Reduced order approaches for variational data assimilation
Applications to ocean models

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Outline

- 4D-Var and reduced order 4D-Var
- Which subspace ?
- Numerical experiments
- Control of the model error
- Towards a hybrid sequential-variational approach ?
- Conclusion

Motivations

- Can we (significantly) reduce the cost of data assimilation in the context of ocean/atmosphere simulation without (significantly) degrading the results ? *(cf K. Kunisch, M. Navon)*
- More generally, can the concept of "order reduction" lead to improvements in data assimilation methods ?

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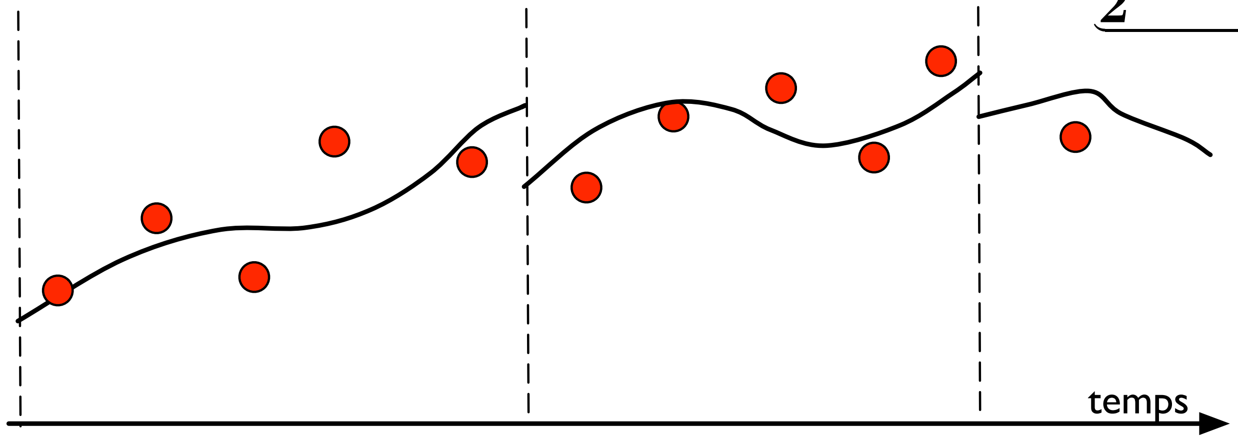
4D-Var data assimilation

Model $\begin{cases} \dfrac{d\mathbf{x}}{dt} = F(\mathbf{x}) & t \in [t_0, t_f] \\ \mathbf{x}(t_0) & \end{cases}$

Observations in time and space : y1 ,..., yN

Find x_0 that minimizes

$$J(\mathbf{x}_0) = \underbrace{\frac{1}{2} \sum_{i=0}^{N} (H(\mathbf{x}_i) - \mathbf{y}_i)^T \mathrm{R}_i^{-1} (H(\mathbf{x}_i) - \mathbf{y}_i)}_{J_o(\mathbf{x}_0)} + \underbrace{\frac{1}{2} (\mathbf{x}_0 - \mathbf{x}^b)^T \mathrm{B}^{-1} (\mathbf{x}_0 - \mathbf{x}^b)}_{J_b(\mathbf{x}_0)}$$



Incremental 4D-Var : find dx that minimizes

$$J(\delta x) = \frac{1}{2}\sum_{i=1}^{N}(H_i M_{t_i,t_0}\delta x - d_i)^T R_i^{-1}(H_i M_{t_i,t_0}\delta x - d_i) + \frac{1}{2}(\delta x)^T B^{-1}\delta x$$

where $\delta x = x_0 - x^b$ and $d_i = y_i - H(x^b(t_i))$

→ Adjoint method : $\nabla J = -p(t_0) + B^{-1}\delta x$

Optimality System :

$$\begin{cases} \dfrac{dx}{dt} = F(x) \\ x(t_0) = x^b + \delta x \\ \dfrac{dp}{dt} + \left[\dfrac{dF}{dx}\right]^T . p = H^T(Hx - y) \\ p(t_f) = 0 \\ \nabla J(\delta x) = 0 \end{cases}$$

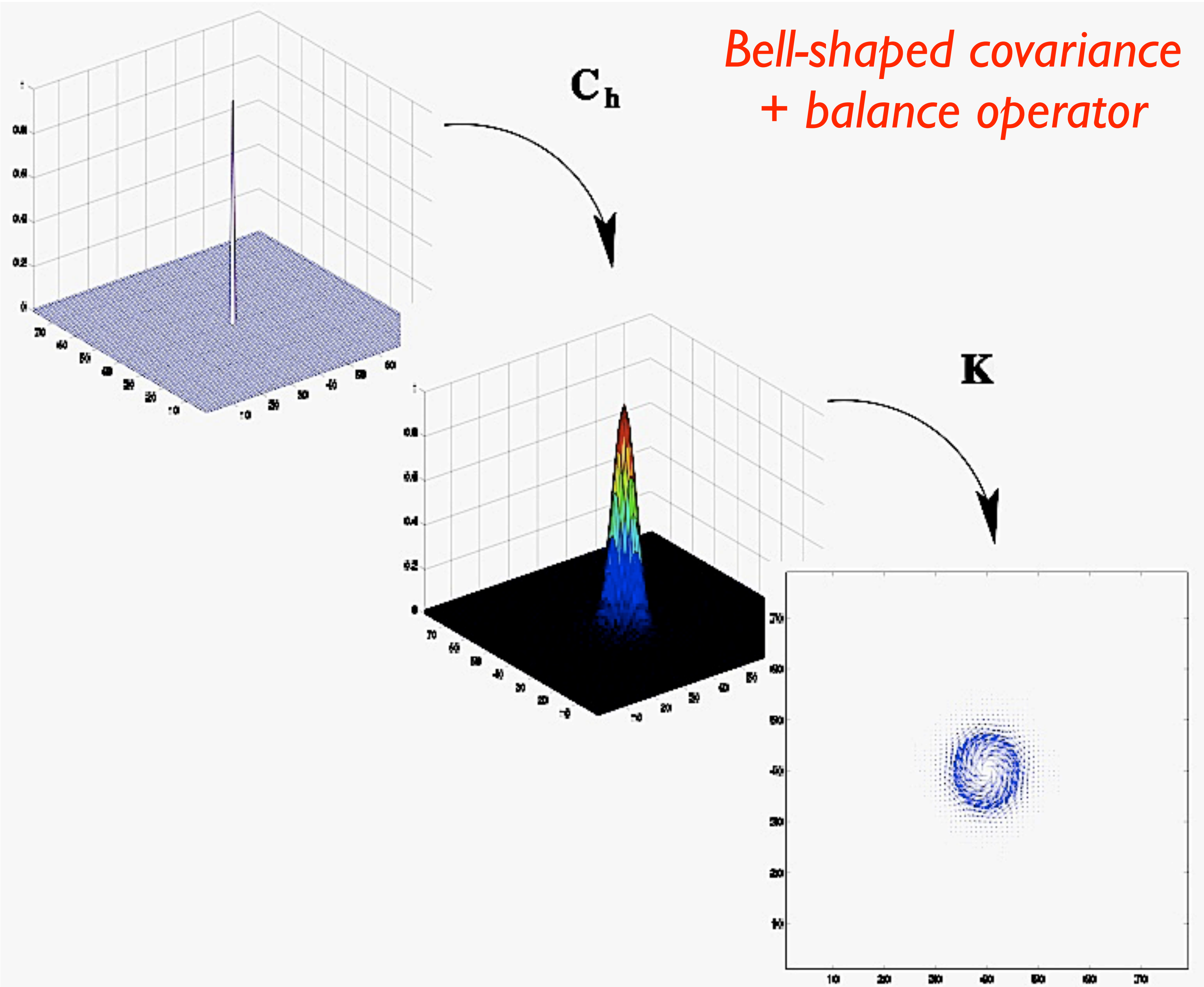
Main difficulties in the context of ocean/atmosphere modelling

- Non-linearities : non convexity, local minima, tangent linear hypothesis
- Huge dimension [x] = 10^6 - 10^7
- Error statistics (R and B) are badly known. However B is fundamental in the process.

Approximation of B

B is represented in most cases somewhat empirically, using +/- analytical models.

- Monovariate covariances : analytical functions for spatial covariances (gaussian, or generalized gaussian), with a particular role of the vertical dimension *(e.g. Weaver et al., 2001)*
- Multivariate covariances : balance relationships, either analytical and/or observed *(e.g. Ricci et al., 2005)*


Bell-shaped covariance
+ balance operator
C_h
K

Reduced order 4D-Var

Data assimilation methods are looking for an optimal correction in a space of huge dimension ⟶ try to describe (most of) this correction in a subspace of low dimension.

Control space Span (L_1, ..., L_r)

$$\delta \mathbf{x} = \mathbf{x}_0 - \mathbf{x}^b = \sum_{i=1}^{r} w_i \mathbf{L}_i = \mathbf{L}\mathbf{w}$$

Cost Function $J_b(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T \mathbf{B}_w^{-1} \mathbf{w}$

with $\mathbf{B}_w = \mathbf{E}\left[(\mathbf{w} - \bar{\mathbf{w}})(\mathbf{w} - \bar{\mathbf{w}})^T\right]$

Covariance matrix in the full space

$$\begin{aligned} \mathbf{B}_r &= \mathbf{E}\left[(\delta\mathbf{x} - \delta\bar{\mathbf{x}})(\delta\mathbf{x} - \delta\bar{\mathbf{x}})^T\right] \\ &= \mathbf{L}\,\mathbf{E}\left[(\mathbf{w} - \bar{\mathbf{w}})(\mathbf{w} - \bar{\mathbf{w}})^T\right]\mathbf{L}^T \\ &= \mathbf{L}\mathbf{B}_w\mathbf{L}^T \end{aligned}$$

(singular low-rank matrix)

+ Minimization in a space of dimension *r* << [x]
+ Almost no modification of the algorithm
- Choice of (L_1, ..., L_r) and estimation of B_w

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In this context, the subspace must represent most of the natural variability of the system. But which definition for the variability ?

- Statistical approach : PODs (EOFs, Principal Components...)

- Dynamical systems: vectors of maximum growth

- ...

EOFs : Empirical Orthogonal Functions
(principal components, Proper Orthogonal Decomposition)

Sample of a model trajectory : $(\mathrm{x}(t_1), \ldots, \mathrm{x}(t_p))$

$L_1, ..., L_r$: directions in which the variance is maximum

They are the first eigenvectors of the empirical correlation matrix $\mathrm{X}\mathrm{X}^T$ with $\mathrm{X} = (\mathrm{X}_1, \ldots, \mathrm{X}_p)$

$$\mathrm{X}_j(i) = \frac{1}{\sigma_i}[\mathrm{x}(t_j) - \bar{\mathrm{x}}]$$

$$\bar{\mathrm{x}} = \frac{1}{p}\sum_{j=1}^{p} \mathrm{x}(t_j) \qquad \sigma_i^2 = \frac{1}{p}\sum_{j=1}^{p} (\mathrm{X}_j(i))^2$$

Vectors of maximal growth

Amplification rate of some perturbation $Z(t_1)$:

$$\rho\left(\boldsymbol{Z}(t_1)\right) = \frac{\|\boldsymbol{M}_{t_1 \to t_2}\left(\boldsymbol{X}(t_1) + \boldsymbol{Z}(t_1)\right) - \boldsymbol{M}_{t_1 \to t_2}\left(\boldsymbol{X}(t_1)\right)\|}{\|\boldsymbol{Z}(t_1)\|}$$

Find $\boldsymbol{Z}_1^*(t_1)$ such that $\rho\left(\boldsymbol{Z}_1^*(t_1)\right) = \max_{\boldsymbol{Z}(t_1)} \rho\left(\boldsymbol{Z}(t_1)\right)$

Degrees of freedom : $[t_1, t_2]$, M , $\|\,.\,\|$, forward / backward

Vectors of maximal growth (2)

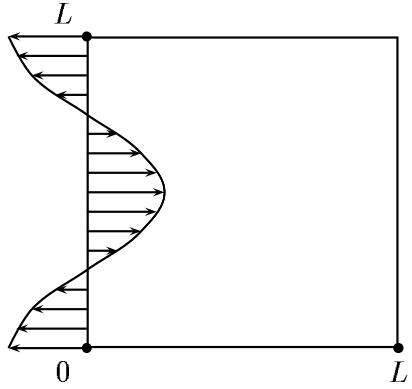
	Tangent linear approximation	Full (nonlinear) model
$[t_1,t_2]$ finite	*singular vectors*	*non-linear singular vectors*
$[t_1,t_2]$ infinite	*Lyapunov vectors*	*breeding vectors*

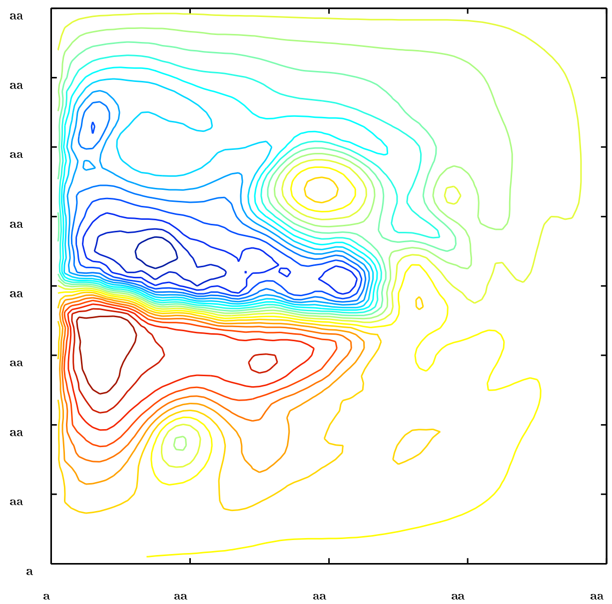
Such vectors are used in particular for stability analysis and for ensemble simulations.

