Sequential methods for ocean data assimilation

From theory to practical implementations (II)

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2. Kalman Filter fundamentals
Assimilation cycle

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

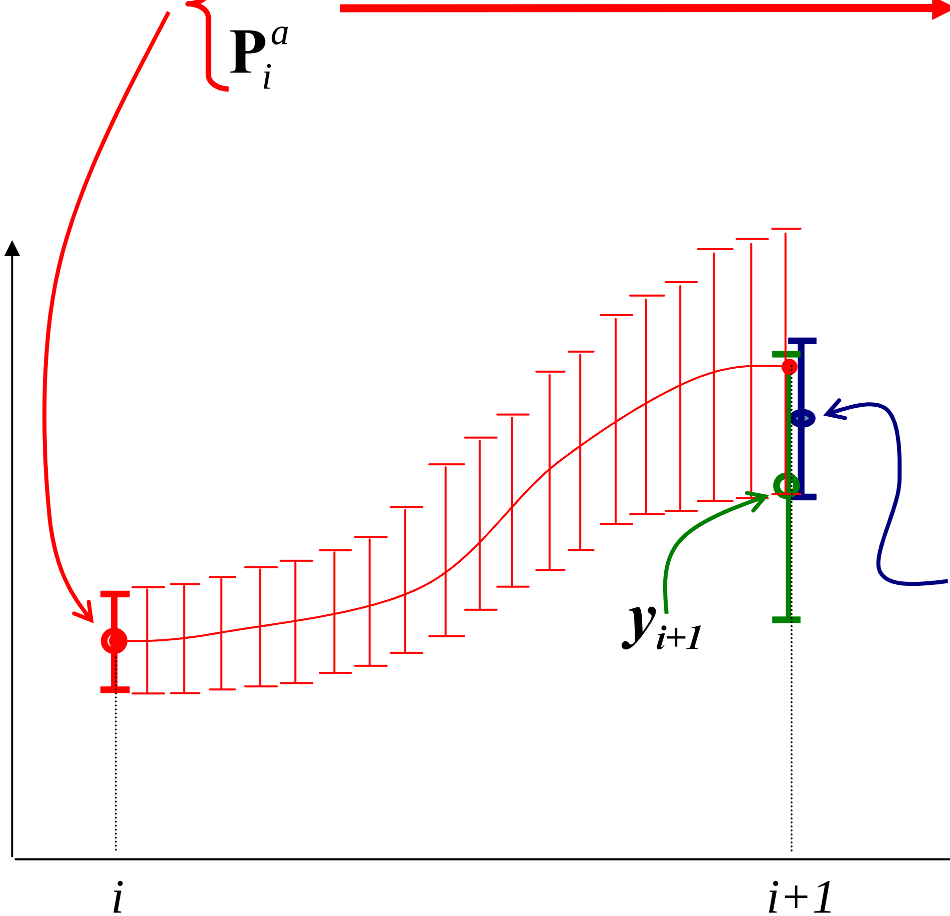
Forecast →

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

Analysis ↓

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

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

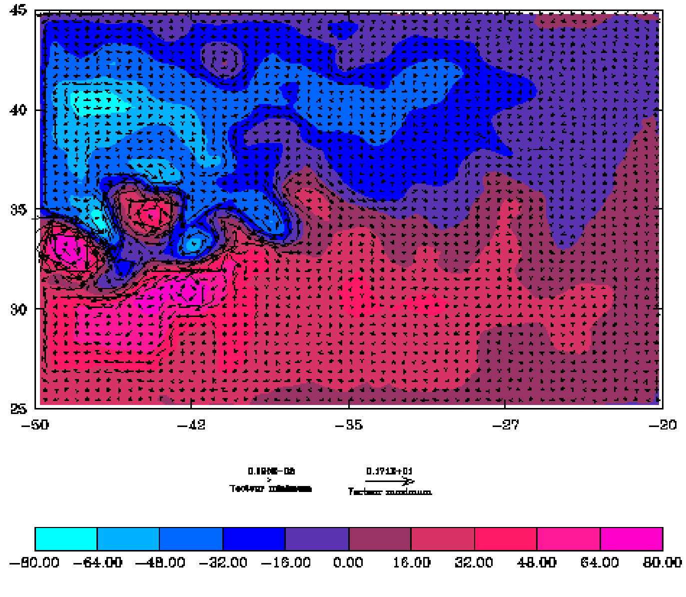


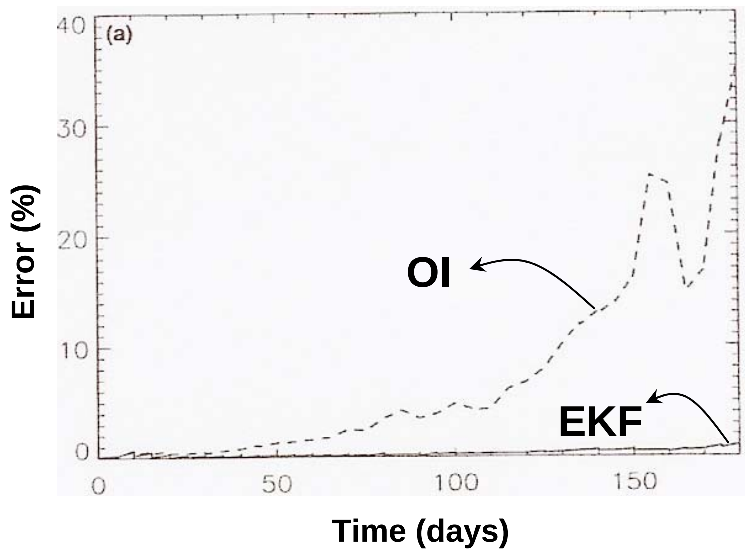
OI vs. EKF

- 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

Idealized double-gyre model (Ballabrera *et al.*, 2001)





OUTLINE

- State-of-the-art
  1. Introduction
  2. Kalman filter: fundamentals
  3. *Applied* ocean data assimilation: specific issues
  4. Simplifications of the KF – Optimal Interpolation

- **Advanced issues**
  5. **Space reduction: state and error sub-spaces**
  6. **Low rank filters: SEEK and EnKF**
  7. **Consistency validation and adaptivity**
  8. **Improved temporal strategies : FGAT and IAU**

5. Space reduction
How ?

- **The concept of space reduction is introduced, with the objectives to :**
  - ✓ Substantially reduce the computational burden of a full Kalman filter, but
  - ✓ Preserve the essential properties of statistical estimation.
- **The reduction can be formulated in terms of <u>state space</u> of <u>error space</u>.**

- **State space reduction by :**
  - ✓ Selection of model state variables (T,S,psi)
  - ✓ Selection of grid points (coarse grid) or large-scale modes
  - ✓ KF for surface (observed) variables only + vertical extrapolation
  - ✓ …
- **Formally:** $w = \mathbf{T}\,x \quad \text{with} \quad dim\,\mathbf{T} = r \times n$

! $\mathbf{T}^{-I}$ *needed to project the KF estimate back to full space* !

5. Space reduction
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**

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

- 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 : $r \sim 10\text{-}100$

5. Space reduction
Error sub-space variants

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

r ~10-100

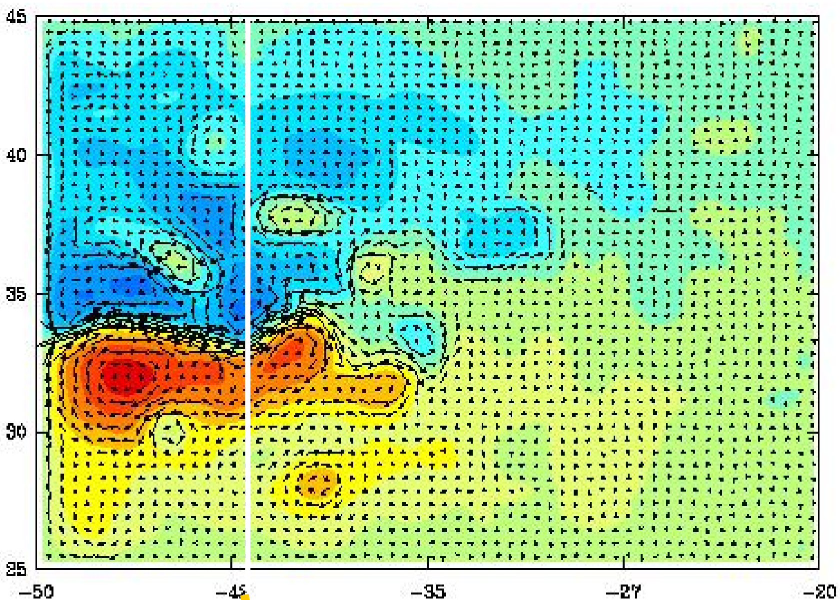
n ~10^6-10^8

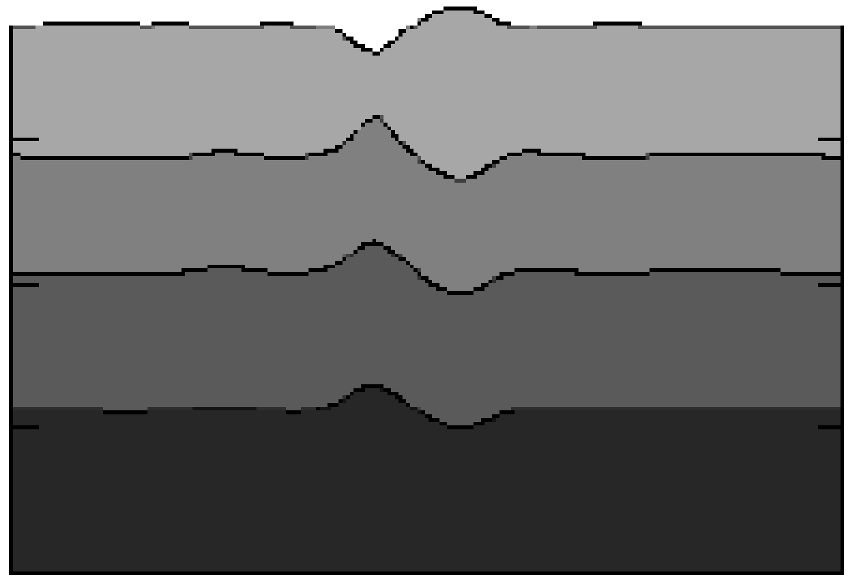
All covariance informations are contained in $\mathbf{S}_0$ *!*

Variants to build the sub-space :

- **EOFs from model variability**: global 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)*
- **Singular or breeding modes** : *for non-linear models*
- **Ensemble of Monte-Carlo perturbations of model states**
- **…**

- **Idealized double-gyre model (MICOM, 4 layers)**





Vertical section through dominant EOF

« 3D Cooper-Haines » mode

EOFs provide a robust description of the covariances between SLA and vertical displacements of isopycnals

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

- ✓ Sampling of historical sequence:

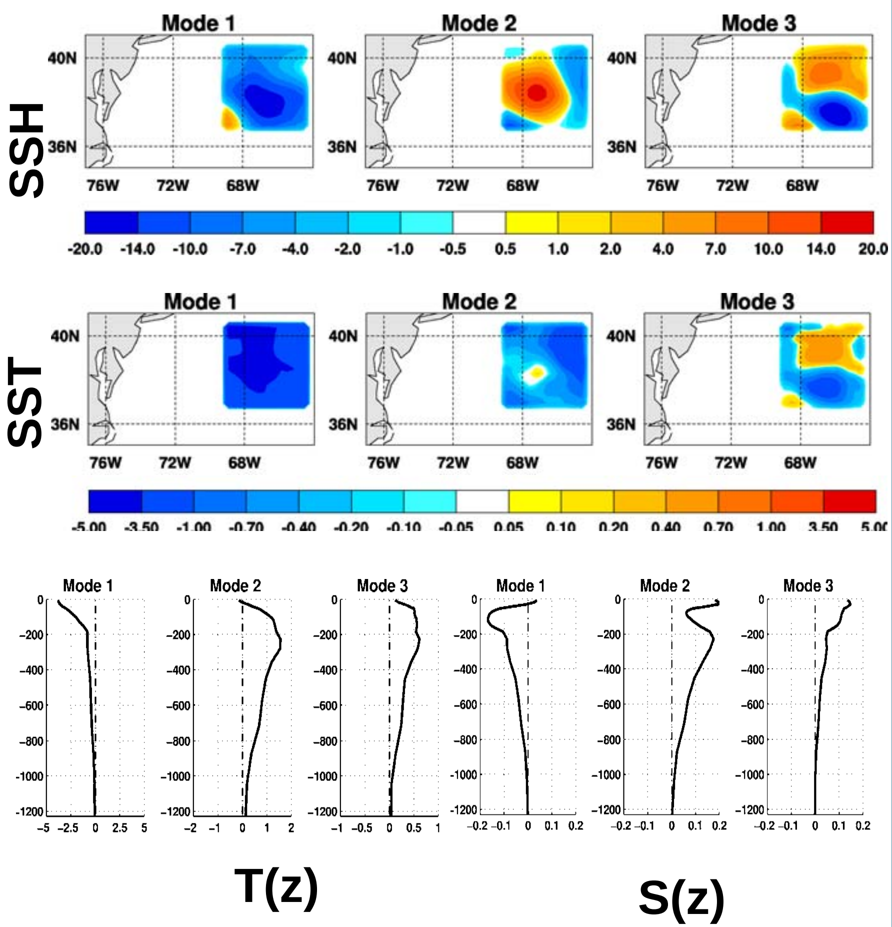
$$x^m(t_{i+1}) = M(t_i, t_{i+1})x^m(t_i) \quad , \quad i = 0,\dots,s-1$$
$$\Rightarrow \mathbf{X} = \left\{ x^m(t_i) - \overline{x^m(t_i)} \right\} \quad \dim n \times s$$

