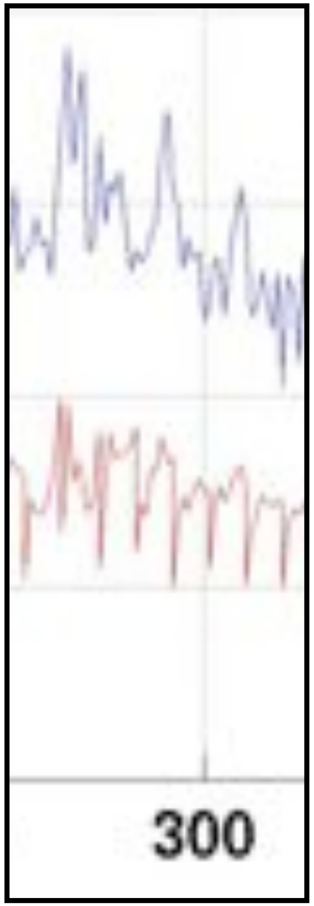


Assimilation of isolated T/S profiles: SSH increment after 1, 2, 3 days of model forecast



7. Improved temporal strategies
« Rejection » of SST data assimilation





7. Improved temporal strategies
Towards a time-continuous DA scheme

2 possible modifications of KF :

- **FGAT (First Guess at Appropriate Time)**
- **IAU (Incremental Analysis Update,** Bloom *et al*., 1996**)**

$$\begin{cases} \boldsymbol{x}_i^a \\ \boldsymbol{P}_i^a \end{cases}$$

Forecast 1

$$\begin{cases} \boldsymbol{x}_{i+1}^f = M\left(\boldsymbol{x}_i^a\right) \\ \boldsymbol{P}_{i+1}^f = \mathbf{M}\mathbf{P}_i^a\mathbf{M}^T + \mathbf{Q} \end{cases}$$

Analysis

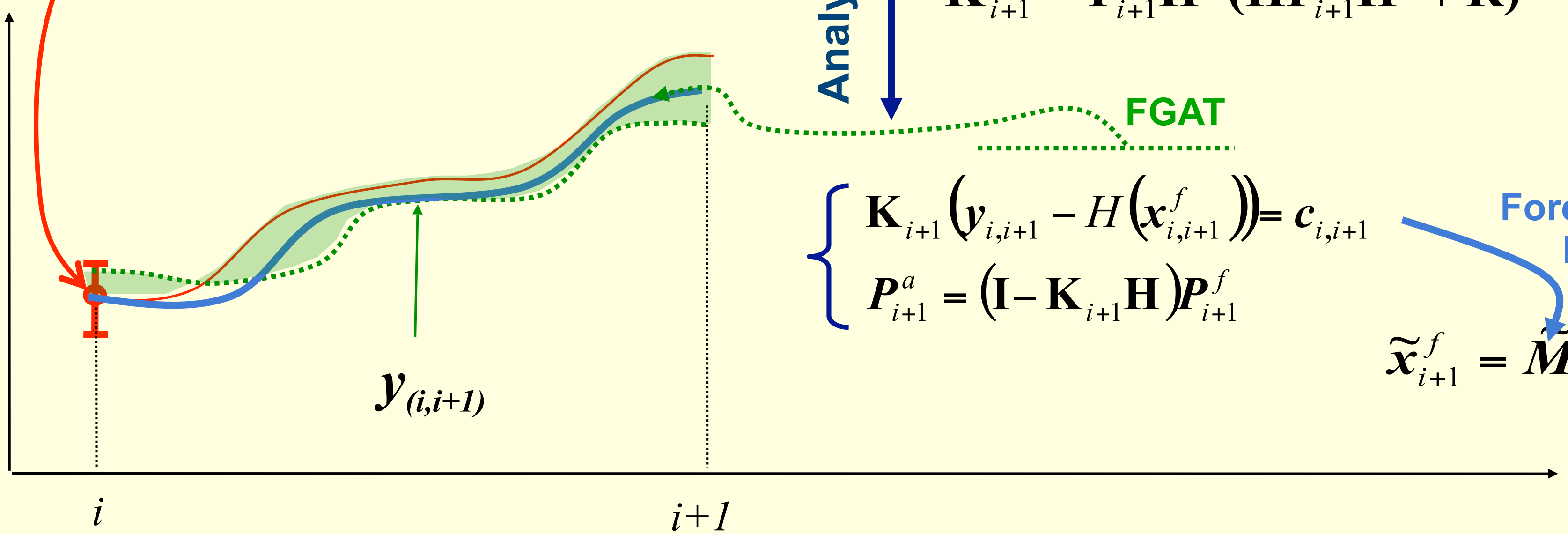
$$\mathbf{K}_{i+1} = \mathbf{P}_{i+1}^f\mathbf{H}^T(\mathbf{H}\mathbf{P}_{i+1}^f\mathbf{H}^T + \mathbf{R})^{-1}$$