Illustration in the context of an idealized shallow water model

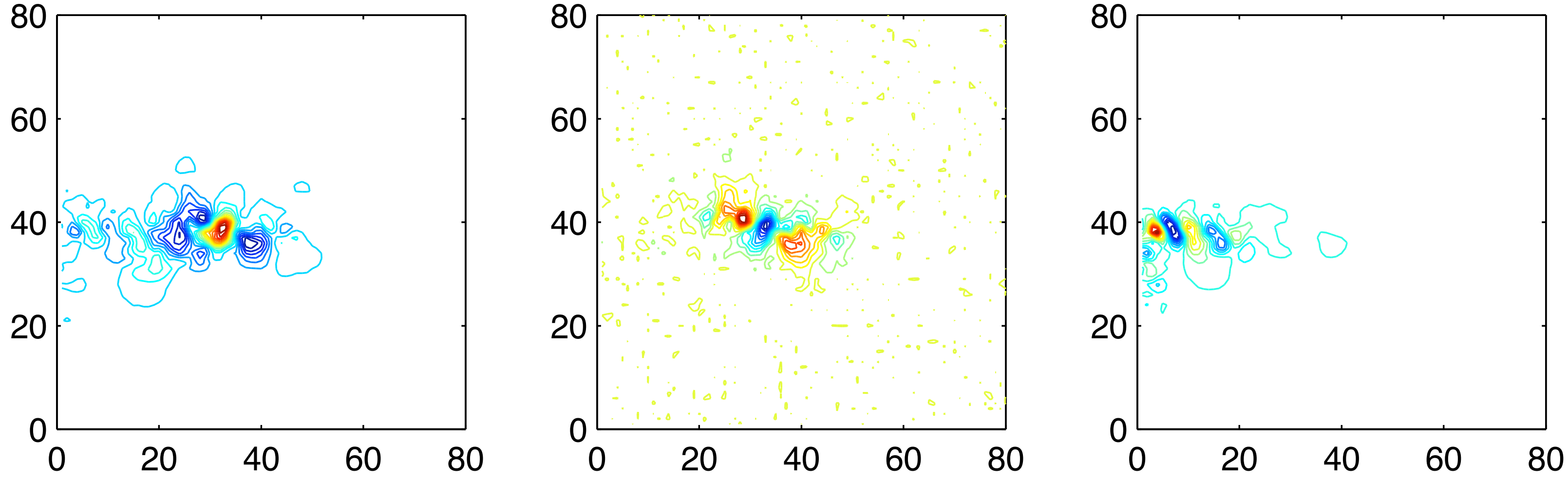
$$\left\{\begin{aligned} \frac{\partial u}{\partial t} + u\,\frac{\partial u}{\partial x} + v\,\frac{\partial u}{\partial y} - fv + g\,\frac{\partial h}{\partial x} + D_x &= F_x \\ \frac{\partial v}{\partial t} + u\,\frac{\partial v}{\partial x} + v\,\frac{\partial v}{\partial y} + fu + g\,\frac{\partial h}{\partial y} + D_y &= F_y \\ \frac{\partial h}{\partial t} + u\,\frac{\partial h}{\partial x} + v\,\frac{\partial h}{\partial y} + h\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) &= 0 \end{aligned}\right.$$

Wind





Snapshot : h



euclidian norm

$$u^2 + v^2 + h^2$$

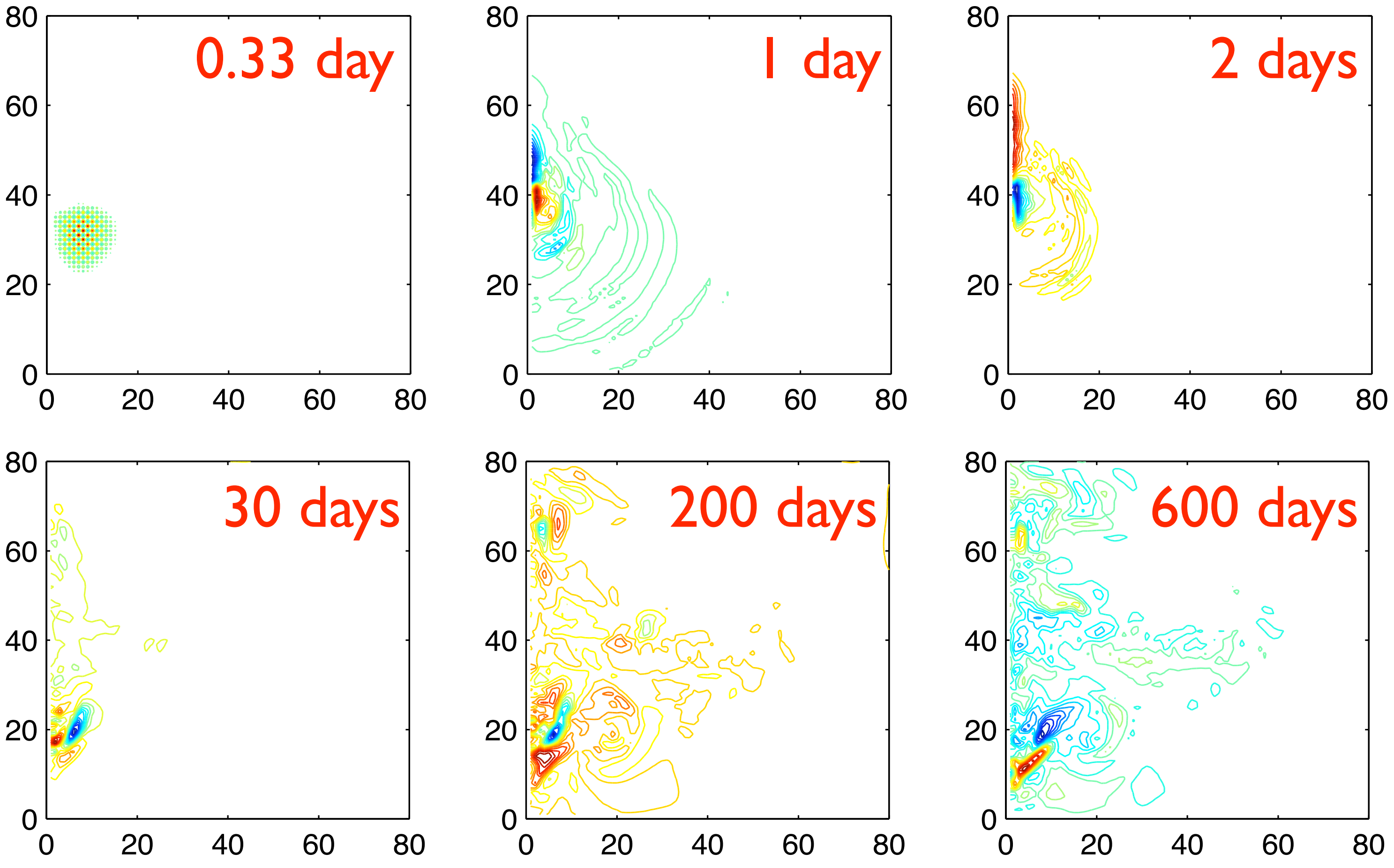
velocity norm

$$\frac{1}{2}(u^2 + v^2)$$

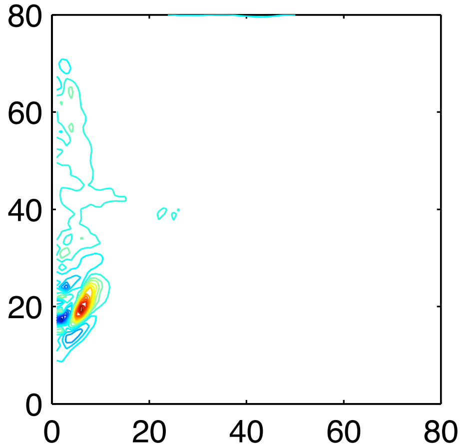
energy norm

$$\frac{1}{2}(u^2 + v^2) + gh$$

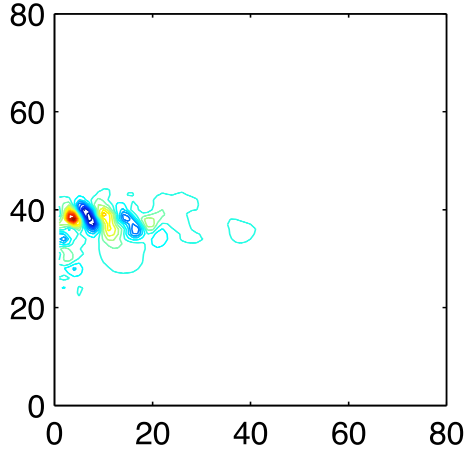
Backward singular vector #1 for different norms



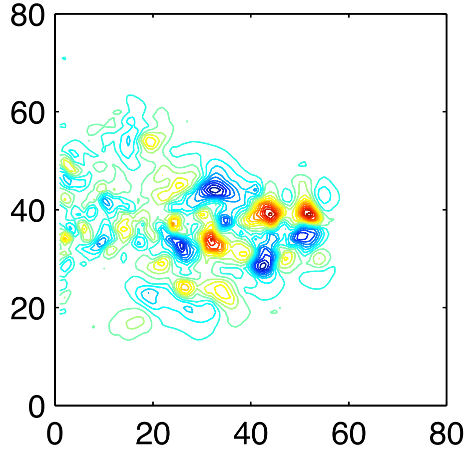
Forward singular vector #1 for different lengths of the time-window



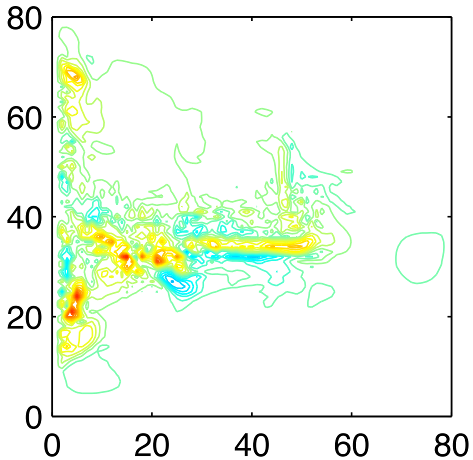
Forward Singular vector #1



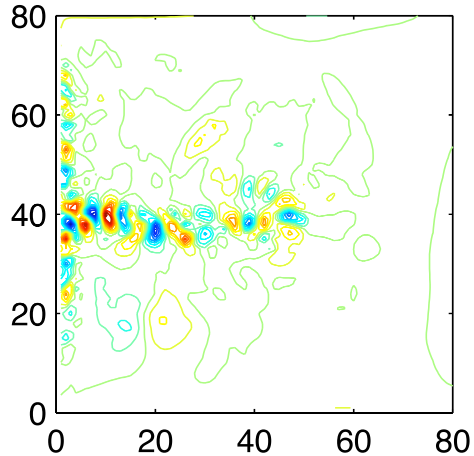
Backward Singular vector #1



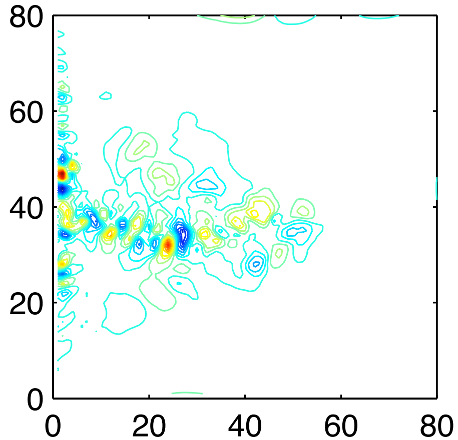
Backward Lyapunov vector #1



Forward Nonlinear Singular vector #1

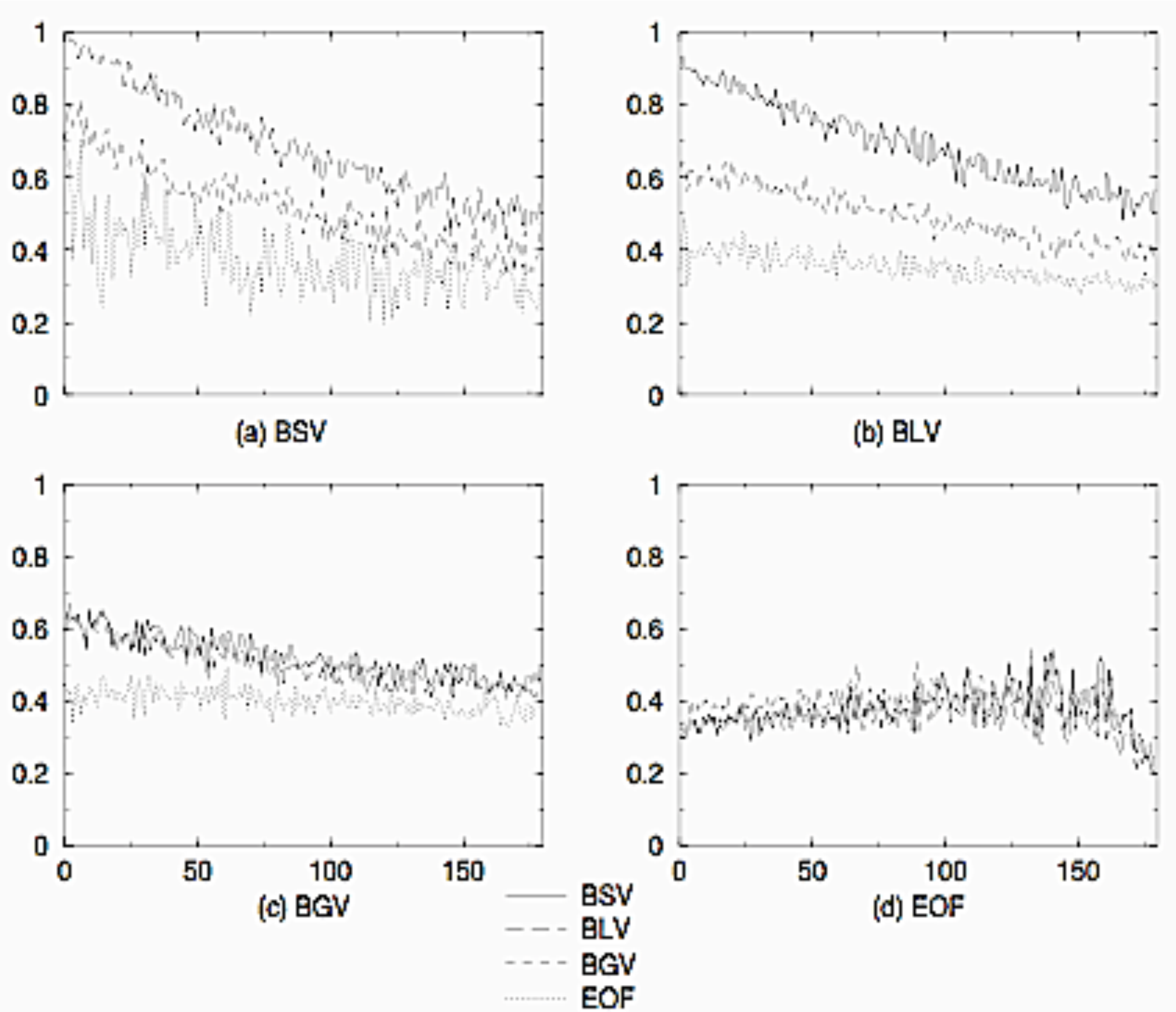


POD #1



Bred mode #1

Colinearity of the different families of vectors



x-axis : # of the vector
y-axis : projection ratio on another family (180 members)