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

$$\mathbf{XX}^T\mathbf{L} = \mathbf{L}\,\Lambda \;\Leftrightarrow\; \mathbf{X}^T\mathbf{XX}^T\mathbf{L} = \mathbf{X}^T\mathbf{L}\,\Lambda = \mathbf{V}\,\Lambda$$
$$\Rightarrow \mathbf{L} = \mathbf{XV}\,\Lambda^{-1}$$

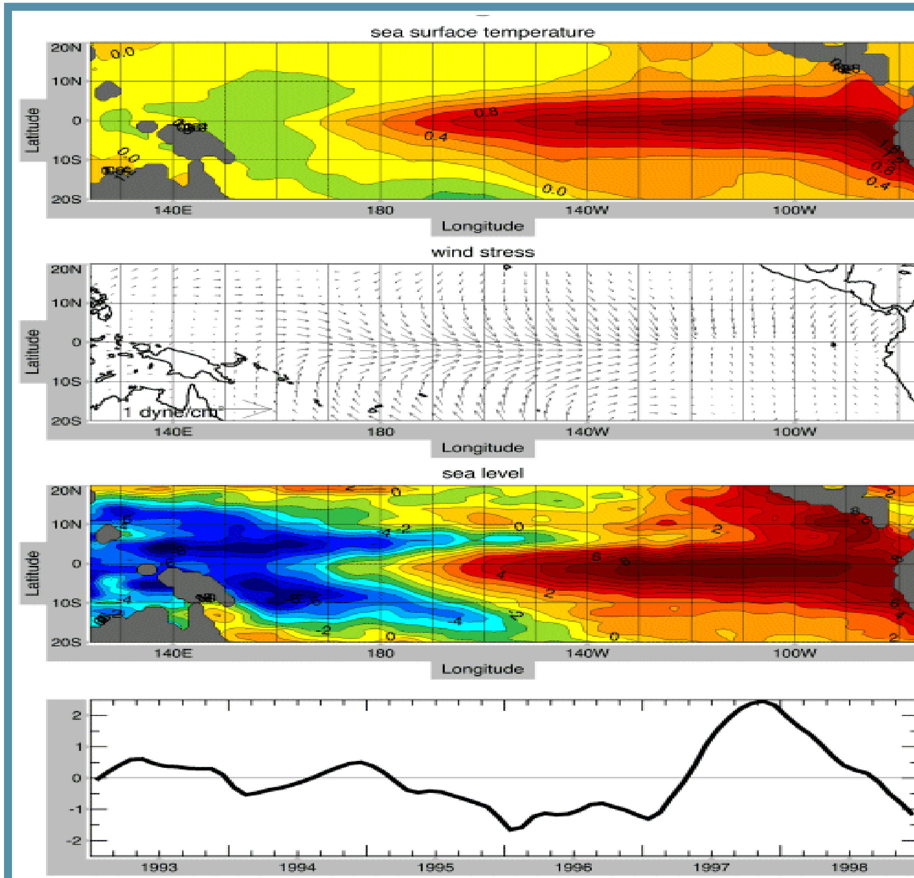
- ✓ Truncation to *r* dominant modes $\Rightarrow \mathbf{S}_0 \quad \text{and} \quad \mathbf{P}_0 \approx \mathbf{S}_0\mathbf{S}_0^T$

5. Space reduction
Error sub-spaces : examples



(from Testut et al., 2001)

Local EOFs



(from Picaut et al., 2001)

Global EOFs

6. Low rank Kalman filters
SEEK filter – forecast equation

Concept:

Use error space reduction $\mathbf{P}_i^a = \mathbf{S}_i^a \, \mathbf{S}_i^{a\,T}$ **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 $\mathbf{Q} \div \mathbf{M} \, \mathbf{P}_i^a \mathbf{M}^T$ to preserve low rank

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

- **« Extended » evolutive :** $\mathbf{S}_{i+1}^f = \mathbf{M}\mathbf{S}_i^a$ (*use tangent linear model : Pham et al., 1998)*
- **« Interpolated » evolutive :** $\mathbf{S}_{i+1}^f \div M\left(\boldsymbol{x}_i^a + \alpha \, \mathbf{S}_i^a\right) - M\left(\boldsymbol{x}_i^a\right)$ (*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)*

Concept: **Use error space reduction** $\mathbf{P}_i^a = \mathbf{S}_i^a \mathbf{S}_i^{a^T}$ **to compute** $\mathbf{K}$

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

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

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

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)*

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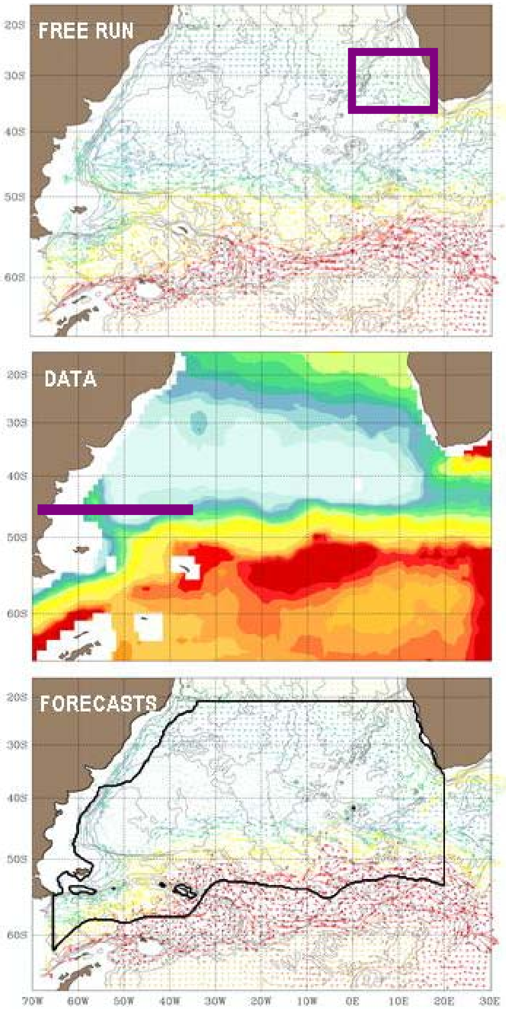
6. Low rank Kalman filters
Local EOFs for mesoscale data assimilation

Free run

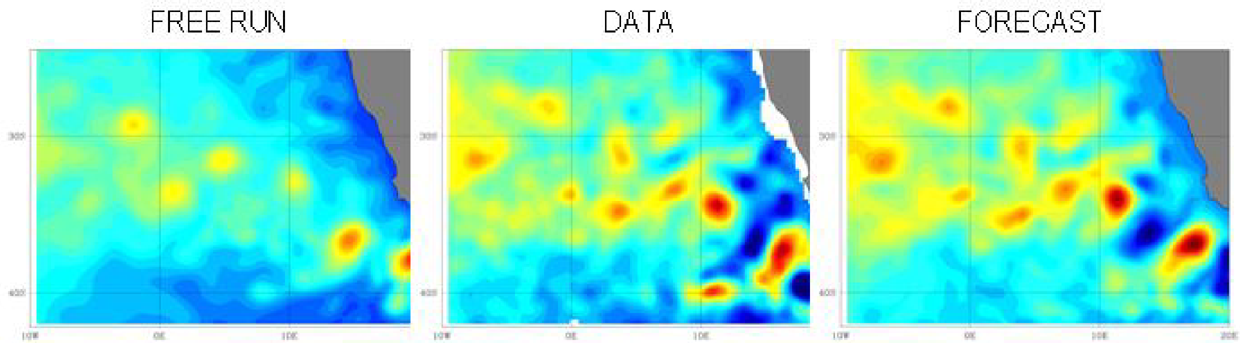
Sclim

Forecast

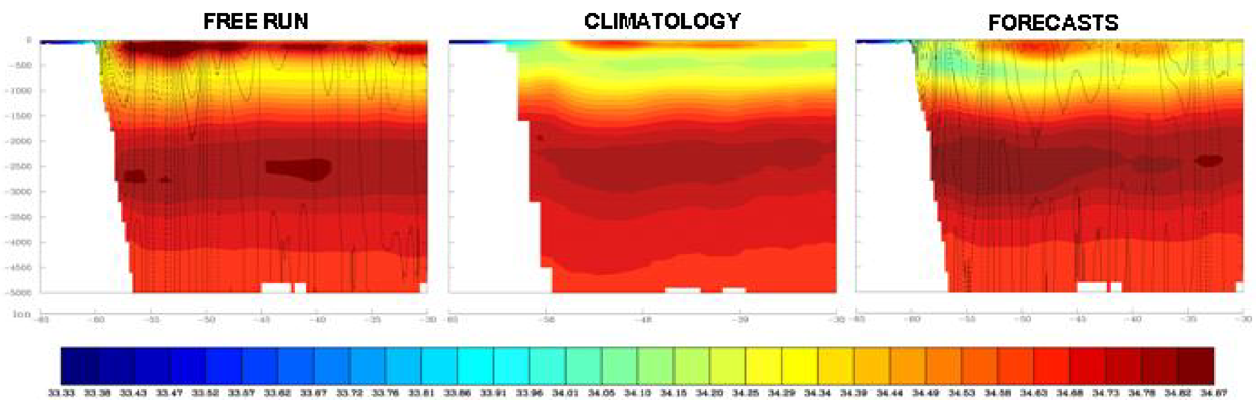


Circulation at 872 m

Agulhas Rings – June 25, 1995



Confluence – mean salinity at 45S



<u>South Atlantic hindcast</u> (Penduff *et al.*, 2003)

- ❑ **OPA model 1/3°, 1993-1996, 6h ECMWF**
- ❑ **Assimilation of SLA (T/P, ERS), SST (AVHRR)**

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:

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

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

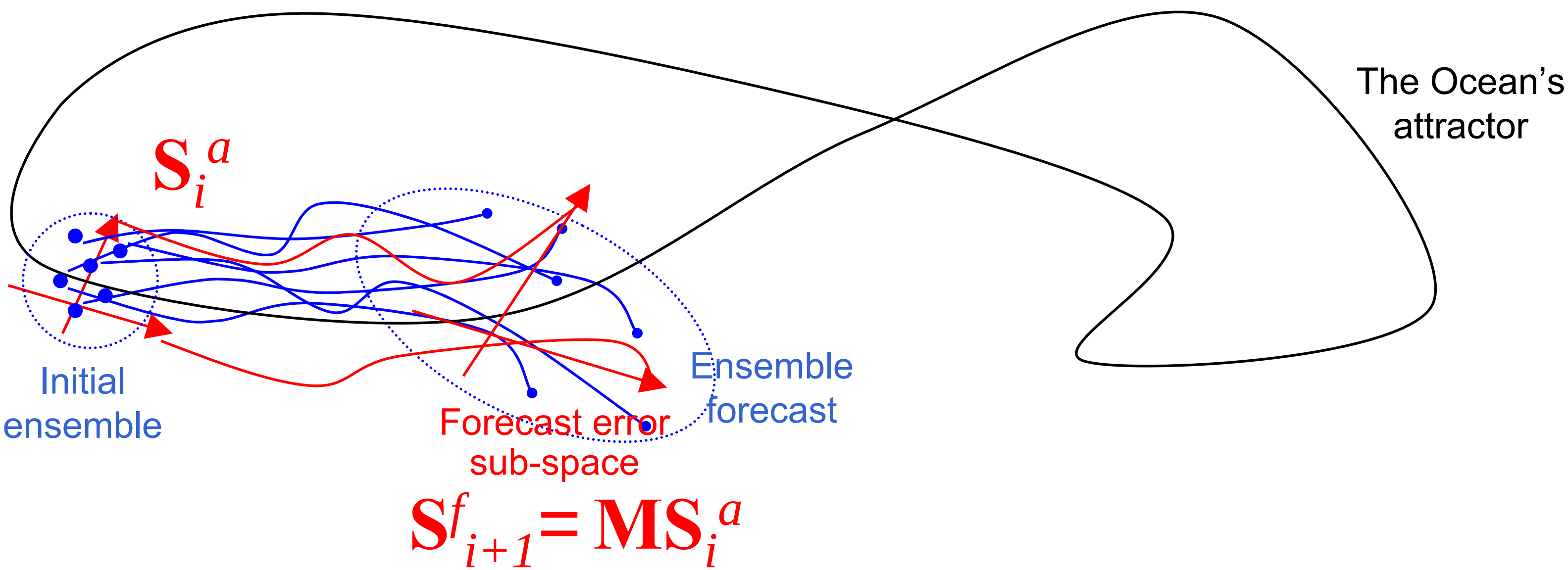
Analysis equation:

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

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

<u>Same philosophy</u> :

Sequential corrections along privileged directions of error growth



Differences between SEEK, EnKF, EnKS : Brusdal et al., JMS, 2003
SEEK, SEIK and EnKF intercomparison : Nerger et al., 2004

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

❑ **Filter error statistics :** $\overline{\boldsymbol{\varepsilon}^o} = 0 \quad \overline{\boldsymbol{\varepsilon}^f} = 0 \qquad \mathbf{R} = \overline{\boldsymbol{\varepsilon}^o \boldsymbol{\varepsilon}^{oT}} \qquad \mathbf{P}^f = \overline{\boldsymbol{\varepsilon}^f \boldsymbol{\varepsilon}^{fT}}$

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

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

❑ **Residuals « seen » by the filter:**

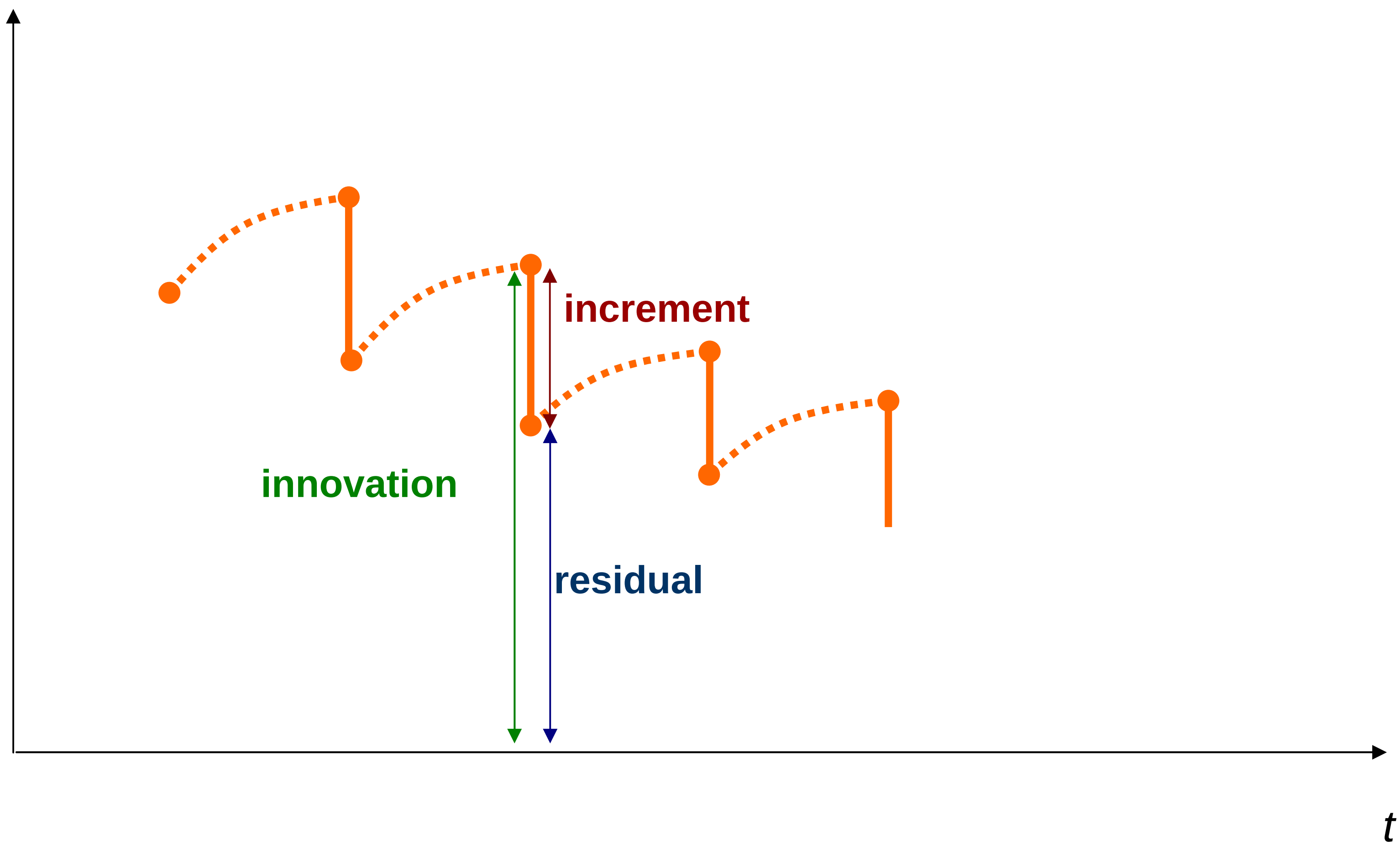
$$\mathbf{r}_i = \mathbf{y}_i - \mathbf{H}\mathbf{x}_i^a = (\mathbf{H}\mathbf{x}_i^t + \boldsymbol{\varepsilon}_i^o) - \mathbf{H}\mathbf{x}_i^a = \boldsymbol{\varepsilon}_i^o - \mathbf{H}\boldsymbol{\varepsilon}_i^a$$

❑ **Increments computed by the filter:**

$$\boldsymbol{x}_i^a - \boldsymbol{x}_i^f = \mathbf{K}_i \left(\boldsymbol{y}_i - \mathbf{H}\, \boldsymbol{x}_i^f \right)$$

7. Validation of DA systems - Adaptivity
Innovation & residual statistics

observation misfit



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

❑ **Unbiased innovation sequence :** $\overline{\mathbf{d}_i} = 0$

❑ **Unbiased residuals (** $\overline{\mathbf{r}_i} = 0$ **) or increments** $\mathbf{H}\overline{(x_i^a - x_i^f)} = 0$

❑ **Consistent error covariances :**

$$\overline{\mathbf{d}_i \mathbf{d}_i^T} = \mathbf{R} + \mathbf{H}\mathbf{P}_i^f \mathbf{H}^T$$

$$\overline{\mathbf{r}_i \ \mathbf{r}_i^T} = \mathbf{R} - \mathbf{H}\mathbf{P}_i^a \mathbf{H}^T$$

❑ χ_p^2 **distribution of** (Bennett, 1992) **:**

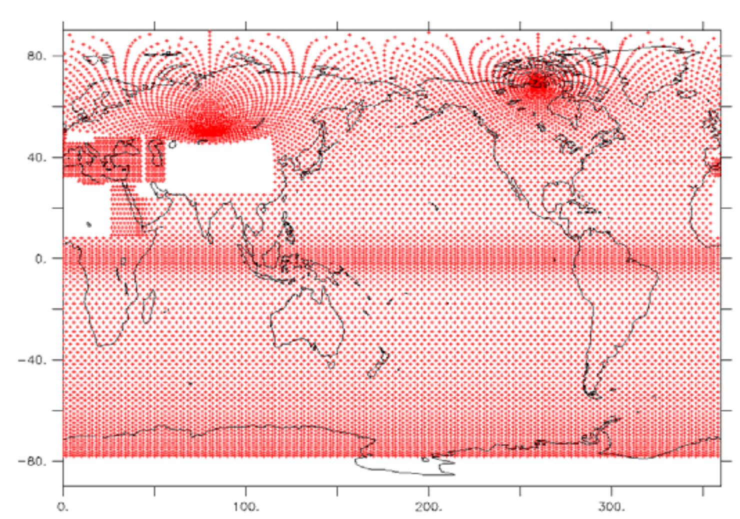
$$J_i = \mathbf{d}_i^T (\mathbf{H}\mathbf{P}_i^f \mathbf{H}^T + \mathbf{R})^{-1} \mathbf{d}_i$$

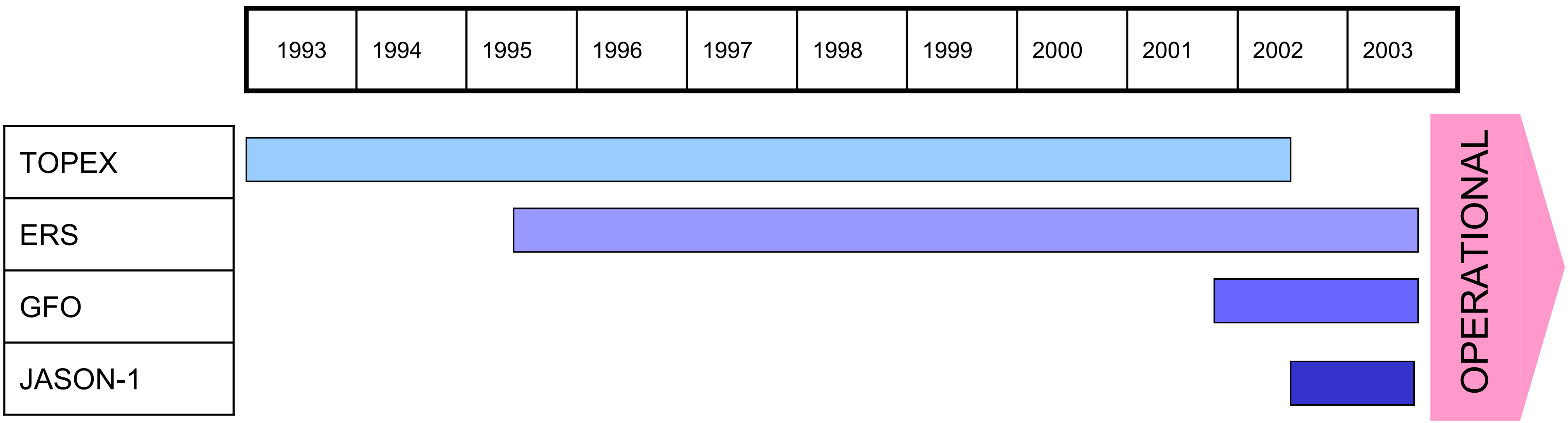
or, for low-rank $J_i = \mathbf{d}_i^T \left\{ (\mathbf{H}\mathbf{S}_i^f)(\mathbf{H}\mathbf{S}_i^f)^T + \mathbf{R} \right\}^{-1} \mathbf{d}_i$

7. Validation of DA systems - Adaptivity

MERCATOR Global : 1993-2002 analysis

- 1 year spin-up (1992)
- 11 years of **weekly** assimilation of SLA





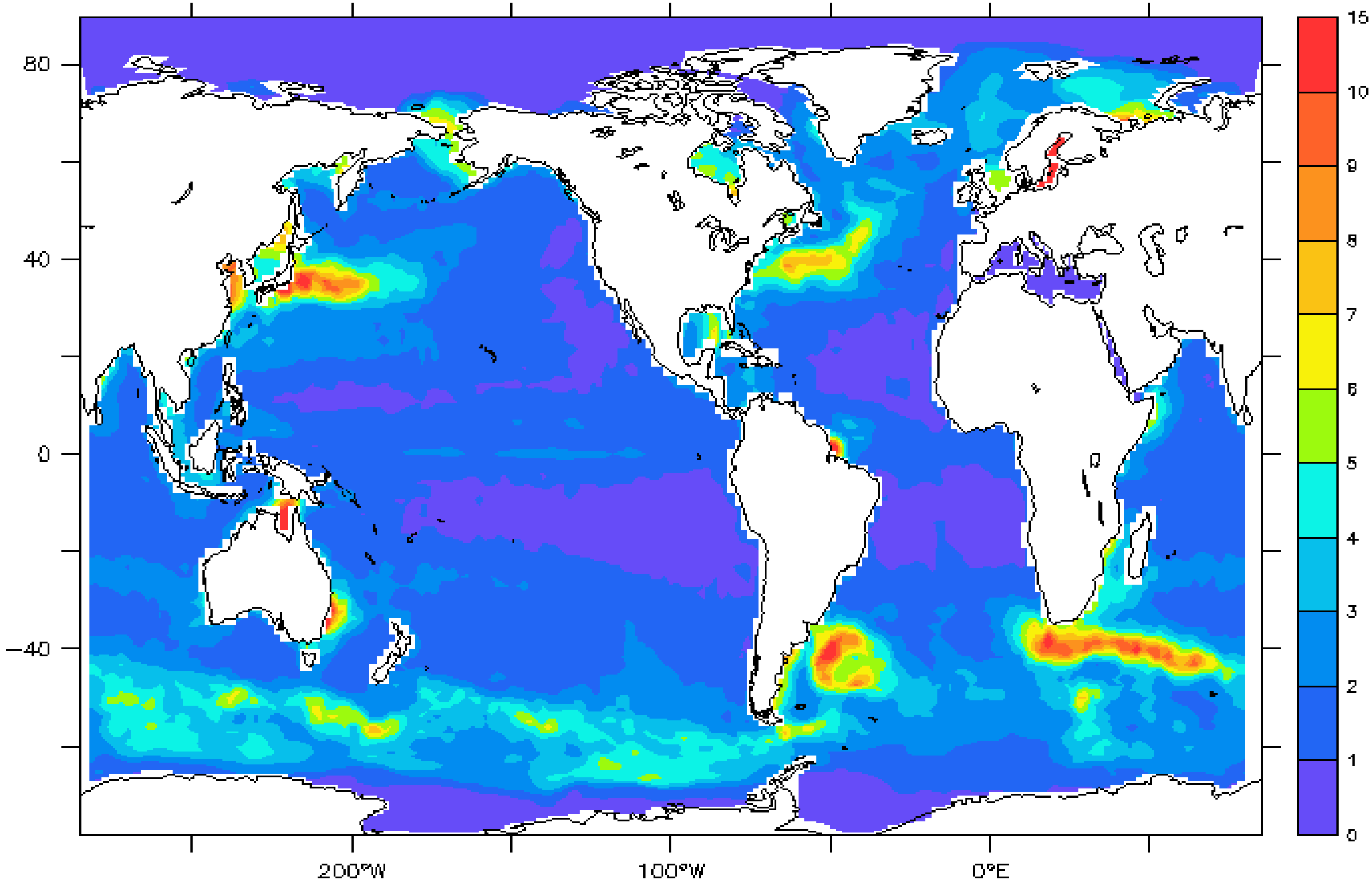
3D state estimation : SAM-1 and SAM-2

- **Optimal interpolation : SAM-1**
  1. SOFA + Cooper/Haines mode (open ocean attractor):
     2D statistical estimation + vertical adjustement : **SAM-1v1**
  2. SOFA + multivariate 1D vertical EOFs (from model or data variability):
     2D +1D statistical estimation : **SAM-1v2**