FGAT

$$\begin{cases} \mathbf{K}_{i+1}\left(\boldsymbol{y}_{i,i+1} - H\left(\boldsymbol{x}_{i,i+1}^f\right)\right) = \boldsymbol{c}_{i,i+1} \\ \boldsymbol{P}_{i+1}^a = \left(\mathbf{I} - \mathbf{K}_{i+1}\mathbf{H}\right)\boldsymbol{P}_{i+1}^f \end{cases}$$

Forecast 2
IAU

$$\tilde{\boldsymbol{x}}_{i+1}^f = \tilde{\boldsymbol{M}}\left(\boldsymbol{x}_i^a\right)$$



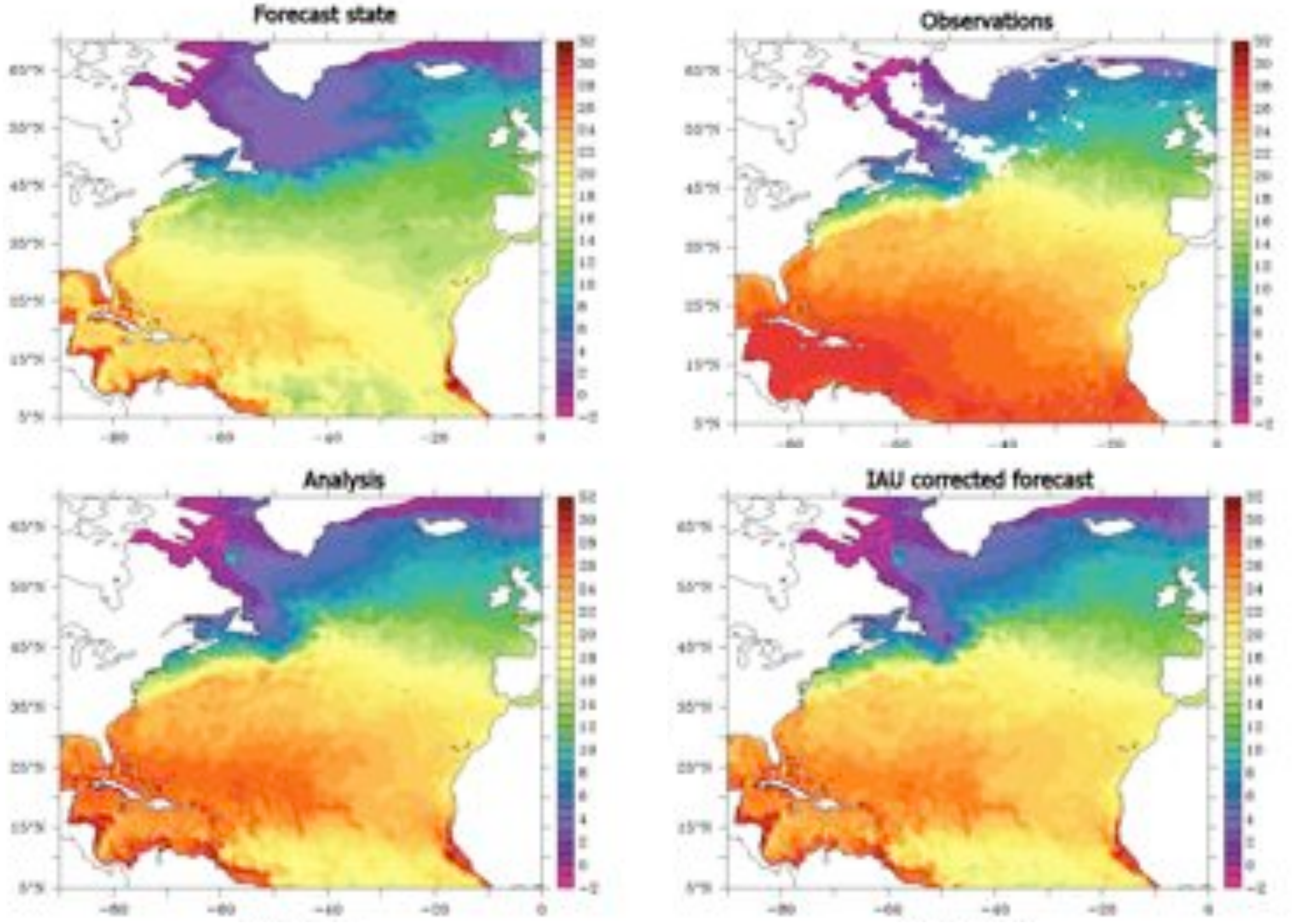
7. Improved temporal strategies
IAU implementation