- Impact of non linearities (bred modes vs Lyapunov vectors)
- Information contained in the PODs is quite "different"

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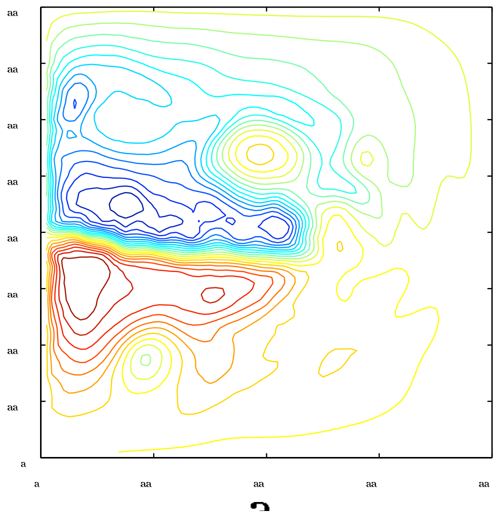
Data assimilation : control of the initial condition

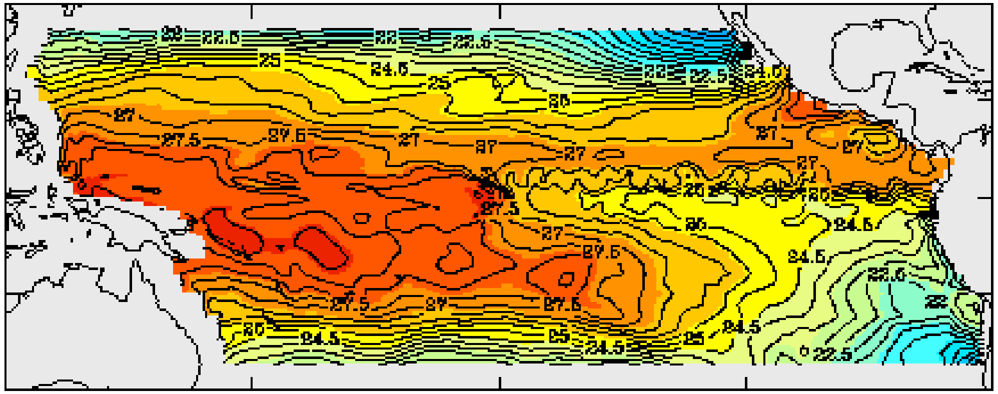
- Use of a POD basis

Preliminary experiments with the idealized shallow water model : PODs lead to good results.



Covariance   Due to the definition of PODs, the covariance matrix in this basis is diagonal : $B_w = \mathrm{diag}(\lambda_1, \ldots, \lambda_r)$

Experiments in a model of the Tropical Pacific ocean



OPA - TDH model

(Weaver et al.)

Primitive Equations

Momentum

$$\frac{\partial u}{\partial t} + \mathrm{U} \cdot \nabla u - \nu \Delta u - f v + \frac{1}{\rho_0} \frac{\partial p}{\partial x} = 0$$

$$\frac{\partial v}{\partial t} + \mathrm{U} \cdot \nabla v - \nu \Delta v + f u + \frac{1}{\rho_0} \frac{\partial p}{\partial y} = 0$$

$$\frac{\partial p}{\partial z} = -\rho g$$

(hydrostatic approximation)

Conservation of mass

$$\mathrm{div}\ \mathrm{U} = 0$$

(Boussinesq approximation)

Equations for tracers

$$\frac{\partial T}{\partial t} + \mathrm{U} \cdot \nabla T = K_T\, \Delta T$$

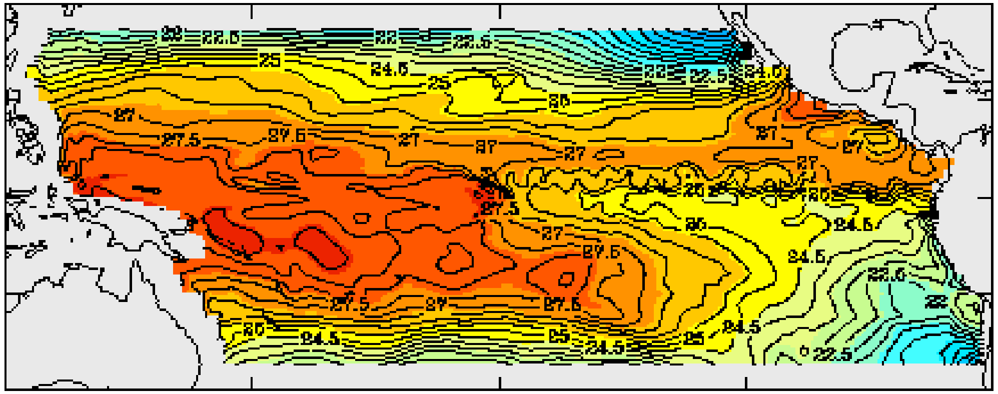
$$\frac{\partial S}{\partial t} + \mathrm{U} \cdot \nabla S = K_S\, \Delta S$$

Equation of state

$$\rho = \rho(T, S, p)$$

+ boundary conditions

Experiments in a model of the Tropical Pacific ocean



OPA - TDH model
(Weaver et al.)

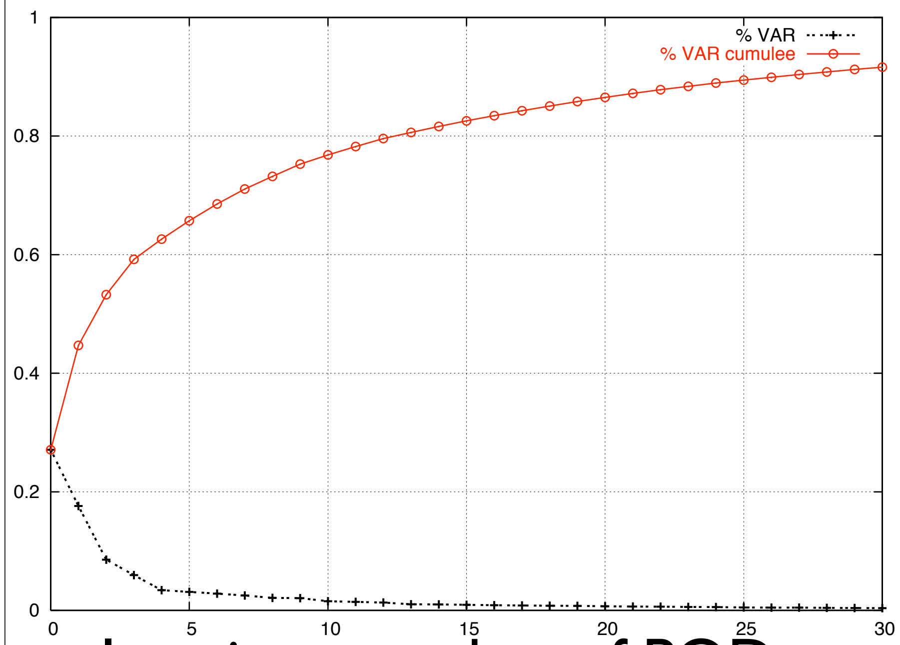
Resolution : 1° x 1/2° - 2° x 25 vertical levels

State variable : [x] ~10^6

Timestep = a few minutes

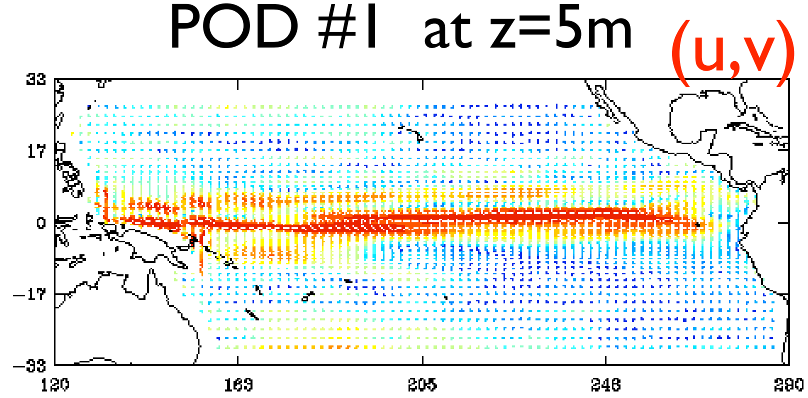
Comparison of Reduced-4D-Var with "usual" 4D-Var using a standard gaussian covariance matrix B

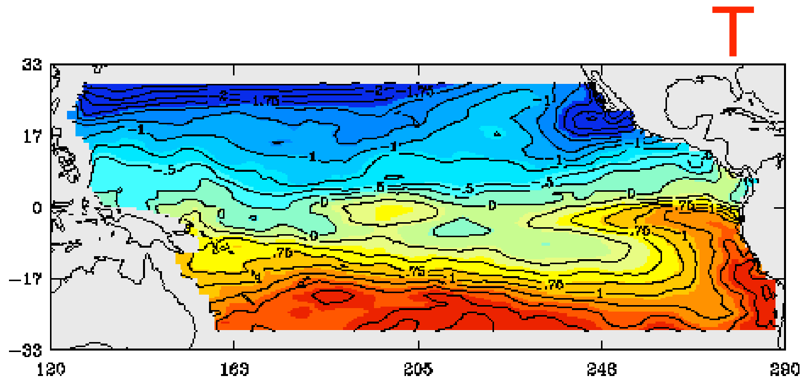
POD analysis of a one-year trajectory of the model

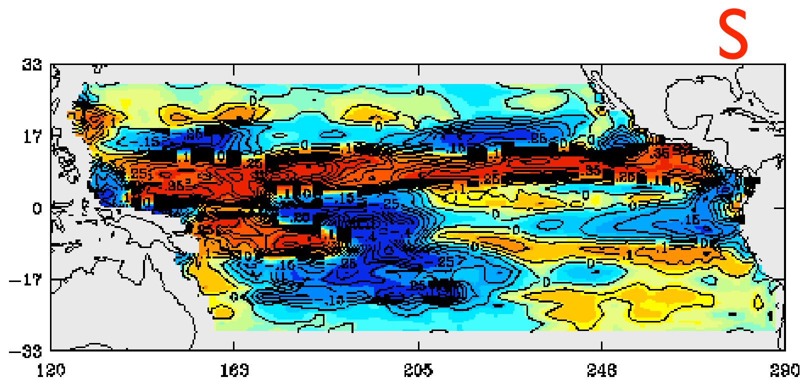


Inertia vs number of PODs

POD #1 at z=5m







Structure of B : assimilation of a single observation

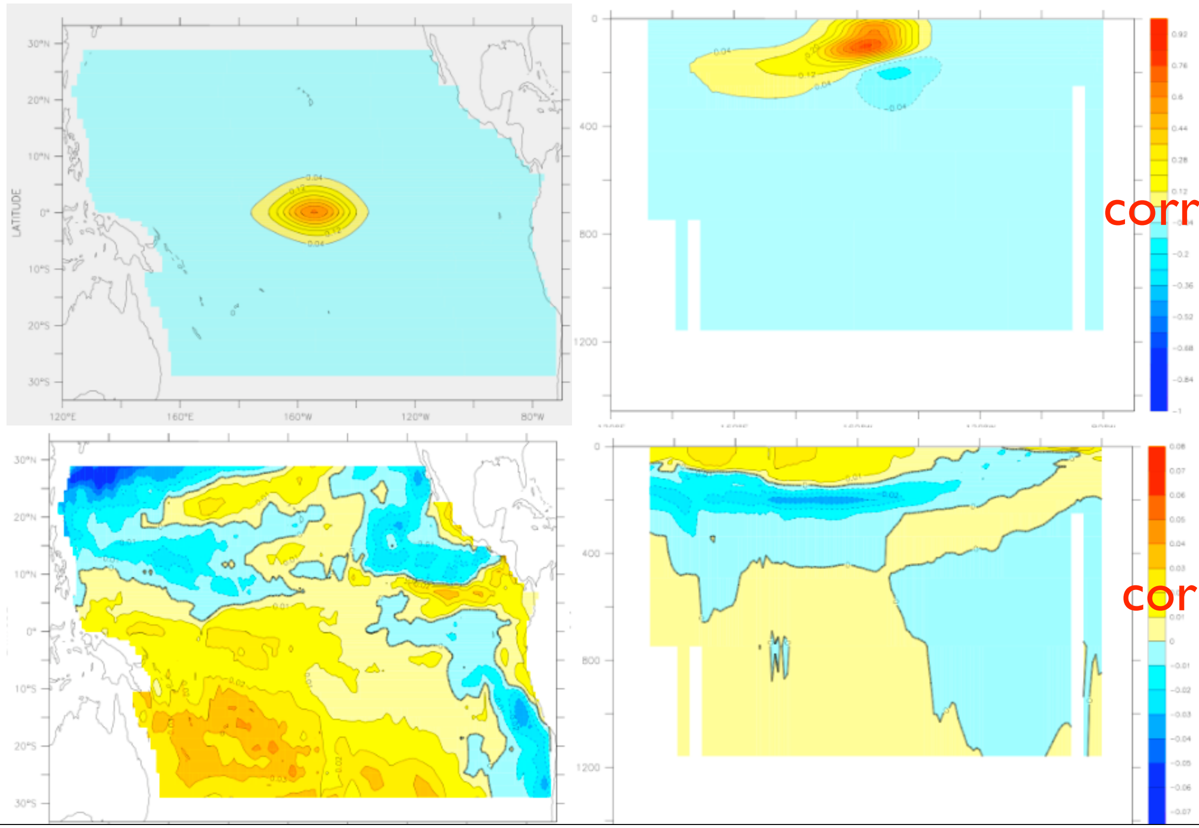
Innovation of 1°C, located on the equator at 160°W, in the thermocline, at the end of a one-month assimilation window