- **Reduced-order Kalman filter : SAM-2**
  1. SOFA + EOFs 3D (multivariate model variability): inversion in observation space : **SAM-2v0**
  2. SEEK + EOFs 3D (multivariate model variability): inversion in error sub-space: **SAM-2v1**

7. Validation of DA systems - Adaptivity
MERCATOR Global : 1993-2002 analysis

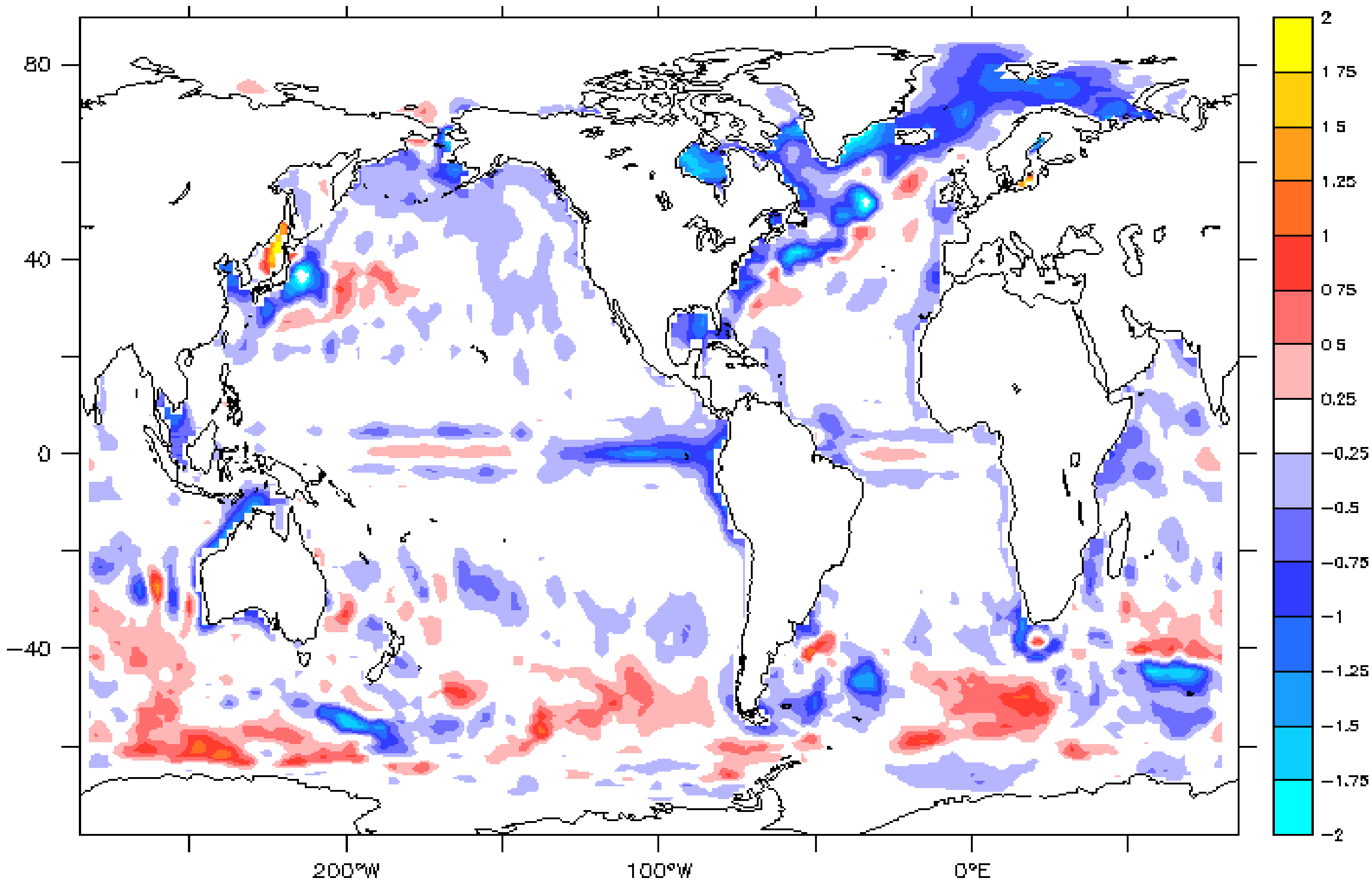
Standard deviation of SLA increment for 1993-2002, (cm)



Mercator global ocean prototype (Ferry *et al.*, 2004)

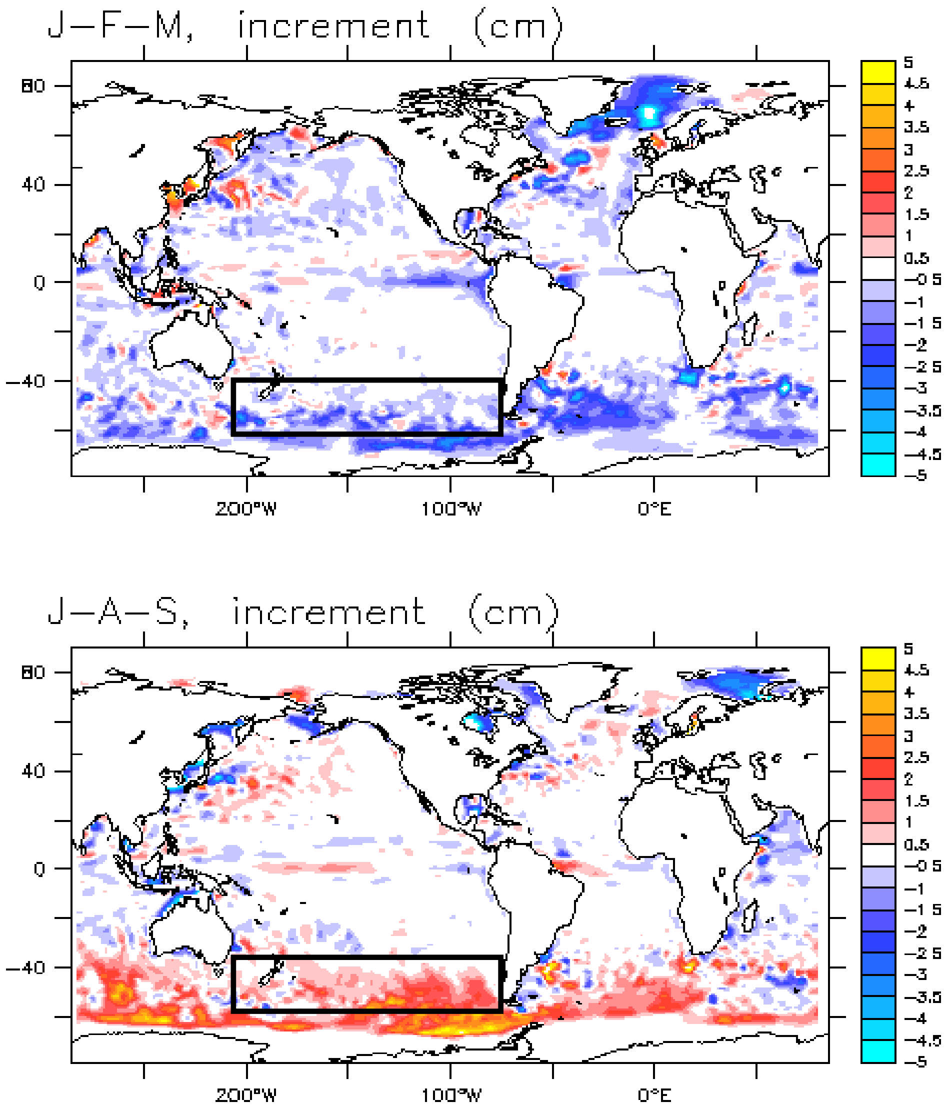
7. Validation of DA systems - Adaptivity
Detection of system biases

Mean SLA increment, 1993-2002, (cm)

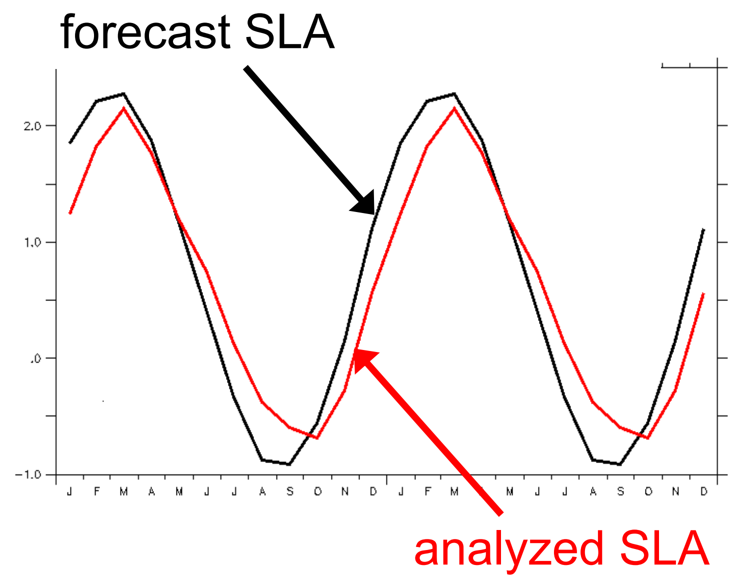


Mercator global ocean prototype (Ferry *et al*., 2004)

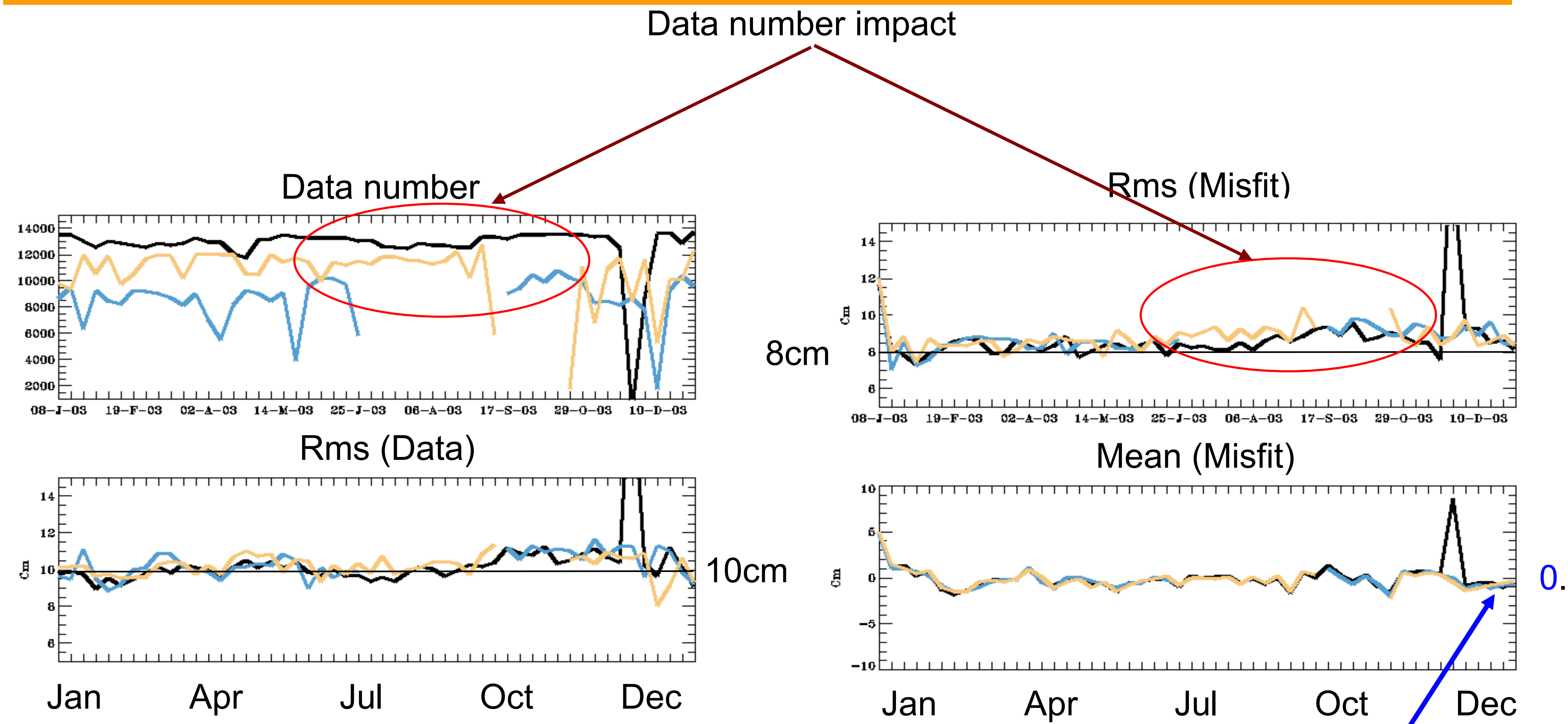
7. Validation of DA systems - Adaptivity
Analysis of system biases