- **Implementation of Incremental Analysis Update in OPA primitive equation model** (Ourmières *et al.*, 2006):
  - Compute innovation using SST/SLA data and FGAT scheme ;
  - Compute Kalman gain and analysis increment at the end of assimilation window using the standard algorithm;
  - Divide temperature and salinity increments by the number of model time steps in assimilation window $\Rightarrow \left(\frac{\delta T}{l}, \frac{\delta S}{l}\right)$
  - Integrate the ocean model on $(t_i\ ,\ t_{i+1})$ once again, with modified equations for temperature and salinity, i.e :

$$\frac{\partial T}{\partial t} + \boldsymbol{u}.\nabla^h T + w\frac{\partial T}{\partial z} = D^h(T) + \frac{\partial}{\partial z}\left(\tilde{\lambda}\frac{\partial T}{\partial z}\right) + \frac{\delta T}{l}$$

7. Improved temporal strategies
IAU - example

- **TEST: SST assimilation – 05/11/92**

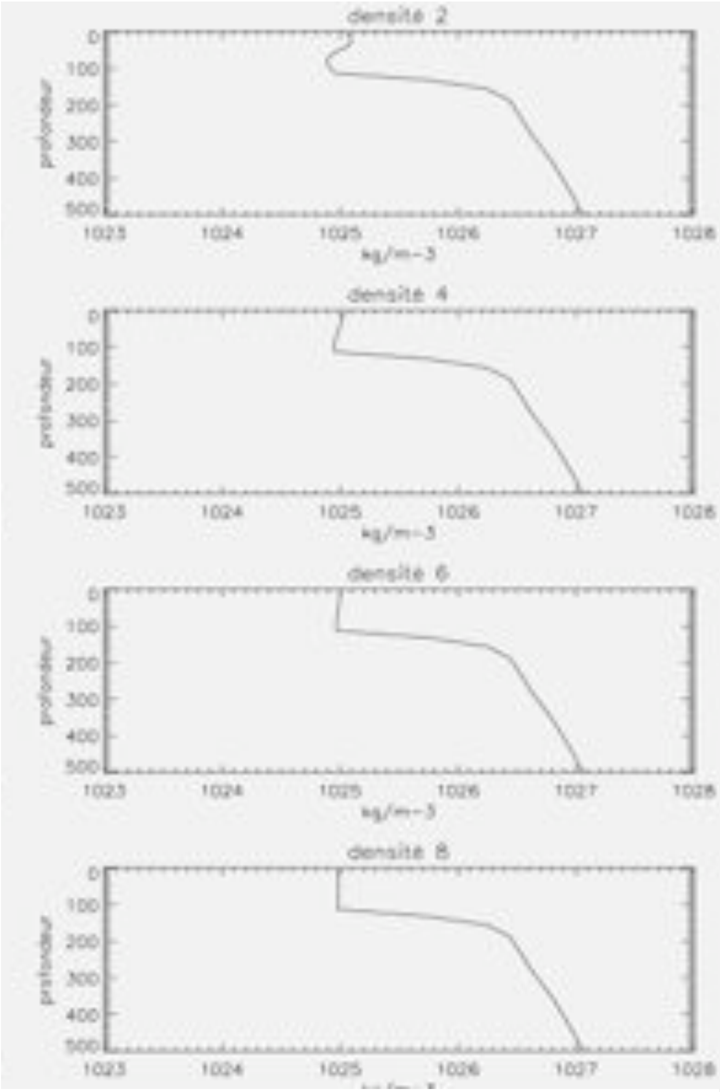


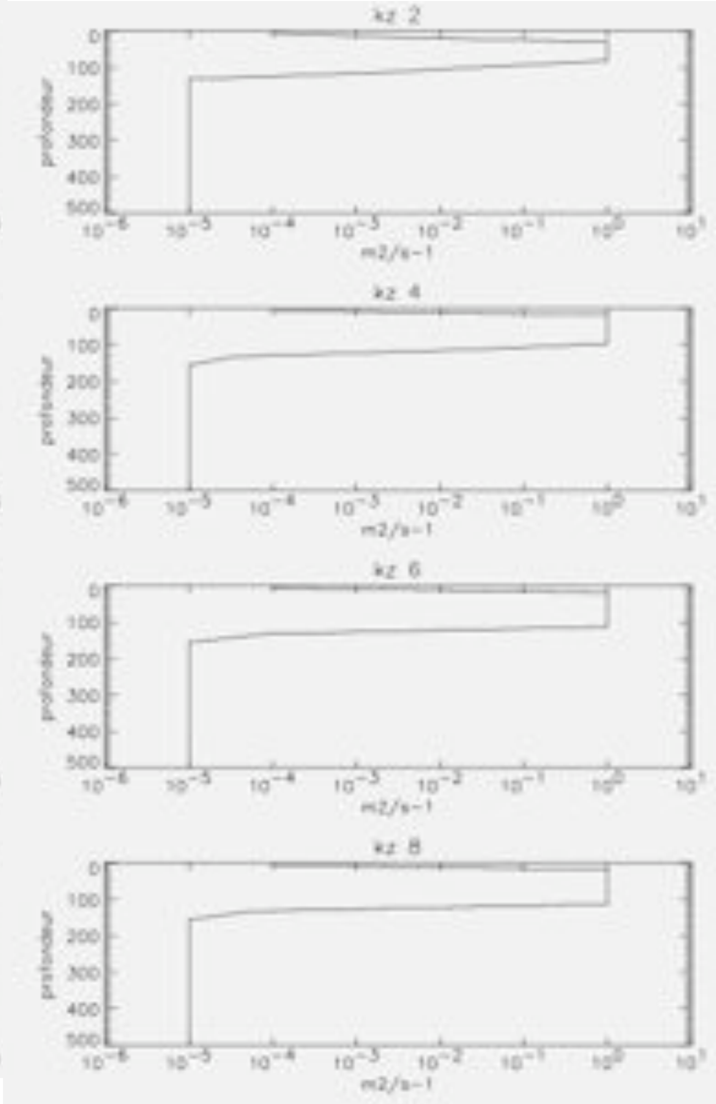
8. Kalman filter with inequality constraints
Motivations

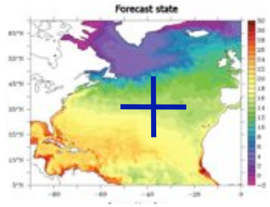
- Inequality constraints are inherent to ocean models
- Examples
  - Concentrations in biogeochemical models must be positive
  - T must be larger than freezing temperature
  - Static stability (a non-linear combination of T/S vertical gradients) must be verified at every assimilation step
  - …
- The traditional Kalman filter framework with gaussian statistics doesn't guarantee equality/inequality constraints
- Empirical correction schemes can be implemented after the statistical analysis step to restore the constraints