Temperature component of δx

z = 5m | vertical section

Full 4D-Var

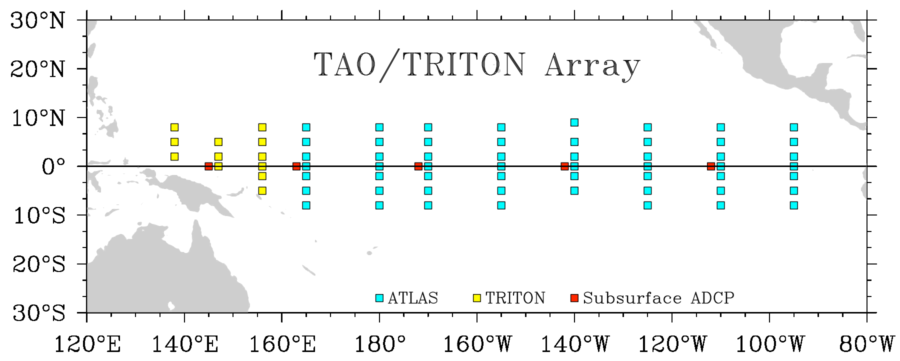
Reduced 4D-Var



maximal correction : 0,94 °C

maximal correction : 0,06 °C

Twin experiments : assimilation of simulated observations



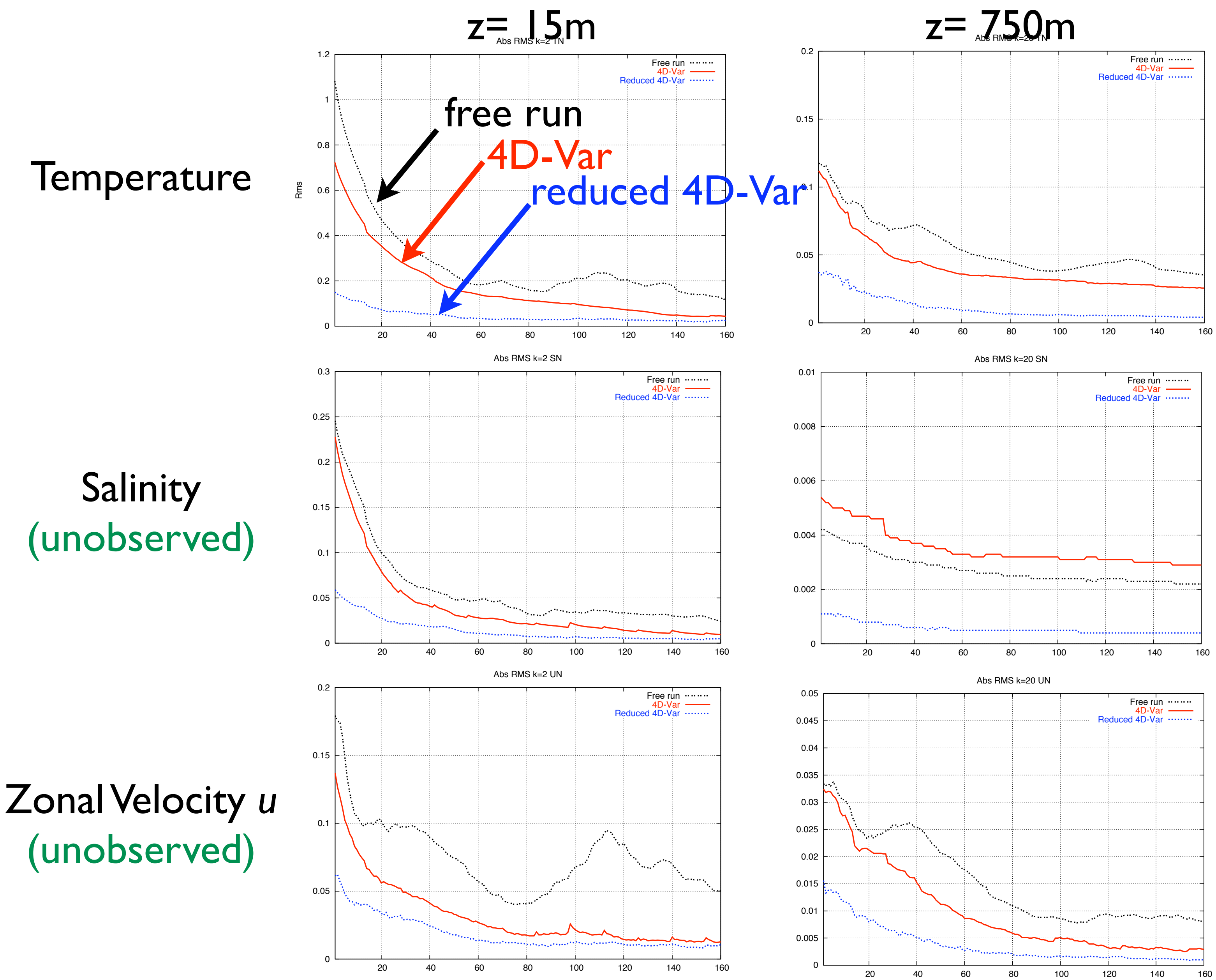
Reference simulation one-year experiment

Simulated data 70 TAO moorings : vertical sampling of T in the 500 first meters (0,17% of [x]), every 6h + gaussian noise

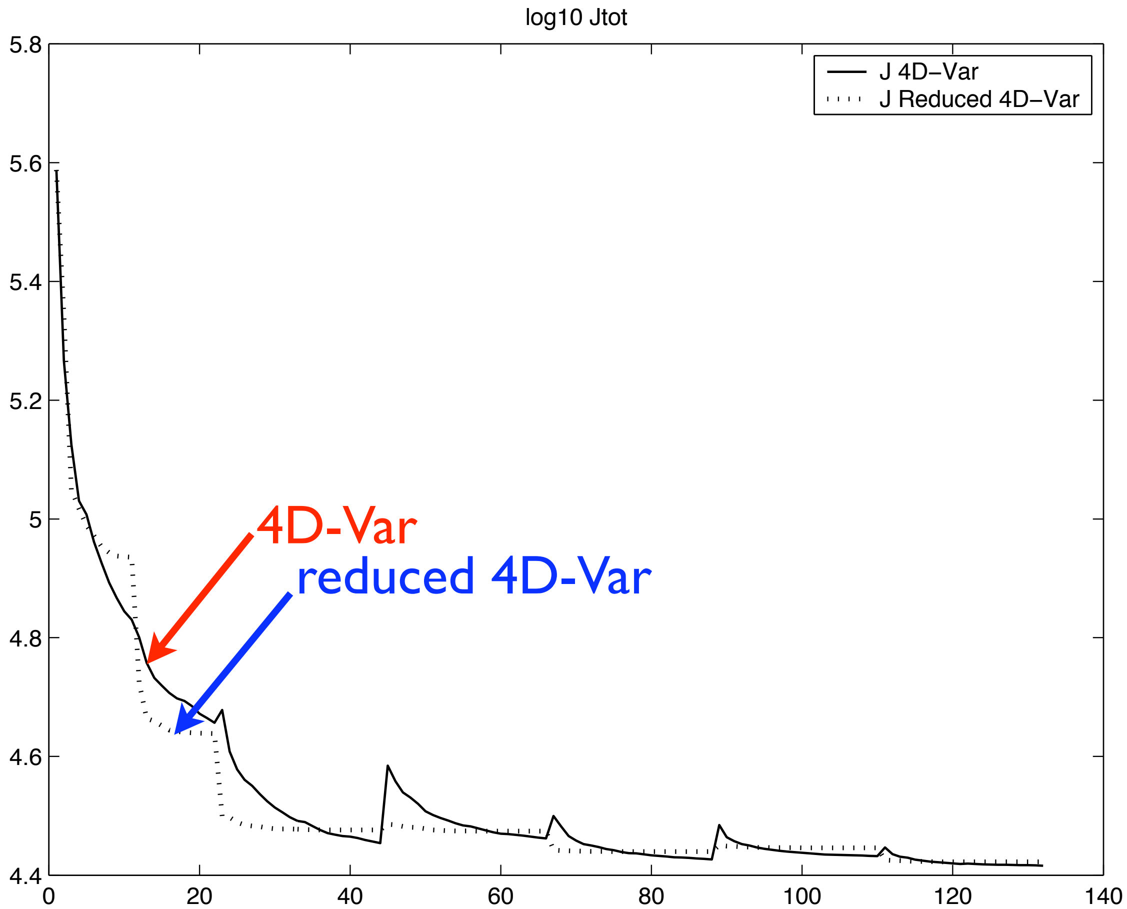
Background x^b a model state three months before

Numerical experiment 12 one-month assimilation windows

L^2 - norm of the error as a function of time



Cost function
(ln J vs iteration #)



6 one-month windows, 22 iterations each

The necessary number of iterations is divided by a factor of 4-5

Assimilation of real data : the role of model error

The model error makes unefficient the POD basis obtained by analysis of a free run.

- Compute PODs from a simulation using data assimilation

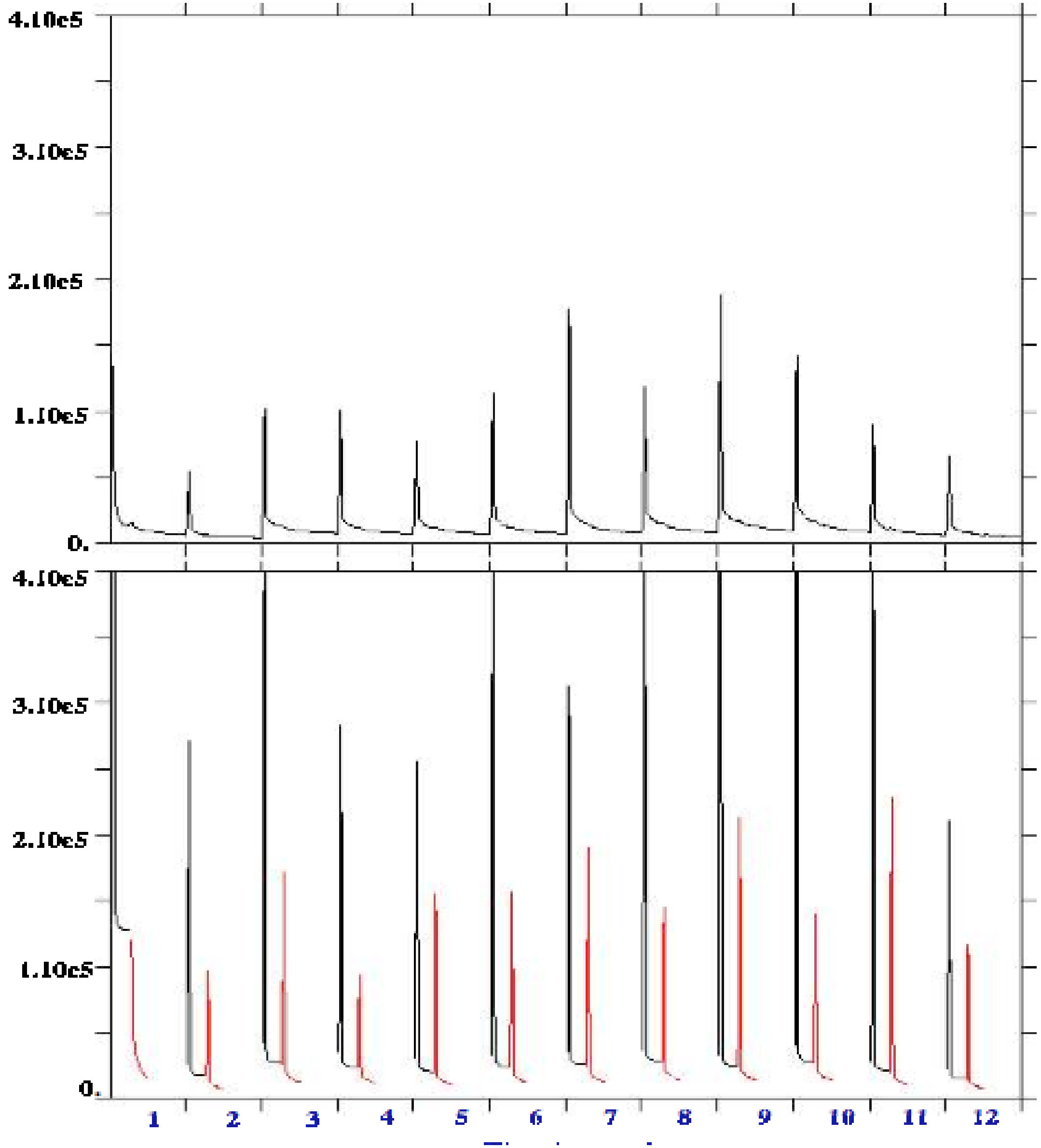
or

- Use Reduced-4D-Var as a preconditionner for full 4D-Var $\longrightarrow$ "two-step 4D-Var"

The number of iterations is divided by a factor of (at least) 2.