❑ Mean seasonal SLA increment



7. Validation of DA systems - Adaptivity
Assimilation diagnostics



Black : Jason1
Blue : Ers2 (Envisat)
Orange : Gfo

No bias

7. Validation of DA systems - Adaptivity *Variants*

Concept: **« on line » modification of prior statistics ($\mathbf{R}$, $\mathbf{Q}$, …) 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 sub-space » :** use residual innovation to generate new error 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 : $\mathbf{P}_{i+1}^{f} \approx \alpha \, \mathbf{P}_{i}^{a}$

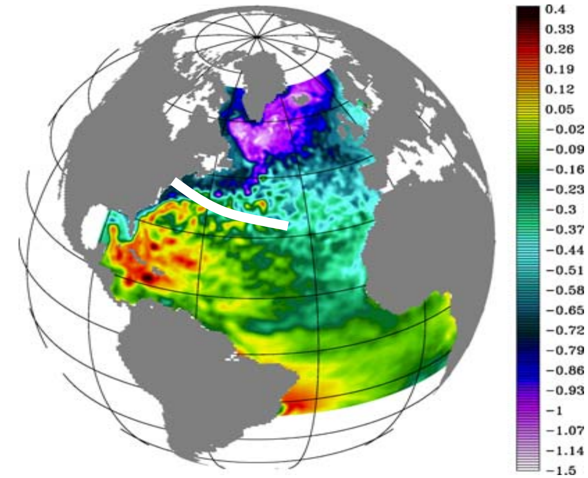
α → determined using innovation statistics history

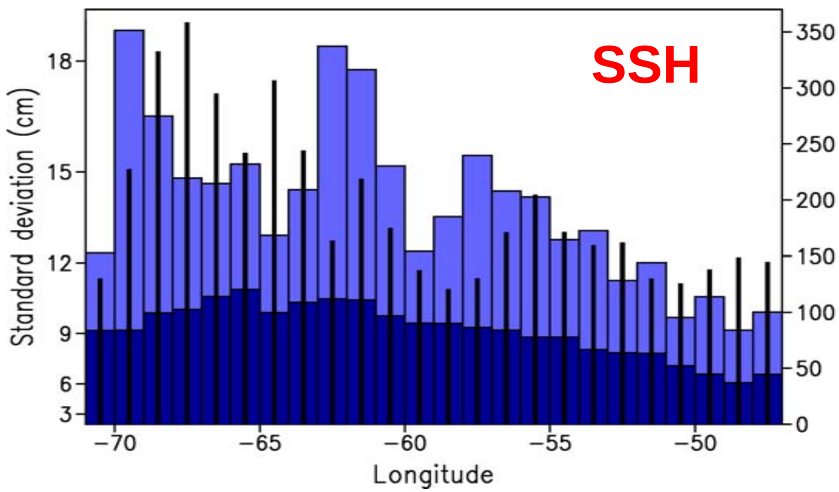
7. Validation of DA systems - Adaptivity
Example (I)

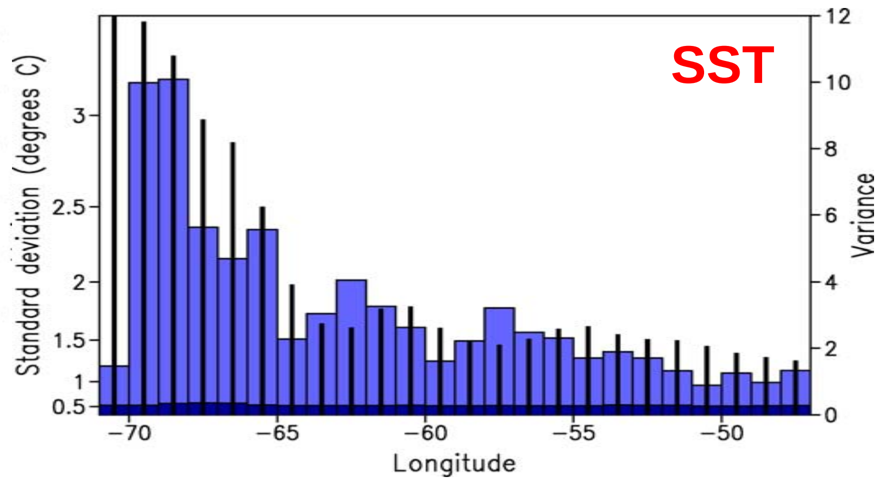
Comparison between 2 estimations of the forecast error variance in a zonal section crossing the Gulf Stream (HYCOM model, Brankart et al., 2003):

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

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

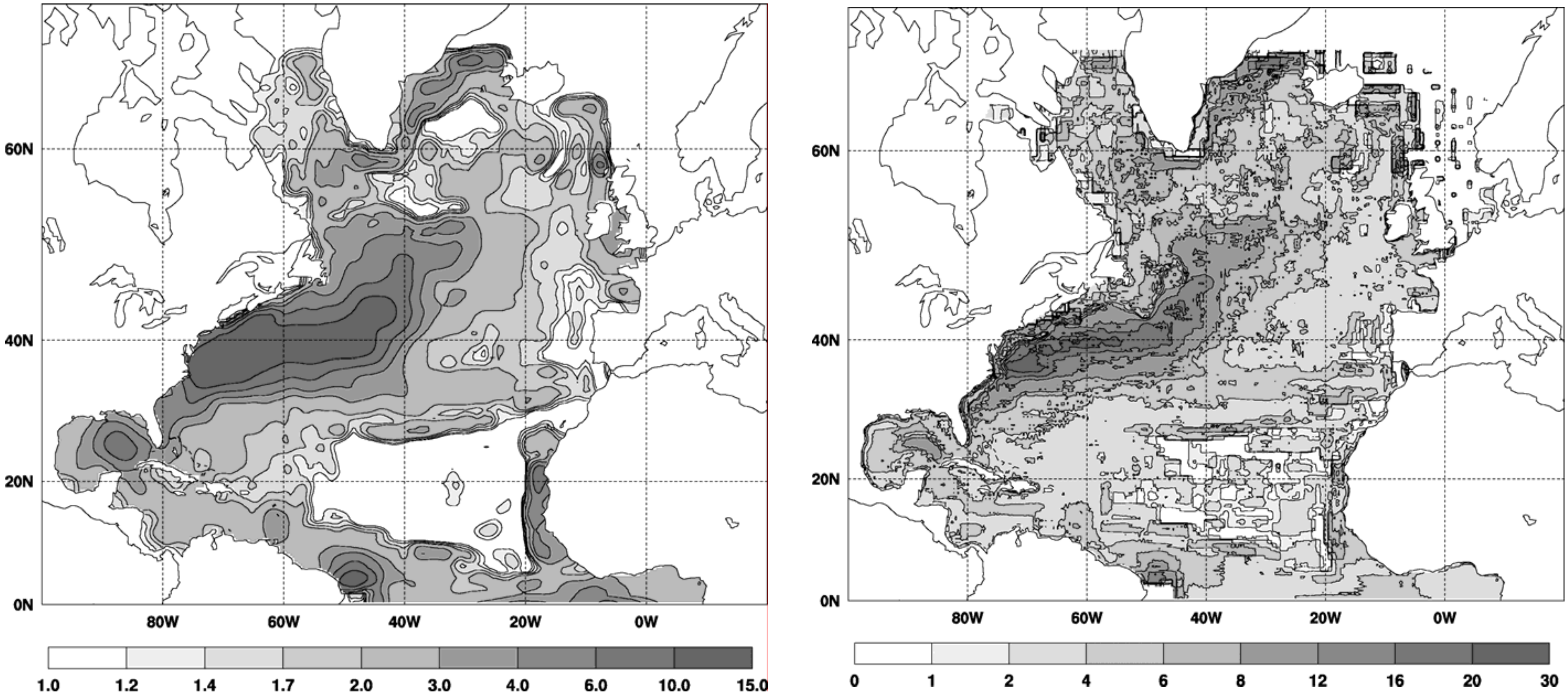






$diag\ (\overline{\mathbf{d}_i^f \mathbf{d}_i^{f^T}})$ $\quad$ diag $\mathbf{R}$ $\quad$ diag $\mathbf{P}^f$

7. Validation of DA systems - Adaptivity
Example (ii)



Model error amplification α

Forecast error estimates

8. Improved temporal strategies
Distributed observations

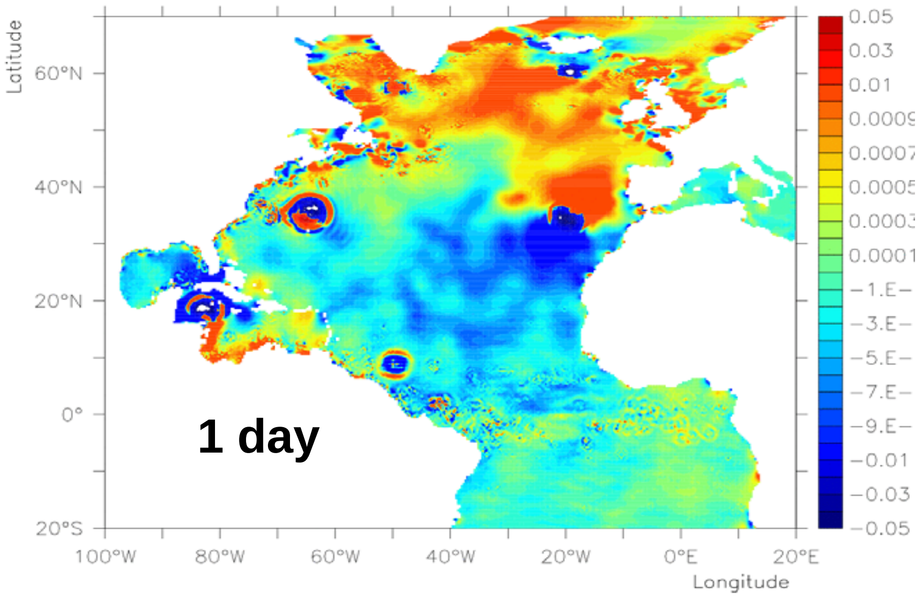
- Ocean observations are continuously distributed in time during the assimilation period; however, it is impossible to rigorously incorporate the data at their exact acquisition time. Therefore, **intermittent data assimilation schemes are *approximate*.**

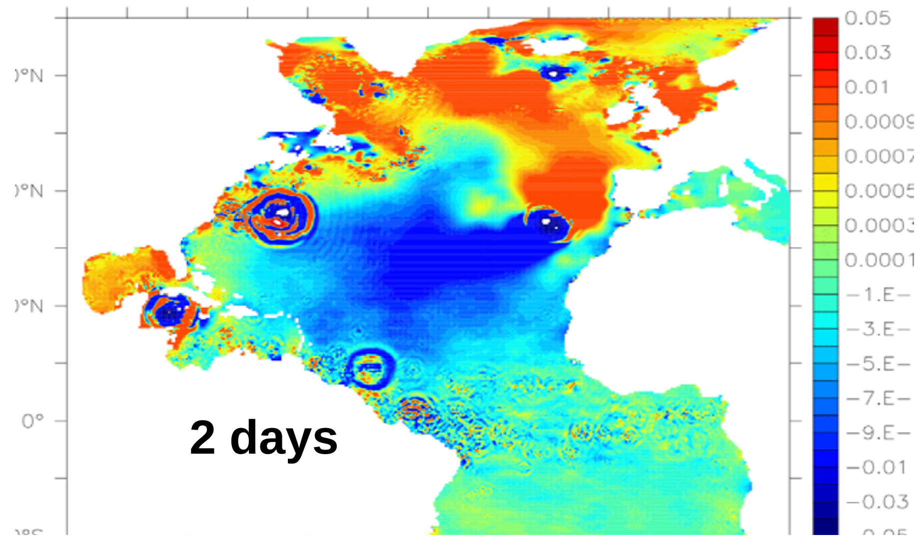
- Typical length of assimilation periods:
  - 3-7 days for mesoscale ocean current predictions;
  - 30 days for initialisation of seasonal climate predictions.