Poster by Claire Lauvernet for more details

8. Kalman filter with inequality constraints
DA-induced static instability



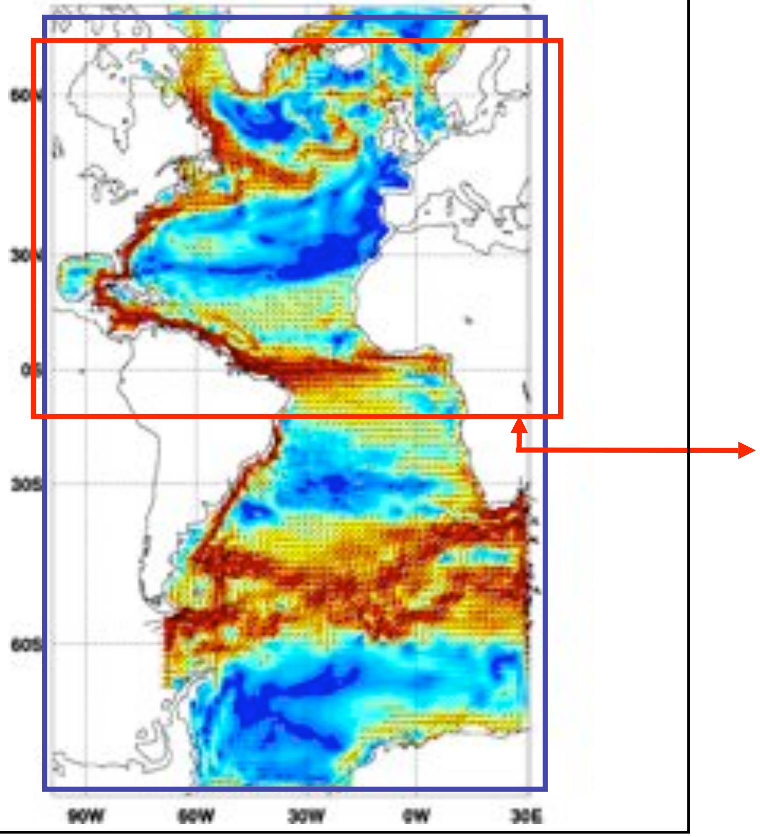




8. Kalman filter with inequality constraints
DA into coupled physical-biological model

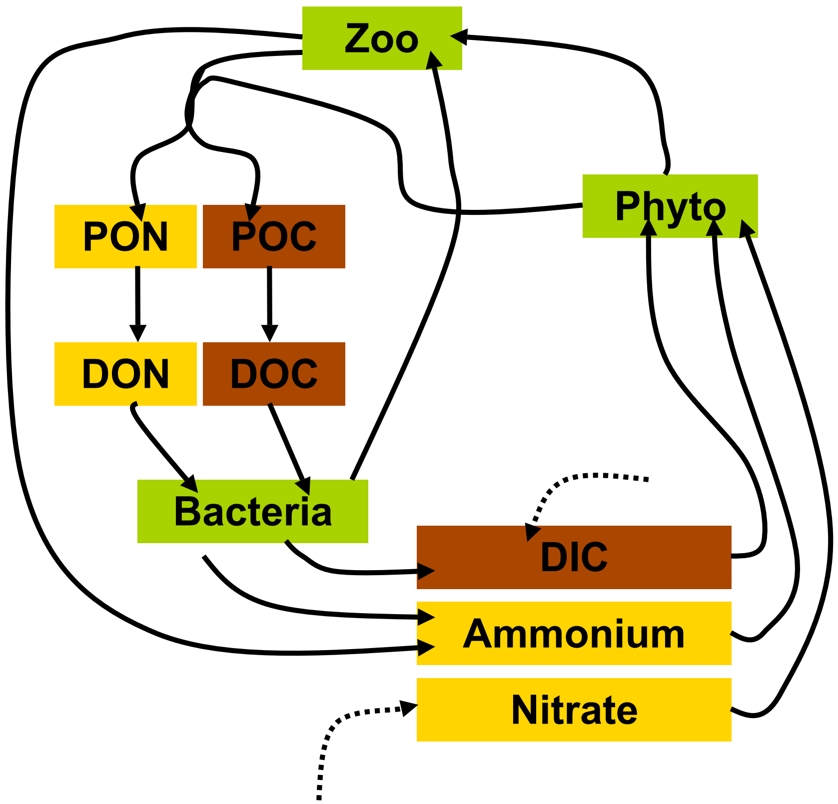
Hydrodynamic model

- OPA code, horizontal resolution 1/3°