4D-Var

two-step 4D-Var



Misfit with observations at (110°W, 0°N)

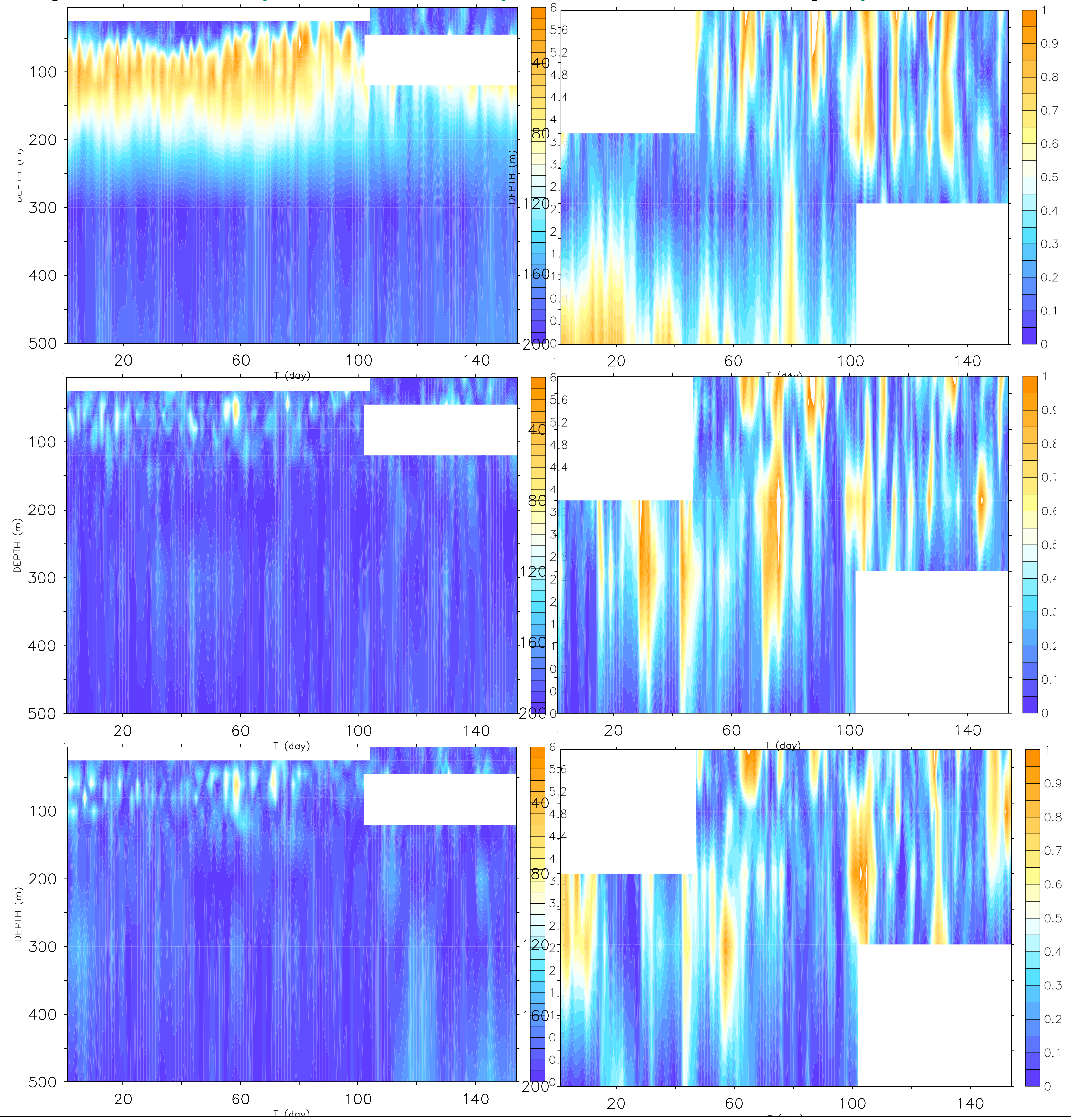
x-axis : time , y-axis : depth

temperature (assimilated) zonal velocity (non assimilated)

model without assimilation

4D-Var

two-step 4D-Var



How could we go further ?

Two aspects limit the effectiveness of reduced order variational data assimilation :

- truncation error (reduction of the dimension of the control space)
- model error (unknown physics)

Tentative approaches :

- weak constraint optimization : control of (part of) the model error
- hybrid stochastic/deterministic approach in order to improve the relevance of the reduced basis

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Explicit control of the model error

$$\begin{cases} \mathrm{x}_{i+1} = M_{i\to i+1}(\mathrm{x}_i) + \mathrm{e}_{i+1} \\ \mathrm{x}_0 = \mathrm{x}^b + \delta\mathrm{x} \end{cases}$$

$$J(\delta\mathrm{x}, \mathrm{e}_1, \ldots, \mathrm{e}_N) = \frac{1}{2}\sum_{i=1}^{N}(H(\mathrm{x}_i) - \mathrm{y}_i)^T \mathrm{R}_i^{-1}(H(\mathrm{x}_i) - \mathrm{y}_i)$$

$$+\frac{1}{2}(\delta\mathrm{x})^T \mathrm{B}^{-1}\delta\mathrm{x} + \frac{1}{2}\sum_{i=1}^{N} \mathrm{e}_i^T \mathrm{Q}_i^{-1}\mathrm{e}_i$$

$$\begin{cases} \nabla_{\delta\mathrm{x}} J = -p_0 + \mathrm{B}^{-1}\delta\mathrm{x} \\ \nabla_{\mathrm{e}_i} J = -p_i + \mathrm{Q}_i^{-1}\mathrm{e}_i \end{cases}$$

Difficulties

- Dimension of the control space : N x [x] !!
- Estimation of Q_i

- Dual approach - minimization in the observation space : *representers (Bennett 92), 4D-PSAS (Amodei 95, Courtier 97, Louvel 01, Auroux 02)*

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- Reduced order modelling of e_i :
  - systematic bias *(Vidard 01, Griffith and Nichols 01, D'Andréa and Vautard 01, Bell et al 02)* : $e_i = \bar{e}$

Control of the model bias

$$\begin{cases} \mathbf{x}_{i+1} = M_{i \to i+1}(\mathbf{x}_i) + \bar{\mathbf{e}} \\ \mathbf{x}_0 = \mathbf{x}^b + \delta \mathbf{x} \end{cases}$$

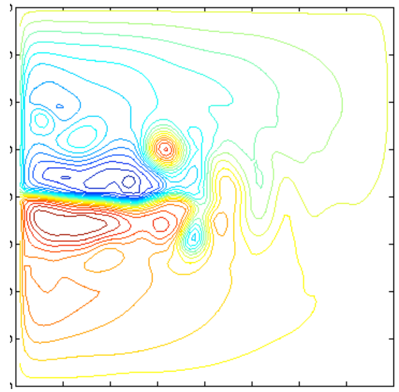
$$J(\delta \mathbf{x}, \bar{\mathbf{e}}) = \frac{1}{2} \sum_{i=1}^{N} (H(\mathbf{x}_i) - \mathbf{y}_i)^T \mathbf{R}_i^{-1} (H(\mathbf{x}_i) - \mathbf{y}_i)$$

$$+ \frac{1}{2} (\delta \mathbf{x})^T \mathbf{B}^{-1} \delta \mathbf{x} + \frac{N}{2} \bar{\mathbf{e}}^T \mathbf{S}^{-1} \bar{\mathbf{e}}$$

$$\begin{cases} \nabla_{\delta \mathbf{x}} J = -p_0 + \mathbf{B}^{-1} \delta \mathbf{x} \\ \nabla_{\bar{\mathbf{e}}} J = - \sum_{i=1}^{N} p_i + N \, \mathbf{S}^{-1} \bar{\mathbf{e}} \end{cases}$$

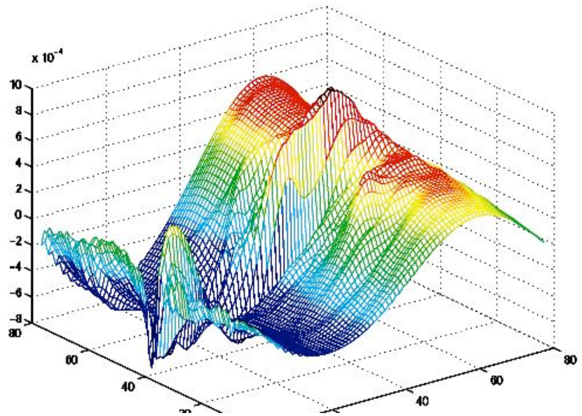
Default choice : S = B

Results with the shallow-water model

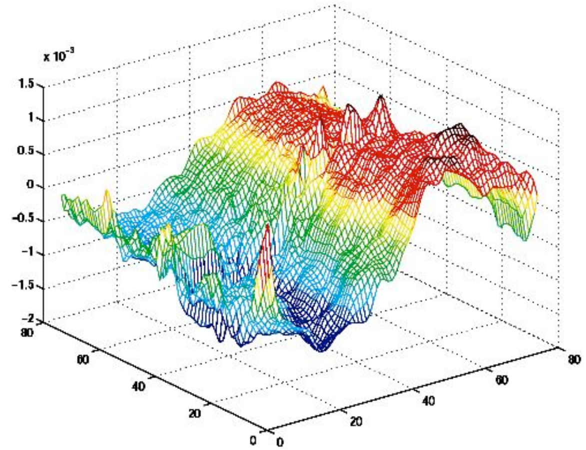


- "Cousin" experiments (a reference model and a perturbed model)
- Obs : sub-sampling of h