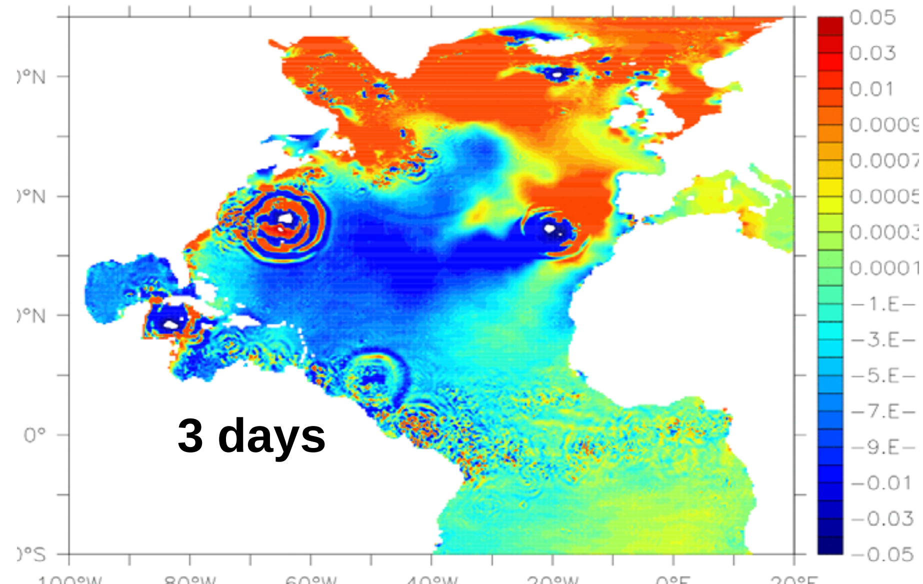
- Two related problems arise with intermittent corrections: shocks to the model, and data rejection.

Strategies to alleviate these problems ?

8. Improved temporal strategies
« Shocks » to model forecasts

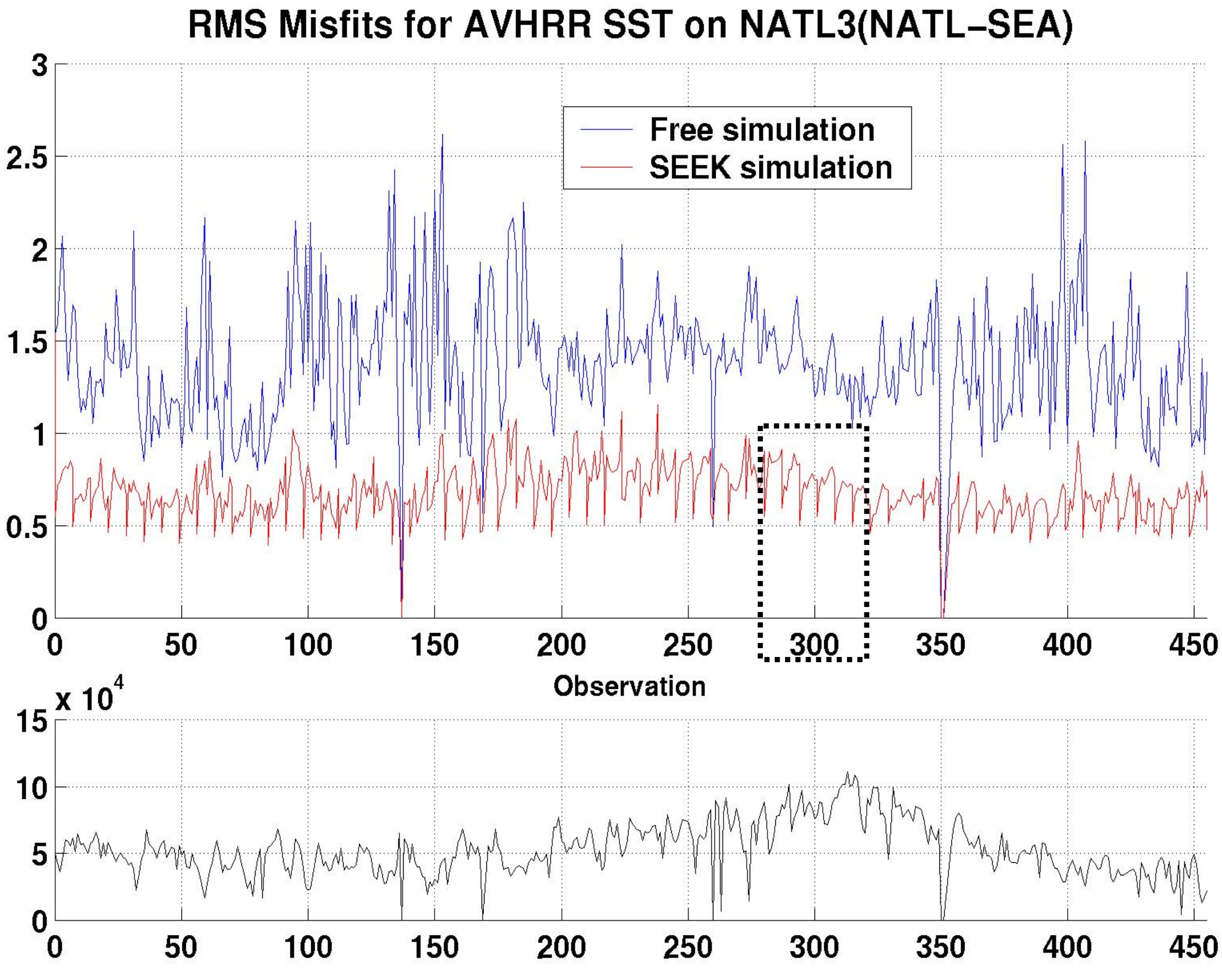


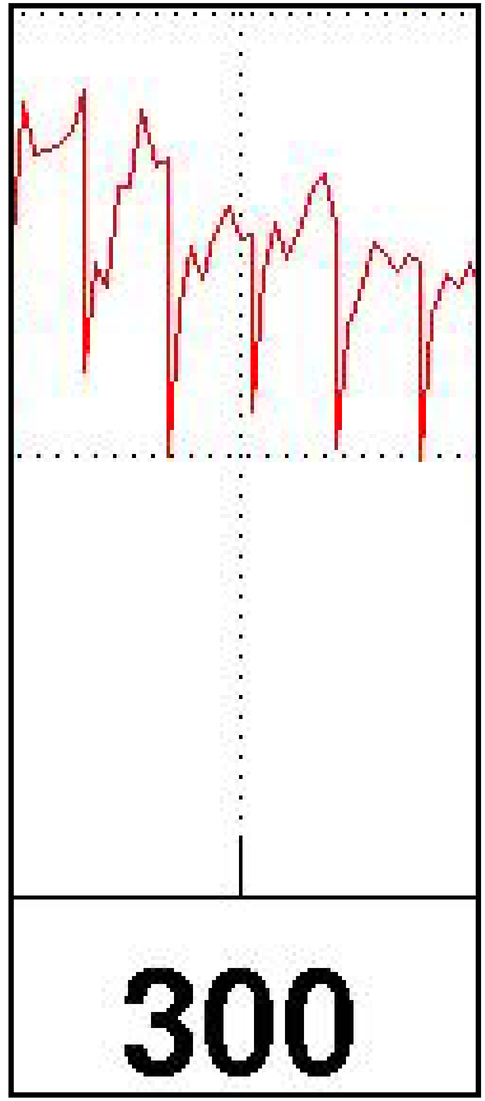




Assimilation of isolated T/S profiles: SSH increment after 1, 2, 3 days of model forecast

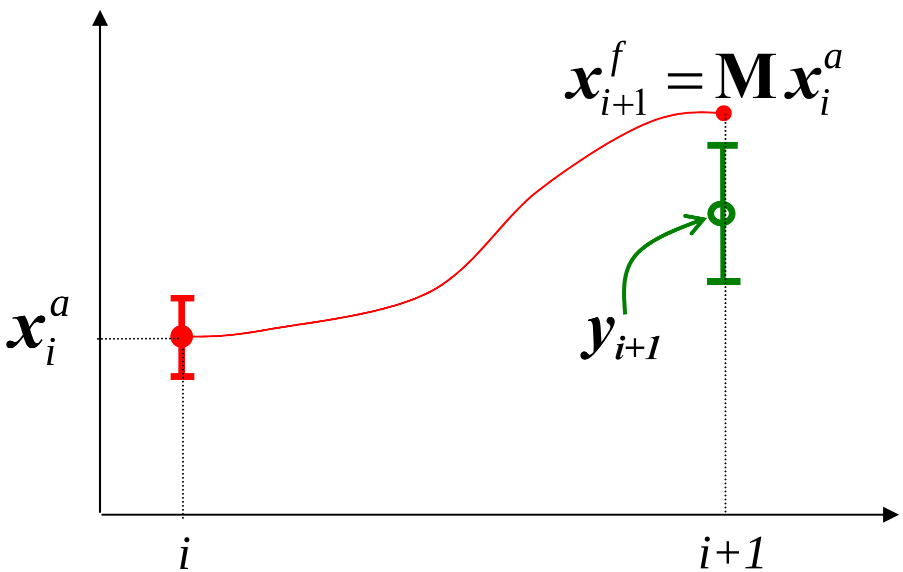
8. Improved temporal strategies
« Rejection » of SST data assimilation