- SST/SLA assimilation using SEEK



Ecosystem model

- FDM formulation in the euphotic zone
- Regeneration model below



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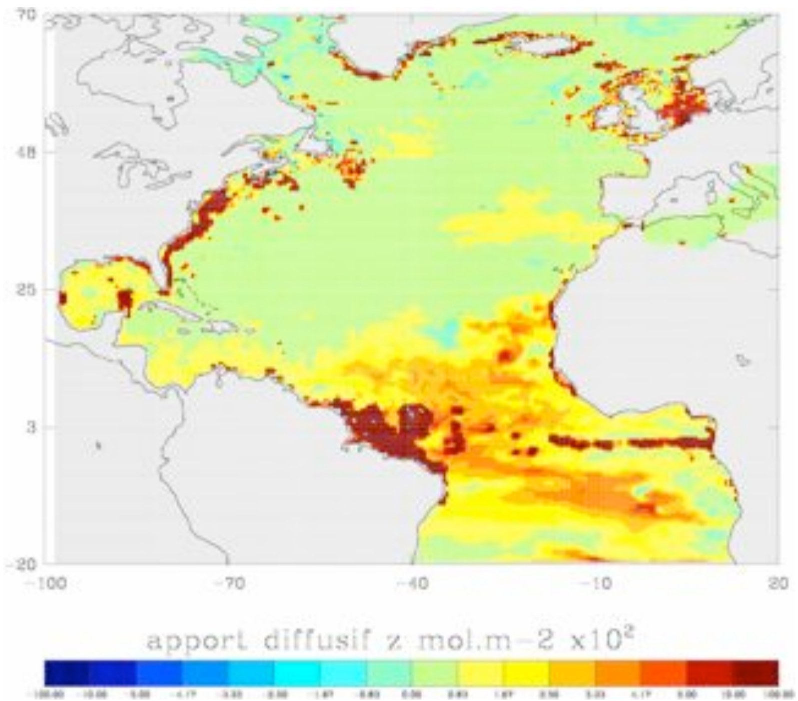
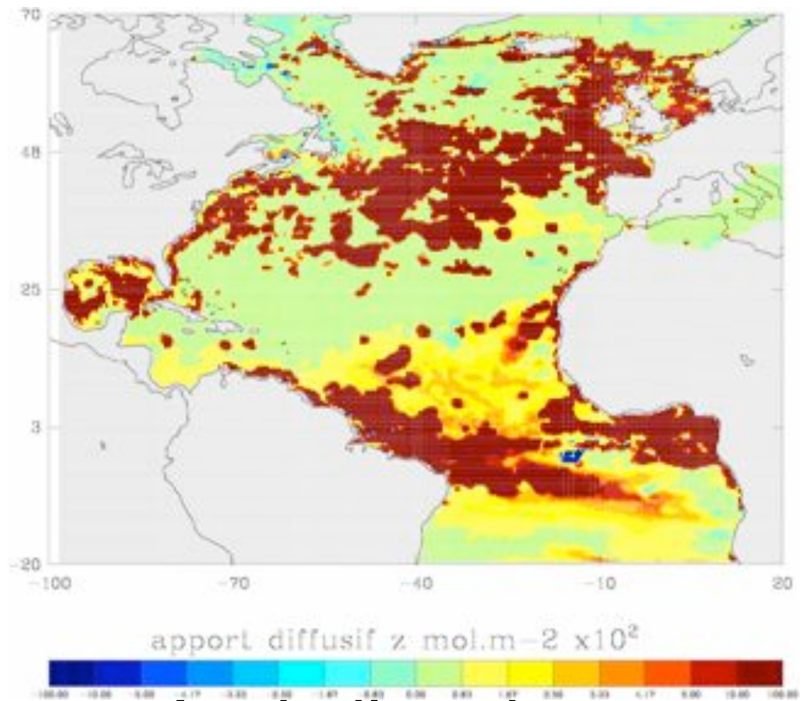
8. Kalman filter with inequality constraints
Impact on nutrient dynamics