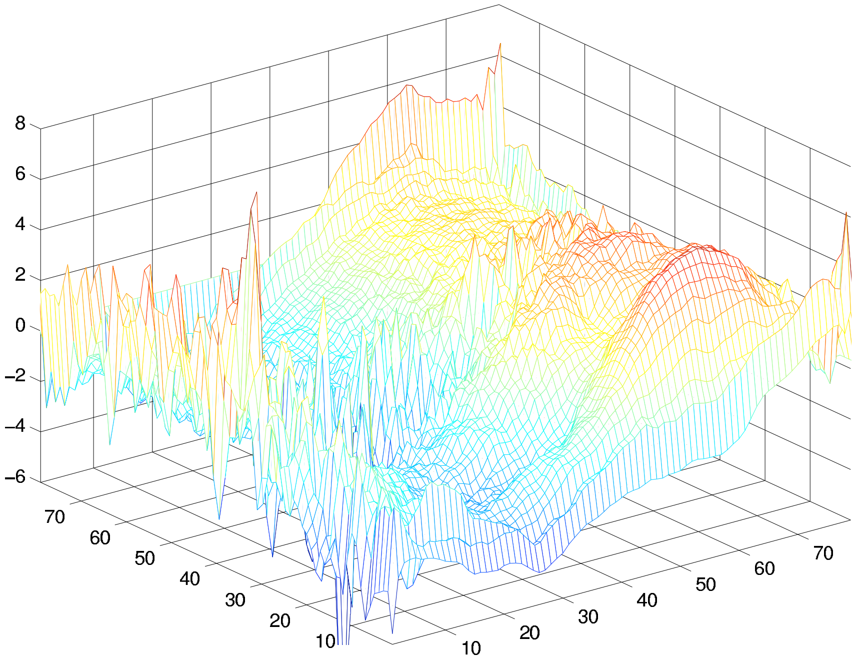
exact bias

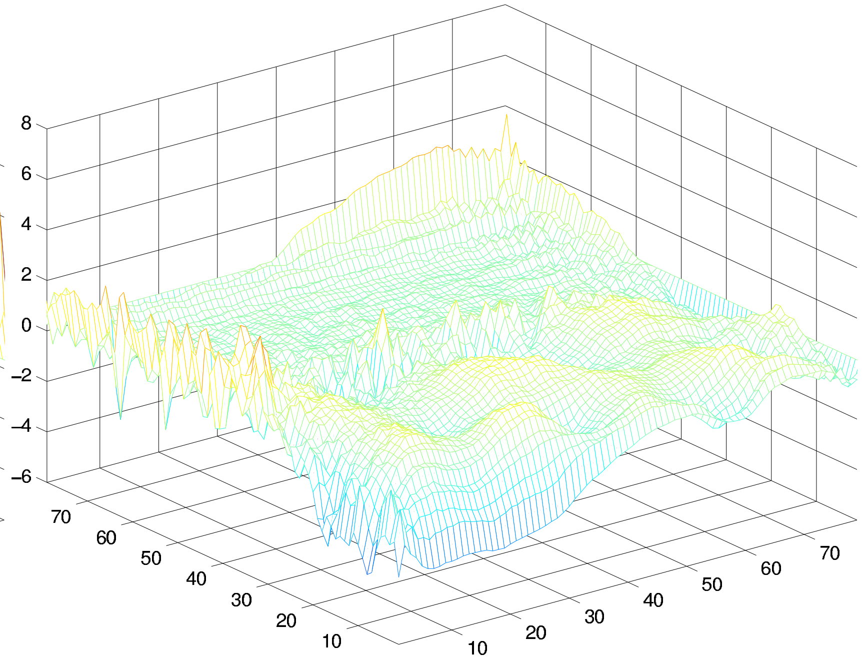


identified bias



Error on the initial correction

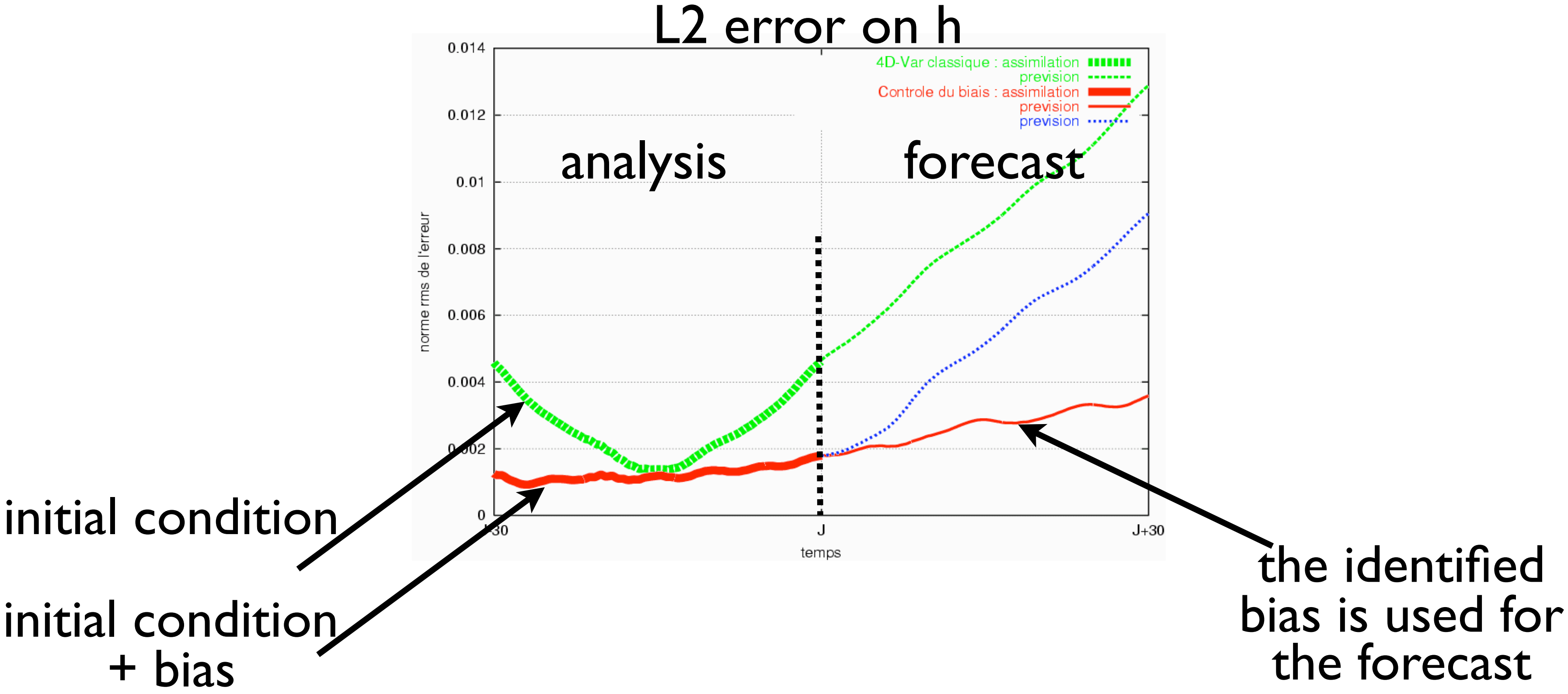




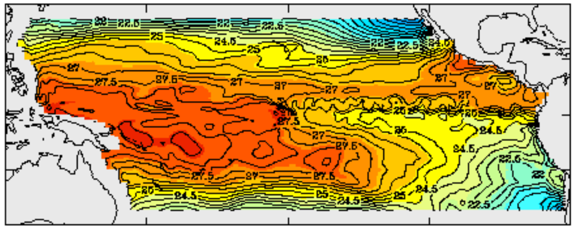
Control of the initial condition only

Control of the initial condition + bias

The use of the identified bias significantly improves the forecast.

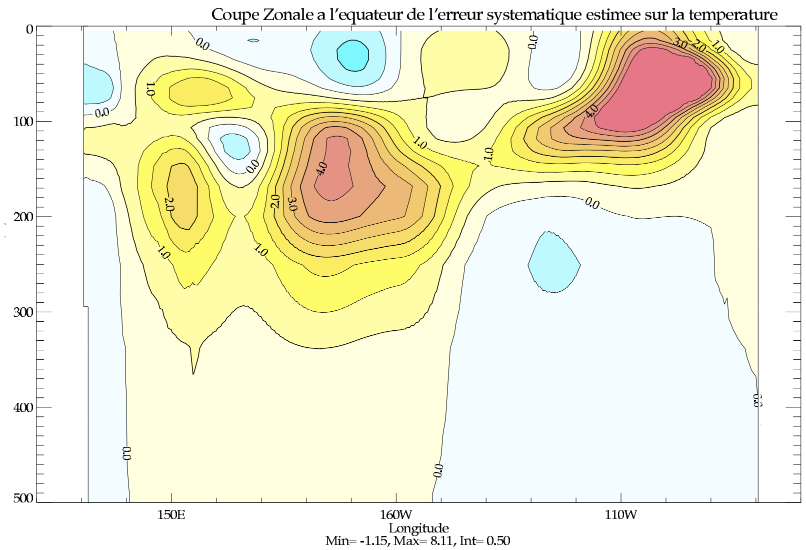


Results with the Primitive Equations Tropical model

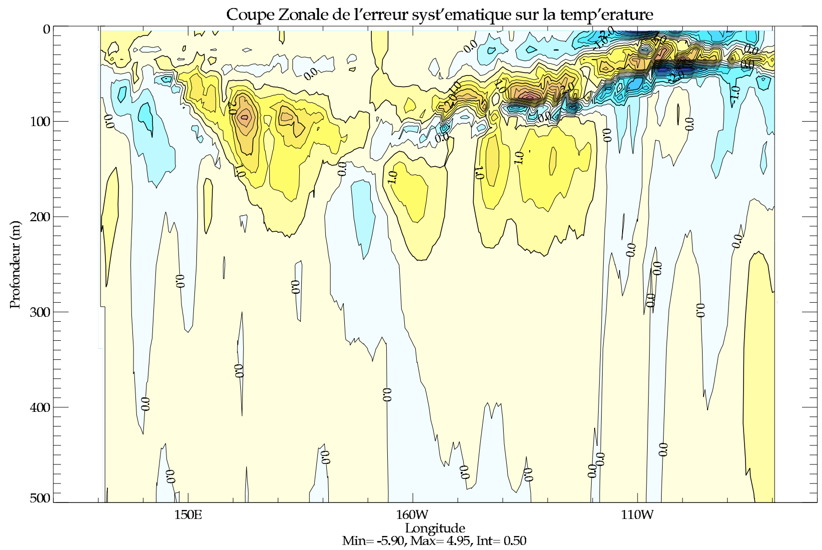


“Cousin experiments”

Bias : vertical section at the equator



estimate

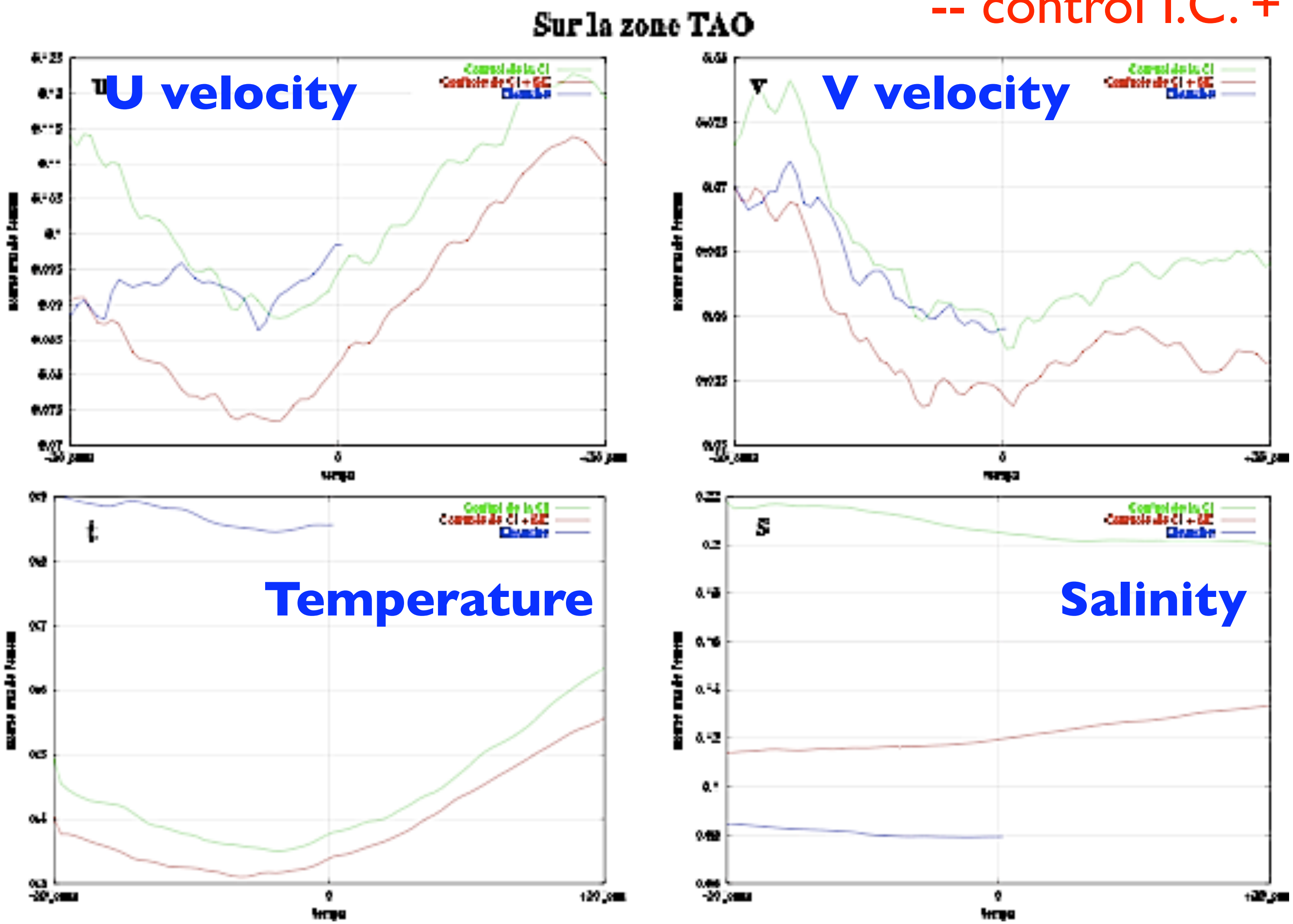


exact bias

Difficulty : definition of the covariance matrix for the bias

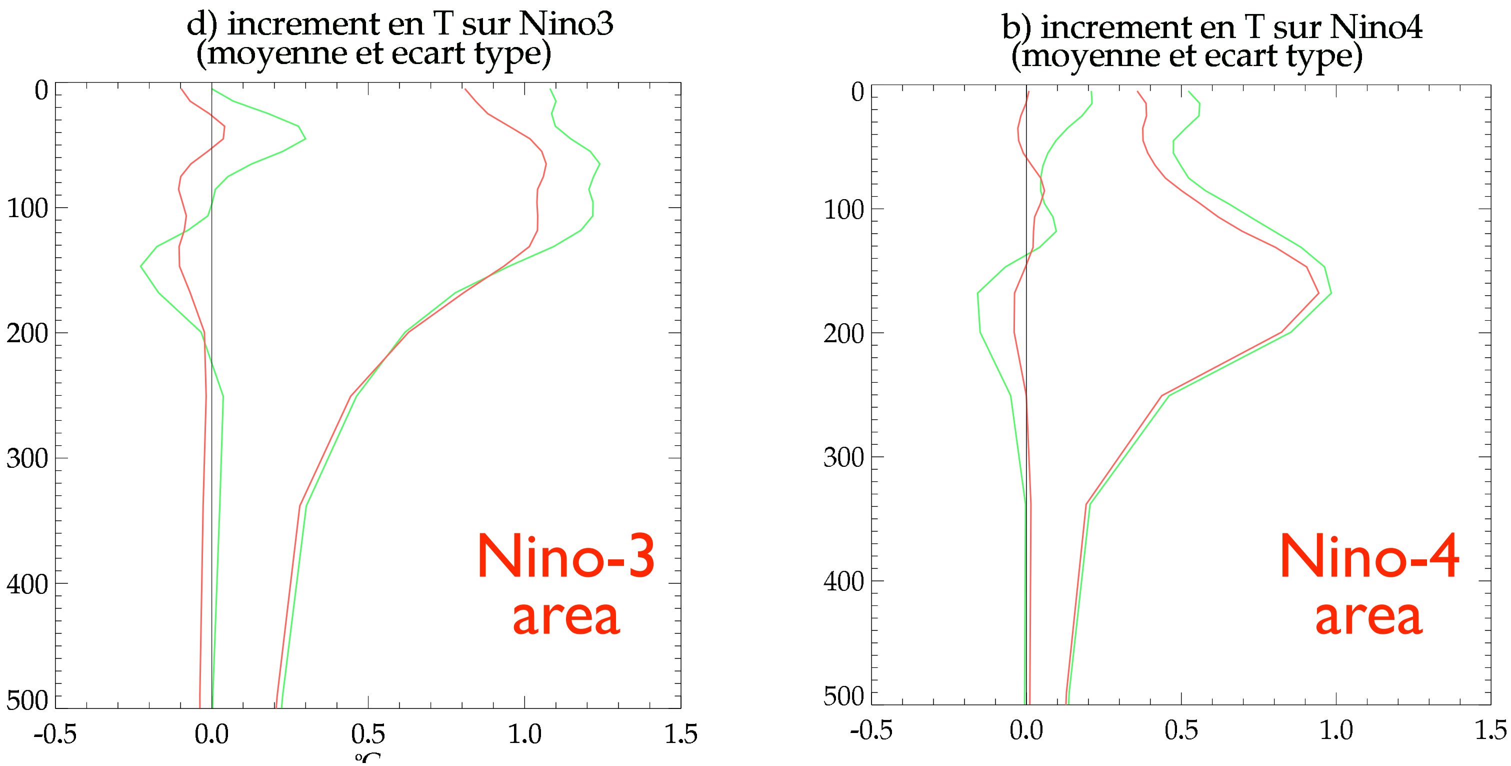
L^2 error

-- background
-- control I.C.
-- control I.C. + bias



Experiments with assimilation of real data

Vertical section of the analysis increments : mean and standard deviation



-- Control of the initial condition

-- Control of the initial condition + bias

The correction is weaker, and closer to zero on average.