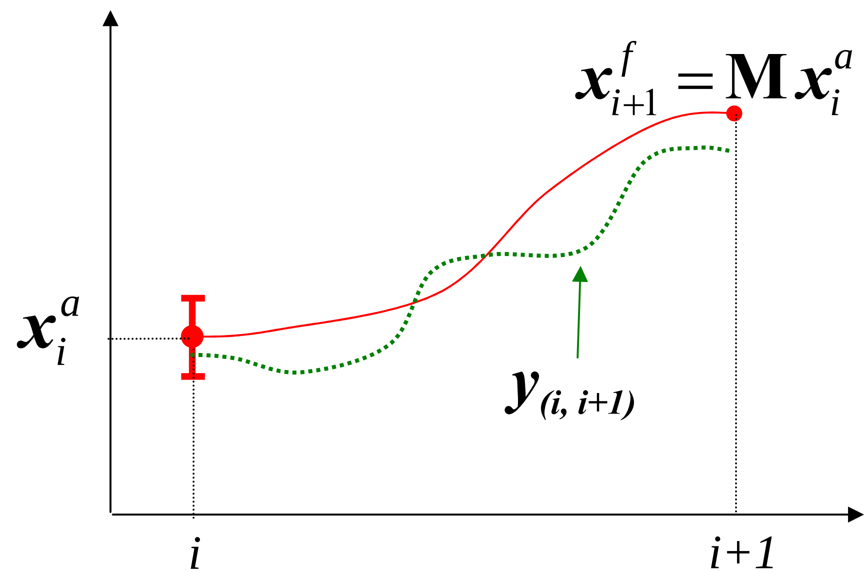


8. Improved temporal strategies
Distributed observations

- **Discrete DA problem**

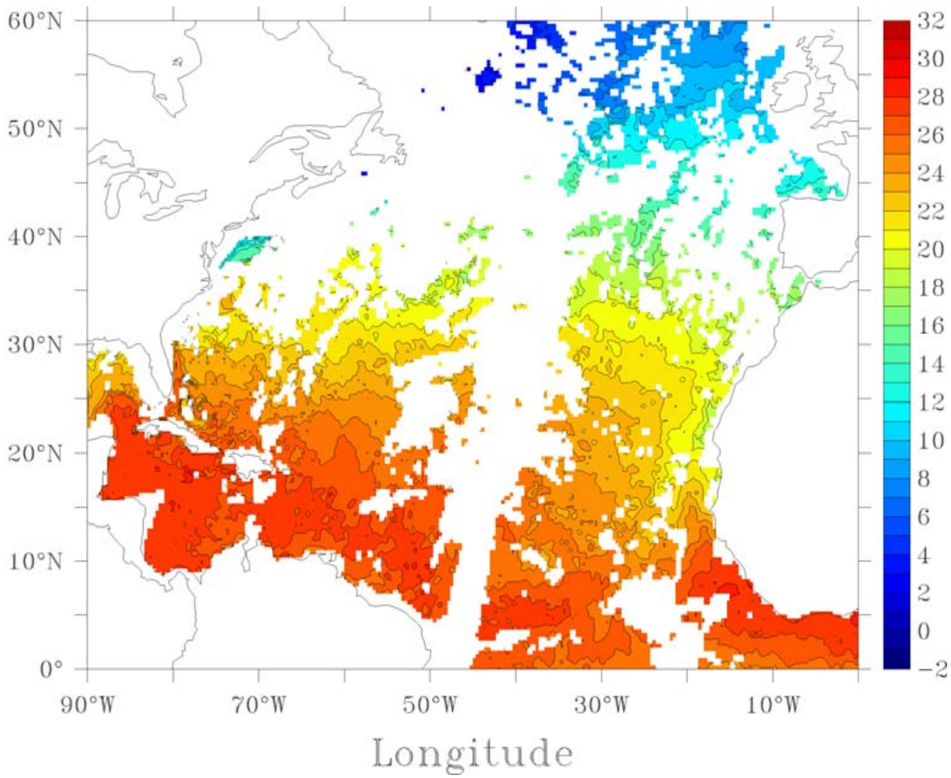


- **Continuous DA problem**

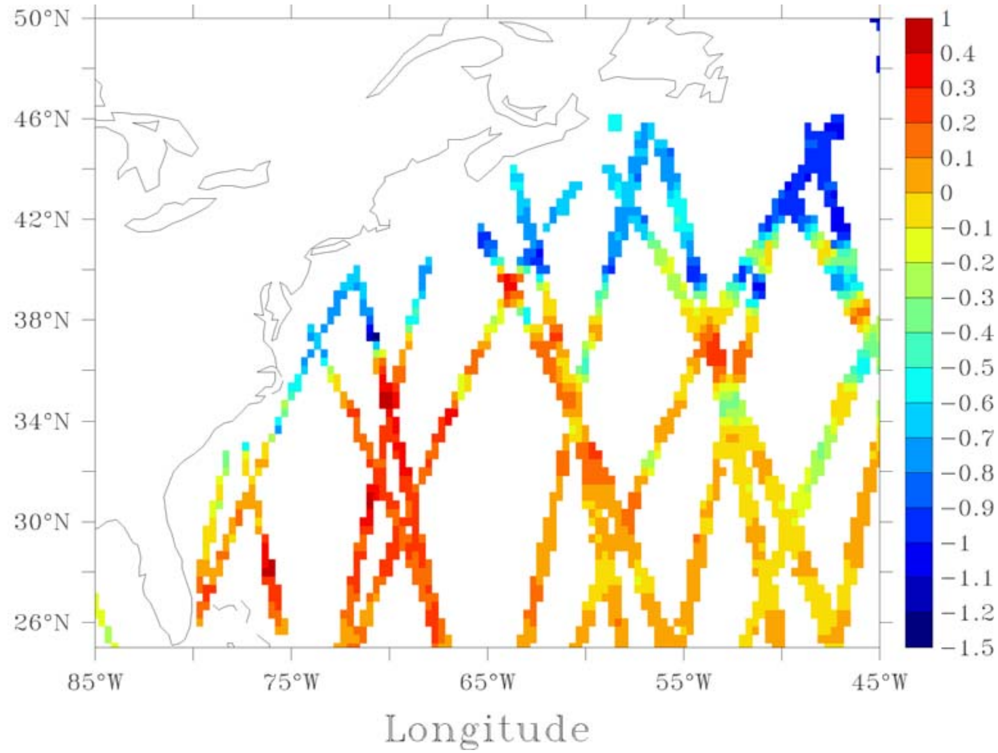


8. Improved temporal strategies
Example: composite data sets

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



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



- The observation vector y_{i+1} contains informations related to different instants.

8. 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**)**

$$\left\{\begin{array}{l} x_i^a \\ P_i^a \end{array}\right. \xrightarrow{\text{Forecast 1}} \left\{\begin{array}{l} x_{i+1}^f = M\left(x_i^a\right) \\ P_{i+1}^f = \mathbf{M}P_i^a\mathbf{M}^T + \mathbf{Q} \end{array}\right.$$

Analysis

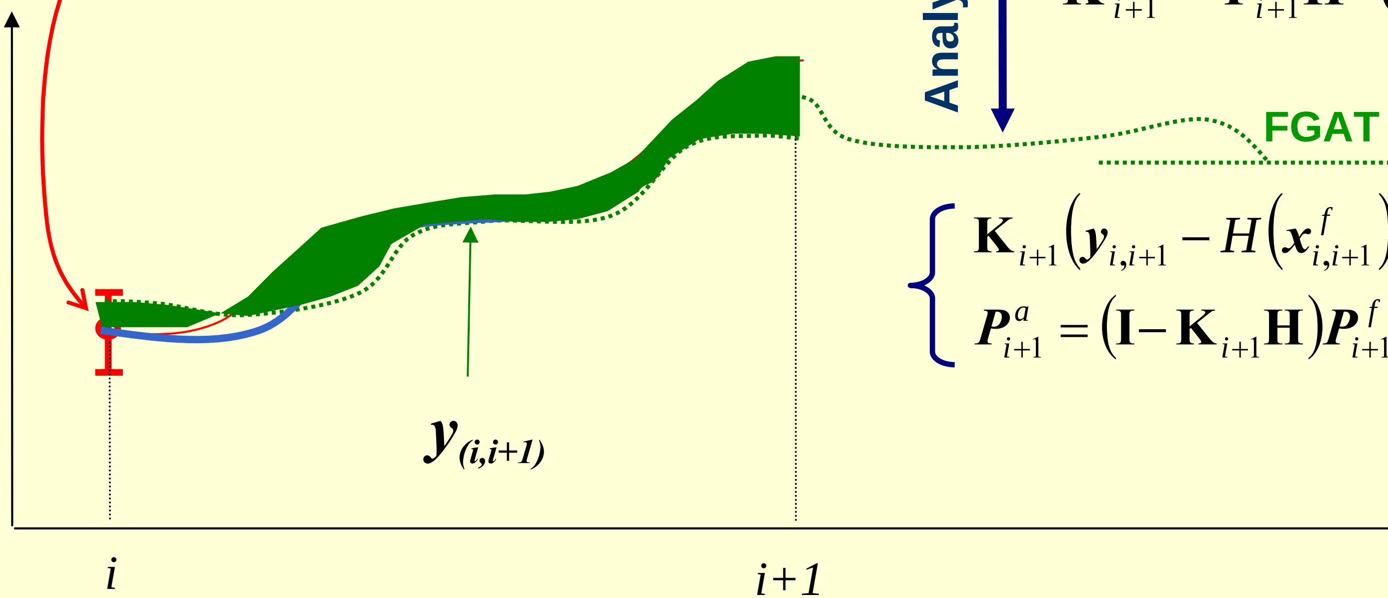
$$\mathbf{K}_{i+1} = \mathbf{P}_{i+1}^f\mathbf{H}^T(\mathbf{H}\mathbf{P}_{i+1}^f\mathbf{H}^T + \mathbf{R})^{-1}$$

FGAT

$$\left\{\begin{array}{l} \mathbf{K}_{i+1}\left(y_{i,i+1} - H\left(x_{i,i+1}^f\right)\right) = c_{i,i+1} \\ P_{i+1}^a = \left(\mathbf{I} - \mathbf{K}_{i+1}\mathbf{H}\right)P_{i+1}^f \end{array}\right.$$

Forecast 2
IAU

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



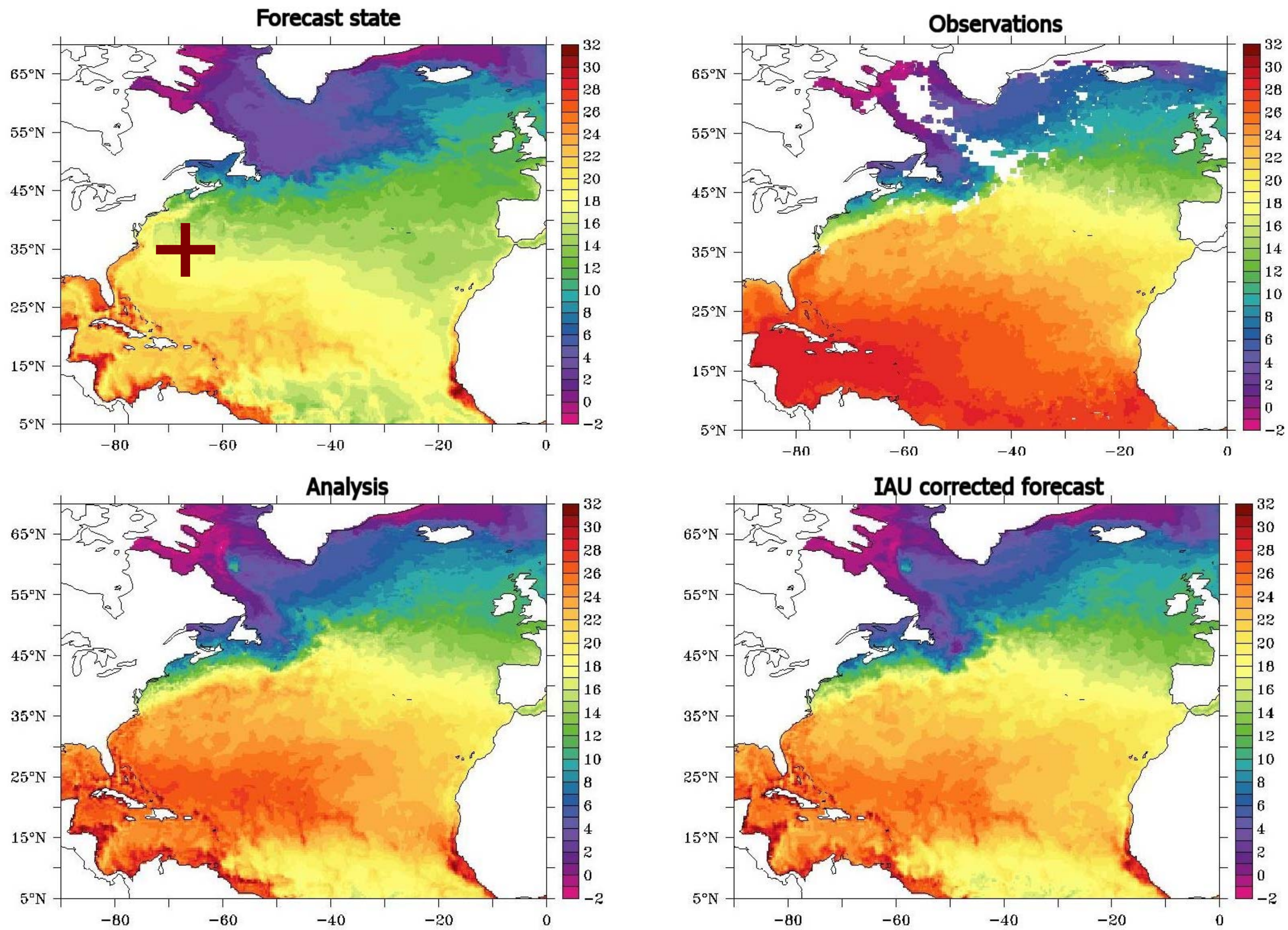
8. Improved temporal strategies
IAU implementation

- **Implementation of Incremental Analysis Update in OPA primitive equation model** :
  - Compute innovation using SST/SLA data and FGAT scheme ;
  - Compute Kalman gain and analysis increment at the end of assimilation window using SEEK 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 OPA model on $(t_i\ ,\ t_{i+1})$ once again, with modified equations for temperature and salinity, i.e :

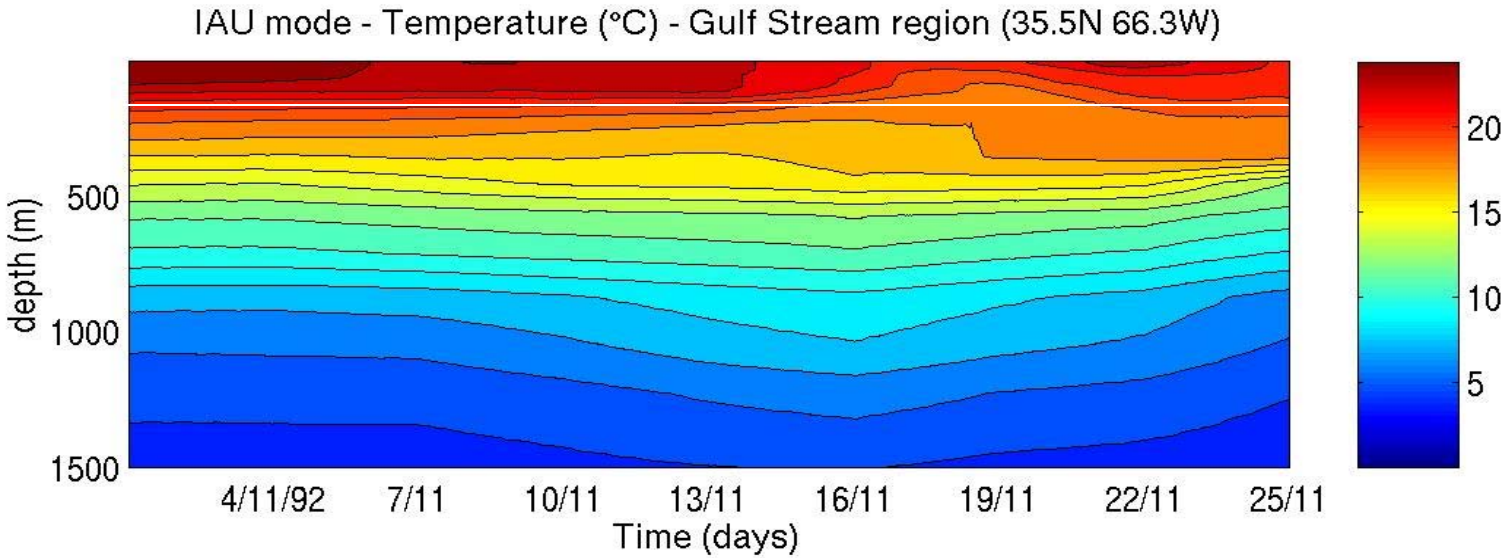
$$\frac{\partial T}{\partial t} + \boldsymbol{u}.\nabla^h T + w\frac{\partial T}{\partial z} = D^h(T) + \frac{\partial}{\partial z}\left(\tilde{\lambda}\frac{\partial T}{\partial z} \right) + \frac{\delta T}{l}$$