Diffusive PO_4 input (mol.m-2) in the euphotic zone



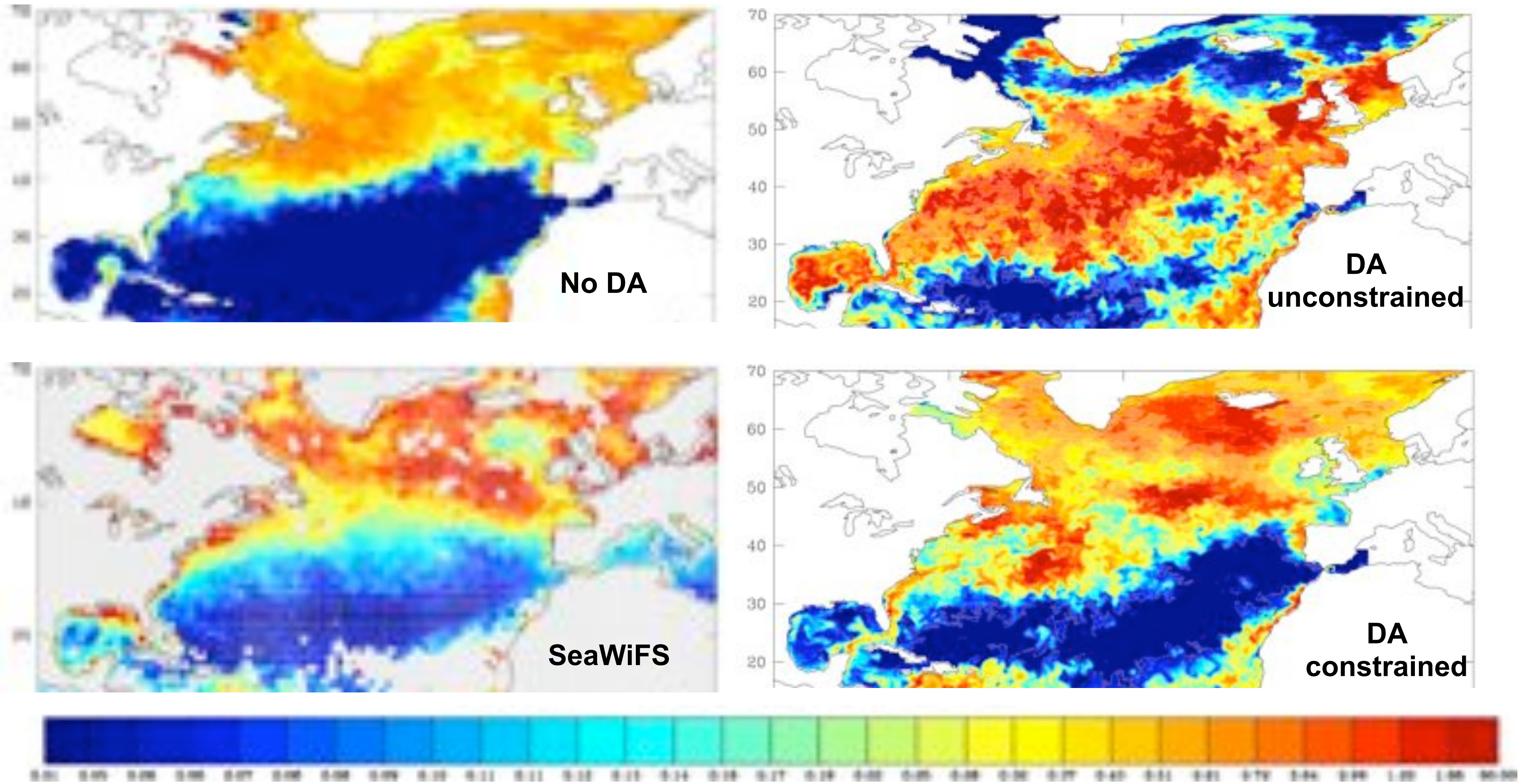
Free run



Assimilated run

8. Kalman filter with inequality constraints
Impact on surface chlorophyll

- **Surface chl_a concentration (mg/m3) – July 1998**



Conlusions

- Statistical schemes derived from the Kalman filter have been successfully developed from theoretical basis to operational oceanographic implementations, for both research and operational applications.

- The specification of adequate error statistics (sub-space, statistical models etc.) is a central issue. Simplified KF (e.g. SEEK with fixed basis) have been very effective to test different statistical models.

- There is no generic method that can be considered as a « plug-and-play » solution. Each particular DA problem requires a good degree of understanding and *ad hoc* developments.

- The next challenge to DA could be to combine local and global inversions (i.e. hybrid 4D-VAR / KF methods).

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