- Dual approach - minimization in the observation space : *representers (Bennett 92), 4D-PSAS (Amodei 95, Courtier 97, Louvel 01, Auroux 02)*
- Reduced order modelling of e_i :
  - systematic bias *(Vidard 01, Griffith and Nichols 01, D'Andréa and Vautard 01, Bell et al 02)* : $\mathrm{e}_i = \bar{\mathrm{e}}$
  - decomposition in a low-rank basis *(Durbiano et al. 01, Vidard et al. 04)* :

$$\mathrm{e}_i = \bar{\mathrm{e}} + \sum_{j=1}^{p} c_j^i \mathrm{L}_j$$

Control of the model error in a reduced space

$$\begin{cases} \mathbf{x}_{i+1} = M_{i\rightarrow i+1}(\mathbf{x}_i) + \bar{\mathbf{e}} + \sum_{j=1}^{p} c_j^i \mathbf{L}_j \\ \mathbf{x}_0 = \mathbf{x}^b + \delta \mathbf{x} \end{cases}$$

$$J(\delta \mathbf{x}, \bar{\mathbf{e}}, \mathbf{c}^1, \ldots, \mathbf{c}^N) = \frac{1}{2} \sum_{i=1}^{N} (H(\mathbf{x}_i) - \mathbf{y}_i)^T \mathbf{R}_i^{-1} (H(\mathbf{x}_i) - \mathbf{y}_i)$$

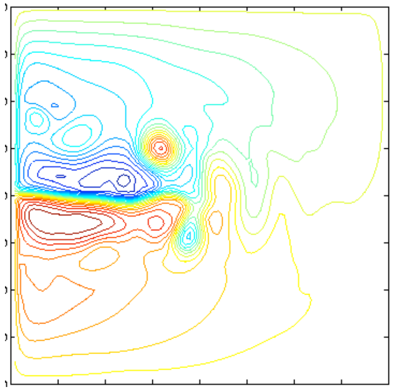
$$+ \frac{1}{2} (\delta \mathbf{x})^T \mathbf{B}^{-1} \delta \mathbf{x} + \frac{N}{2} \bar{\mathbf{e}}^T \mathbf{S}^{-1} \bar{\mathbf{e}}$$

$$+ \frac{1}{2} \sum_{i=1}^{N} \mathbf{c}^{iT} \mathbf{Q}_p^{-1} \mathbf{c}^i$$

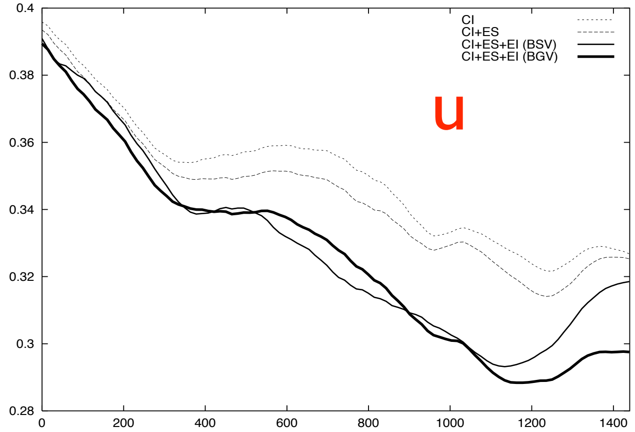
$$\begin{cases} \nabla_{\delta \mathbf{x}} J = -p_0 + \mathbf{B}^{-1} \delta \mathbf{x} \\ \nabla_{\bar{\mathbf{e}}} J = -\sum_{i=1}^{N} p_i + N\, \mathbf{S}^{-1} \bar{\mathbf{e}} \\ \nabla_{\mathbf{c}_i} J = -\mathbf{L}^T p_i + \mathbf{Q}_p^{-1} \mathbf{c}_i \end{cases}$$

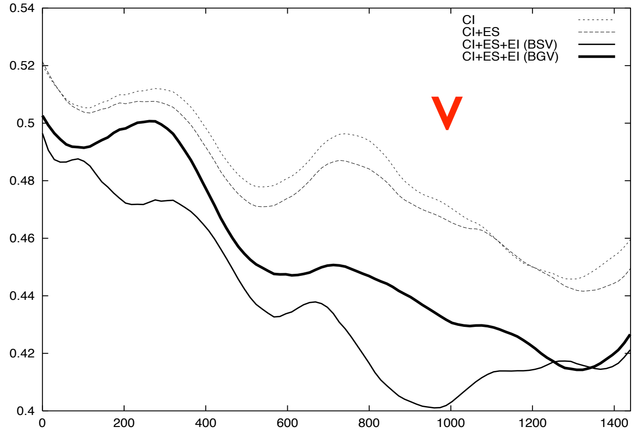
Numerical results with a shallow-water model

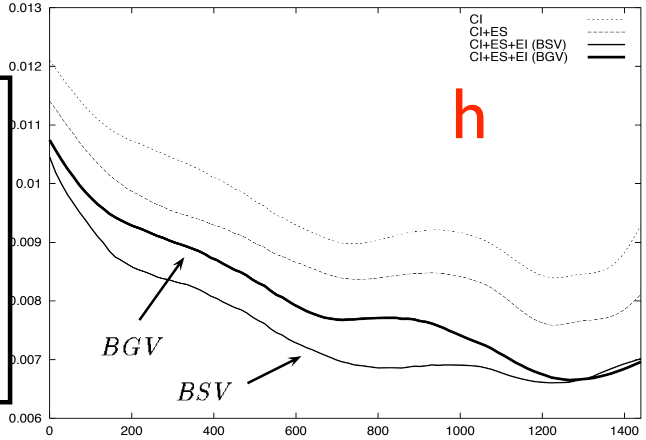
- "Cousin" experiments (a reference model and a perturbed model)
- Obs : sub-sampling of h



L^2 norm of the error

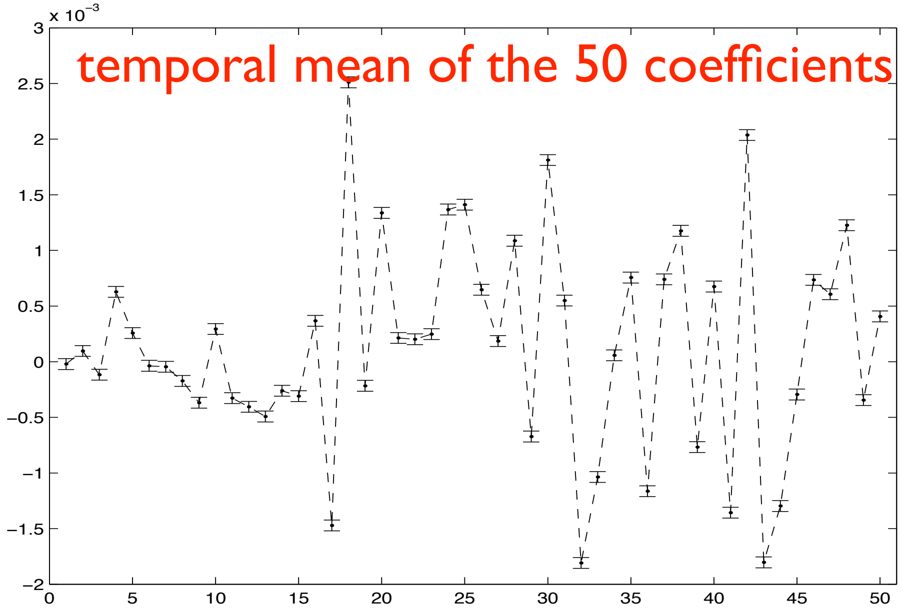


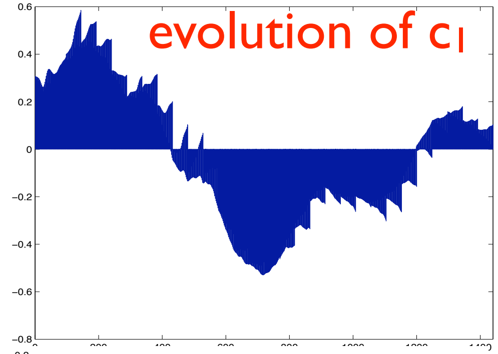


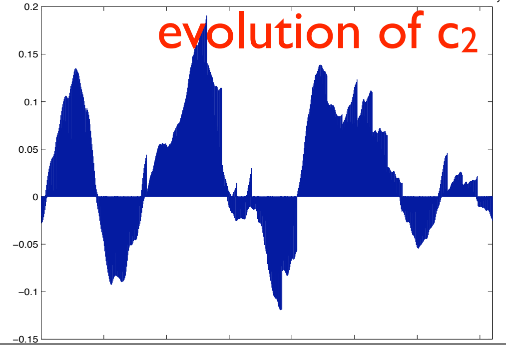


Control of :
I.C.
I.C. + bias
I.C. + bias + time-varying part

The identified part of the error is indeed unbiased.







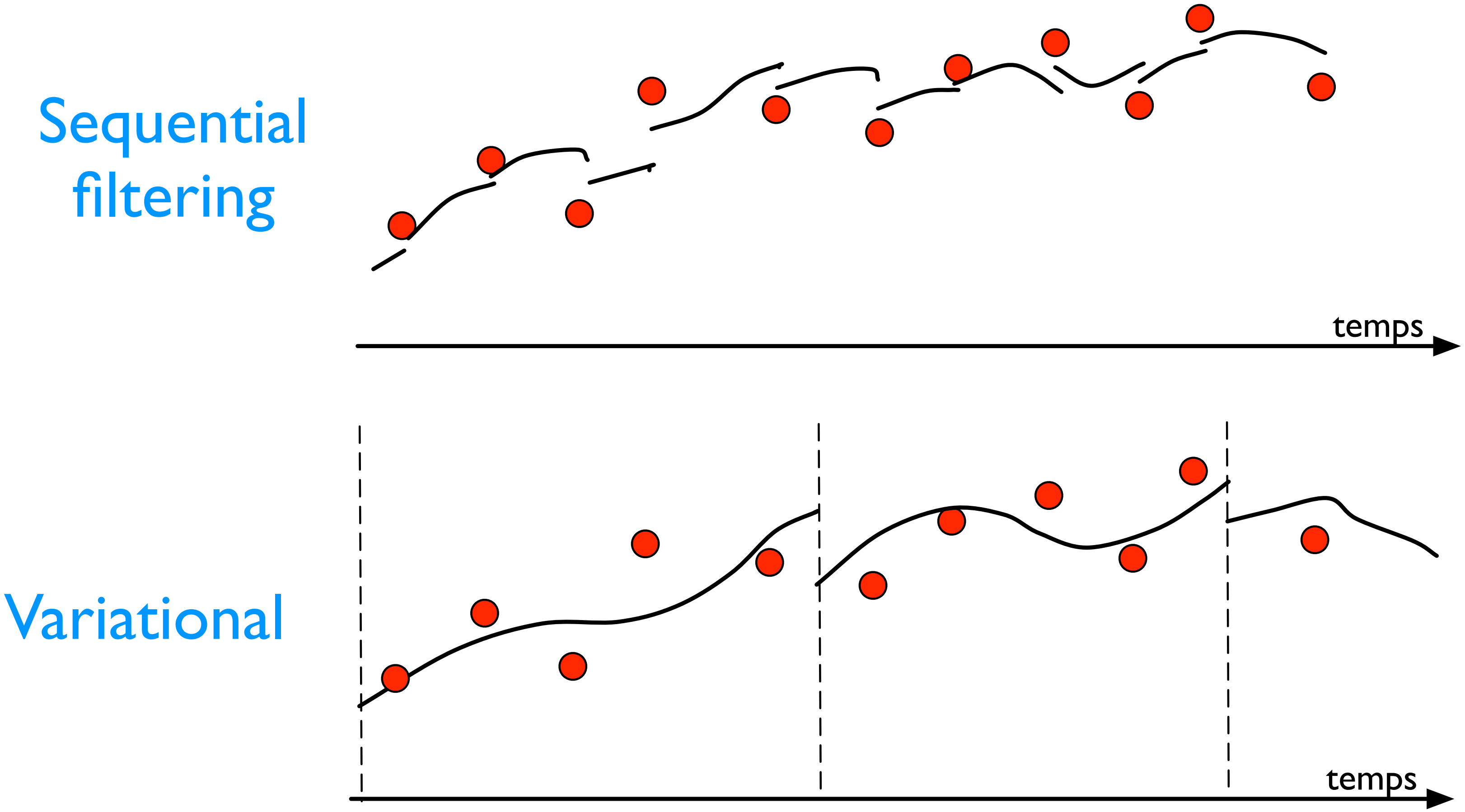
This identification seems useless to improve the forecast.
But it can be used to improve the model itself.

Outline

- 4D-Var and reduced order 4D-Var
- Which subspace ?
- Numerical experiments
- Control of the model error
- Towards a hybrid sequential-variational approach ?
- Conclusion

A hybrid sequential-variational approach

How can we make the basis evolve in time, in order to be more relevant ? ⟶ Sequential data assimilation methods do compute an evolution of the covariance matrices.



Reduced rank Kalman filter : SEEK filter *(Pham et al. 98)*

$$\mathbf{x}^t(t_{k+1}) = \mathbf{M}(t_k, t_{k+1})\mathbf{x}^t(t_k) + \mathbf{e}(t_k)$$

Initialization

$$\mathbf{x}^a(t_0) = \mathbf{x}_0$$
$$\mathbf{P}^a(t_0) = \mathbf{P}_0 = \mathbf{S}_0\mathbf{S}_0^T \quad \text{with } S_0(n,r)$$

Forecast

$$\mathbf{x}^f(t_{k+1}) = \mathbf{M}(t_k, t_{k+1})\mathbf{x}^a(t_k)$$
$$\mathbf{P}^f(t_{k+1}) = \mathbf{M}(t_k, t_{k+1})\mathbf{P}^f(t_k)\mathbf{M}^T(t_k, t_{k+1}) + \mathbf{Q}_k$$
$$= \mathbf{M}(t_k, t_{k+1})\mathbf{S}^f(t_k)(\mathbf{S}^f(t_k))^T\mathbf{M}^T(t_k, t_{k+1}) + \mathbf{Q}_k$$

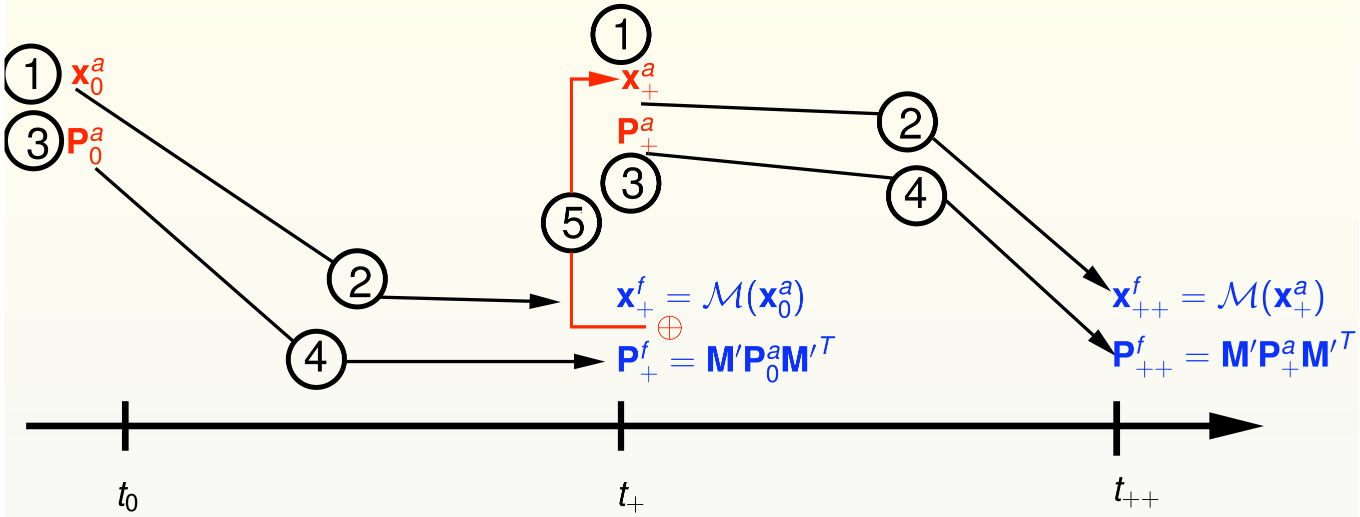
Correction

$$\mathbf{x}^a(t_{k+1}) = \mathbf{x}^f(t_{k+1}) + \mathbf{K}_{k+1}\left[\mathbf{y}_{k+1} - \mathbf{H}_{k+1}\mathbf{x}^f(t_{k+1})\right]$$
$$\mathbf{K}_{k+1} = \mathbf{P}^f(t_{k+1})\mathbf{H}_{k+1}^T\left[\mathbf{H}_{k+1}\mathbf{P}^f(t_{k+1})\mathbf{H}_{k+1}^T + \mathbf{R}_{k+1}\right]^{-1}$$
$$\mathbf{P}^a(t_{k+1}) = \mathbf{P}^f(t_{k+1}) - \mathbf{K}_{k+1}\mathbf{H}_{k+1}\mathbf{P}^f(t_{k+1})$$
$$= \mathbf{S}_{k+1}^a(\mathbf{S}_{k+1}^a)^T$$

Idea : build a hybrid method, where we add to the reduced order 4D-Var an equation for the evolution of the correction basis.

- Theoretical fundation (Veersé, 2000) : some kind of "equivalence" between incremental 4D-Var and Kalman smoother.
- Numerical experiments :
  - Preliminary experiments in a simplified implementation (filter instead of smoother - Robert et al. 2006)
  - On going experiments : exact implementation

Hybrid method : use the evolution of B provided by the SEEK filter/smoother in the reduced-order 4D-Var

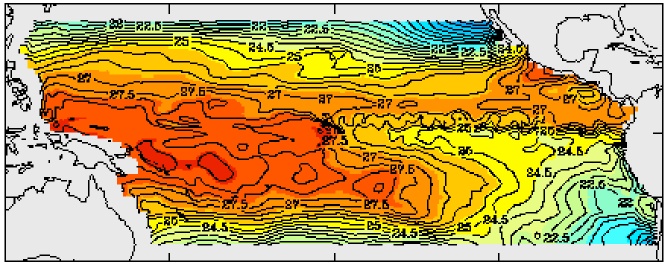


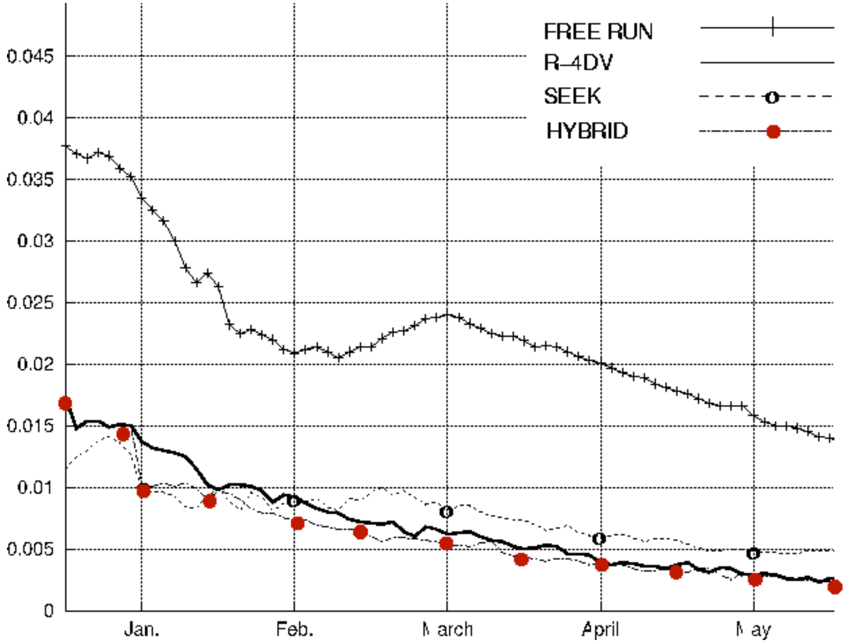
1. $\mathbf{x}_0^a = \mathbf{x}_0^f + \delta\mathbf{x}_0$ [via 4D-VAR] on $[t_0, t_+]$
2. $\mathbf{x}_+^f = \mathcal{M}(\mathbf{x}_0^a)$
3. $\mathbf{P}_0^a$ [via smoother]
4. $\mathbf{P}_+^f = \mathbf{M}'\mathbf{P}_0^a\mathbf{M}'^T$
5. $\mathbf{P}_+^f$ injected into 4D-VAR on $[t_+, t_{++}]$
6. 4D-VAR on $[t_+, t_{++}]$ coincides with the first step of the algorithm

- B is initially the same for both methods
- The reduced-order 4D-Var performs the analysis
- B evolves in time using the equation of the SEEK filter/smoother

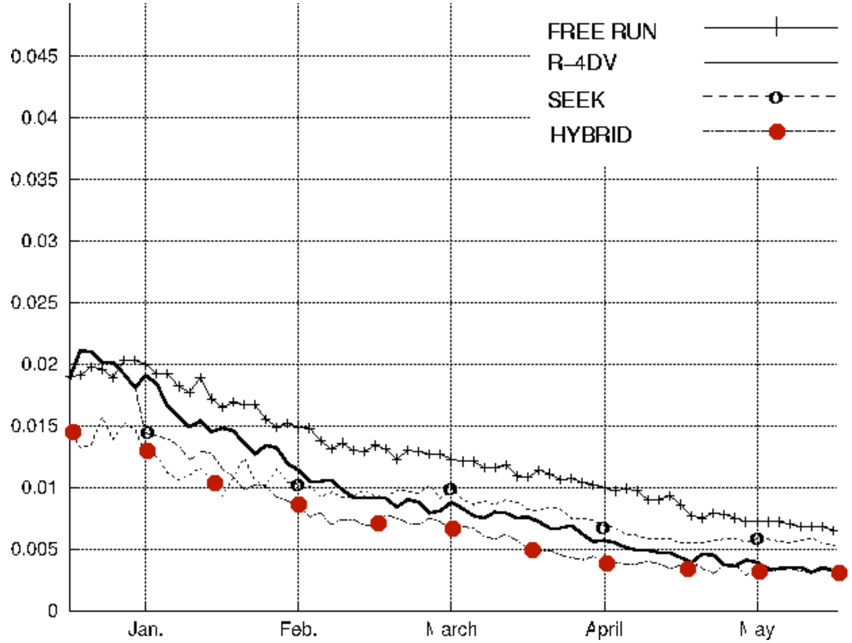
Results with a simplified implementation

Twin experiments
Tropical Pacific ocean





L^2 error on *u* - months 1-6

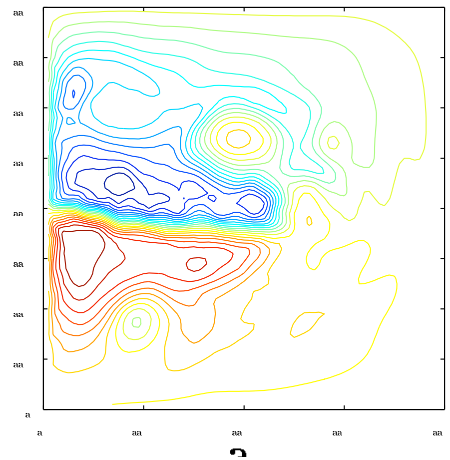


L^2 error on *v* - months 1-6

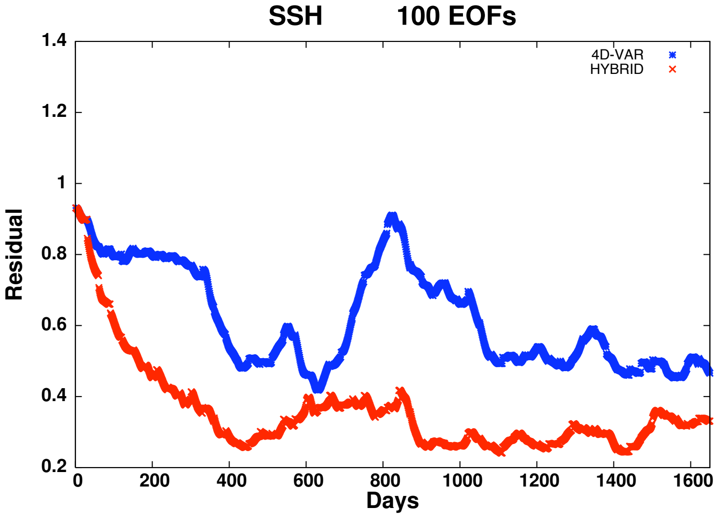
Hybridization seems potentially able to improve the results

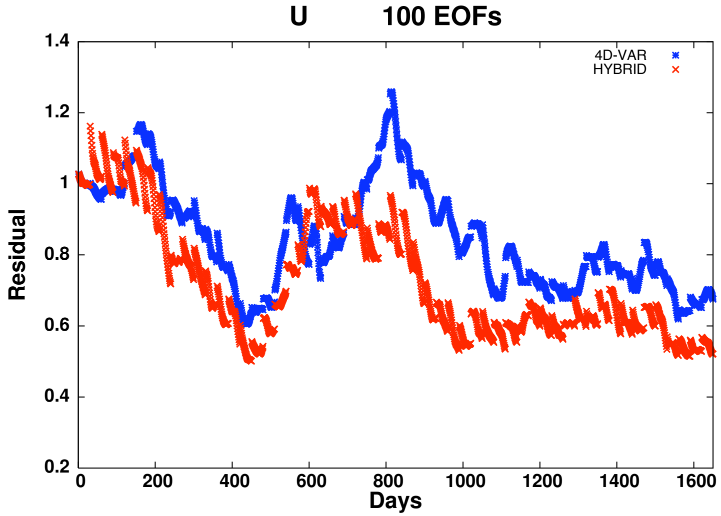
Preliminary results with a "correct" implementation

Twin experiments with the idealized shallow water model



▸ The hybrid metho can lead to some systematic improvement, both on observed and unobserved variables.





Present investigations :

- Are these results robust ?
- Which “stable” criteria to define the basis ?
- Does the subspace initially spanned by PODs converge ?
- What could be learnt from the (evolution of the) structure of the reduced rank error covariance matrix ?

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Summary

- A reduced-order 4D-Var has been implemented. It greatly reduces the dimension of the control space (from 10^6 - 10^7 to 20-30), and it provides a naturally multivariate formulation for B.
- When the model is perfect (twin experiments), this method leads to improved results for a much lower cost.
- When the model is not perfect (real data), this method can be used as a preconditioner for "full" 4D-Var. This two-step method leads to similar results as 4D-Var, for a lower cost (factor of 2).
- A hybrid method is presently under investigation, to improve the evolution of B.

- Other vectors than PODs can also be of interest. There is (to my knowledge) almost no theoretical results concerning nonlinear vectors (NL Singular vectors, Bred modes - *Mu, Kalnay, Toth...*).

- Order reduction / modal decomposition ideas can also be used for other purposes... (example : in the observation space, project the observation on some basis in order to assimilate only the relevant information)

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