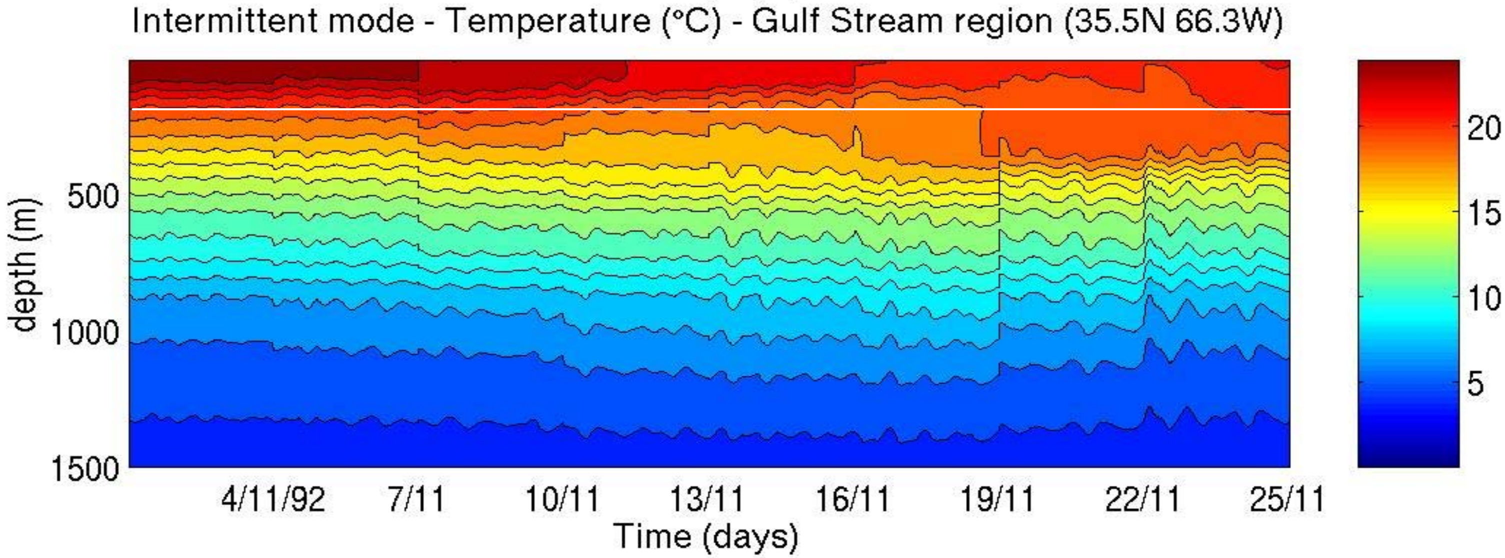
8. Improved temporal strategies
IAU – example (i)

- **SST estimates – 05/11/92**



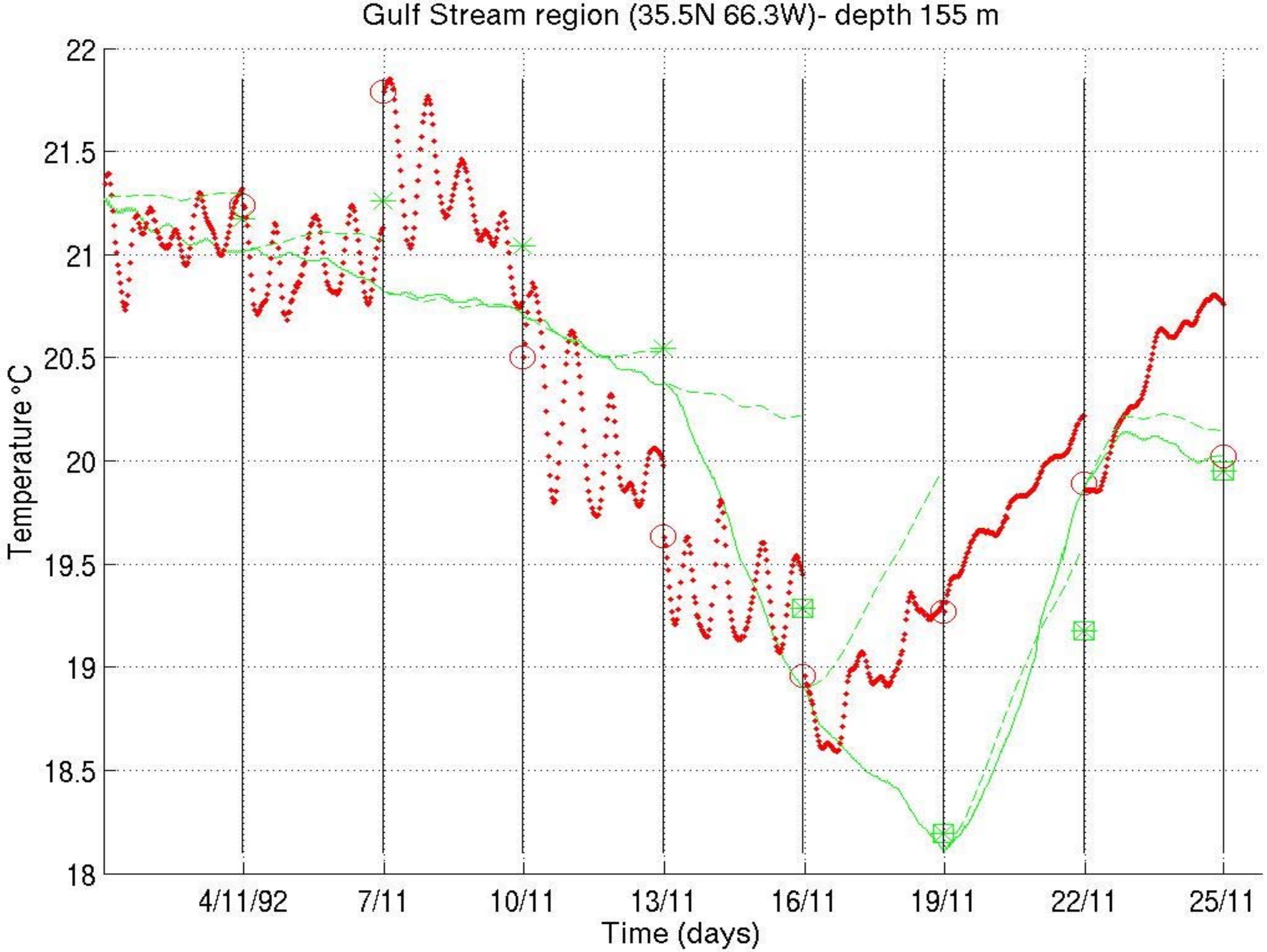
8. Improved temporal strategies
IAU – example (ii)





8. Improved temporal strategies
IAU – example (ii)

- **Temperature “mooring” – 11/92**



9. Statistical filter with inequality constraints

Motivations

- Inequality constraints are inherent to ocean models

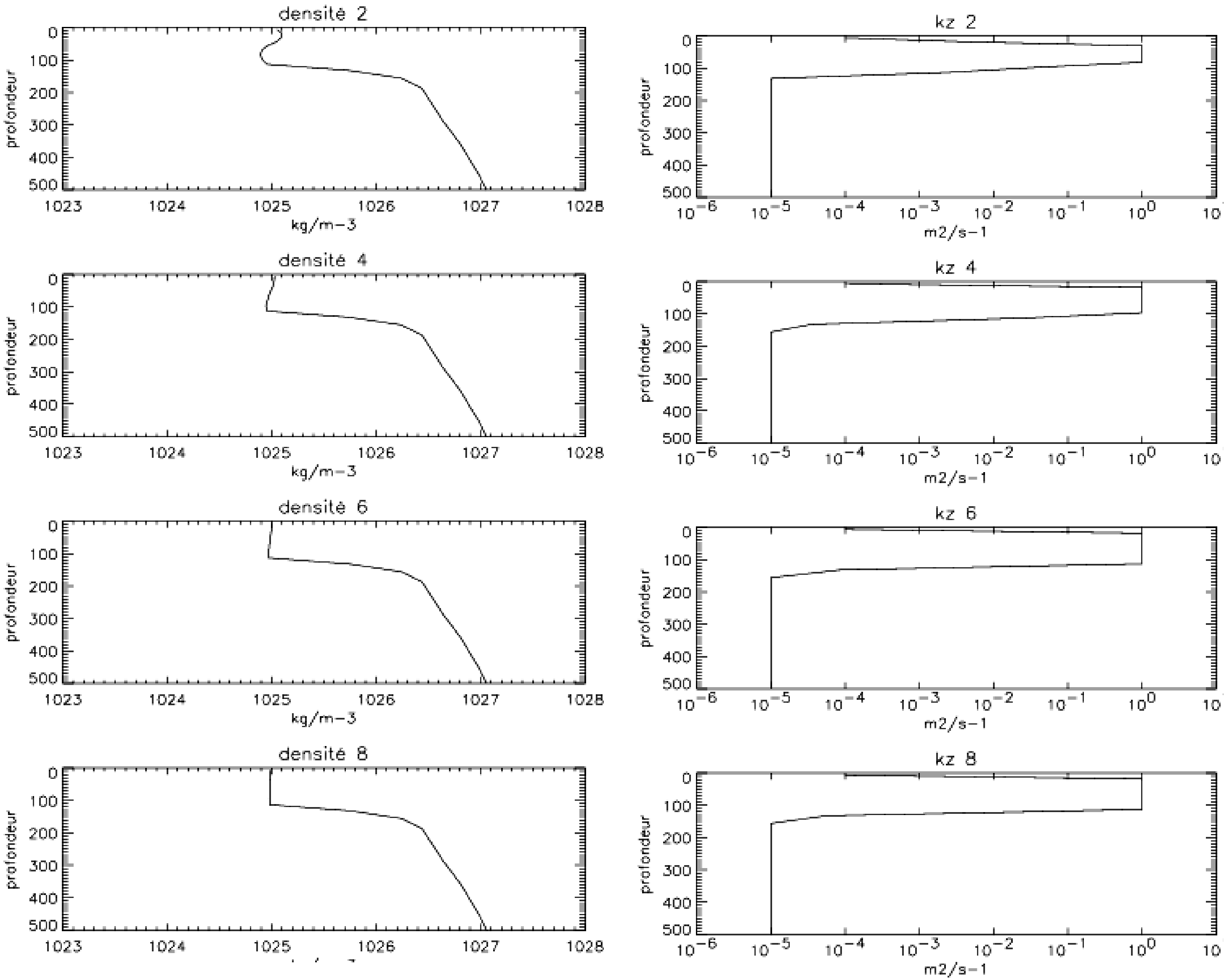
- Examples
  - Concentrations in biogeochemical models must be positive
  - T must be larger than freezing temperature
  - Static stability (a non-linear combination of T/S vertical gradients) must be verified at every assimilation step
  - …

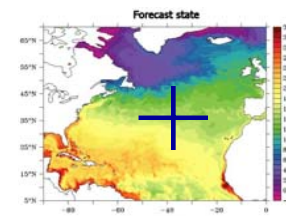
- The traditional Kalman filter framework with gaussian statistics doesn’t guarantee equality/inequality constraints

- Empirical correction schemes can be implemented after the statistical analysis step to restore the constraints

9. Kalman filter with inequality constraints

DA-induced static instability





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Conclusions

- **A fact** : A limited number of schemes have been successfully developed from theoretical basis to operational implementations (Mercator, HYCOM)

- **Learnings** : 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.

- **A word of caution** : 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* customization.

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

5. Global prototype
SAM-1, univariate

Schematically: